IMPACT OF ALLUVIAL GOLD MINING ON SURFACE WATER QUALITY IN THE REVUÈ BASIN-MANICA DISTRICT, MOZAMBIQUE

by

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I hereby declare that this study represents my own unaided work and has not otherwise been submitted in part or in whole for any degree or diploma to any other tertiary institution. Where use has been made of the work of others it is referenced or duly acknowledged in the text.

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February, 2000

ABSTRACT

The upper part of the Revuè basin in the Manica District, Mozambique is located in a mountainous area underlain by rocks of the Manica greenstone belt. This greenstone belt has alluvial gold deposits in the Revuè river and its tributaries Chua and Zambuzi. Alluvial gold in the Manica District has been mined by local people using artisanal mining methods (panning) and by small scale companies. The recovery process of gold involves washing of the auriferous gravel with large quantities of water and the surface water quality has been impaired in this process. The aim of this dissertation is to assess the impact of alluvial gold mining on surface water quality in the Revuè basin. Physical and chemical characteristics of the surface water were determined upstream of, within and downstream of the mining area and in the main tributaries immediately before flowing into the Revuè river. Upstream of the mining area the water is clear and the rock types of the Manica greenstone belt are likely to be the only source of metals dissolved in the water. Metal concentrations are generally low except Cd, Mo and Ni but the water in this area meets all World Health Organization (WHO) recommendations for drinking water. In contrast within the mining area there are signs of pollution. The water is cloudy and the highest concentrations of most metals are found in the lower part of this area where mining activity is very intense. Thus, the alluvial gold mining is responsible for elevated metal concentrations and constitutes the major point source of pollution in the Revuè basin. Water quality within the mining area has been affected and metals Ba, Pb and Mn have concentrations exceeding the WHO recommended values for drinking water. Downstream of the mining area the impounded water in the Chicamba Dam, which is the source of potable water for Chimoio City, reduces the water flow in the Revuè river and sedimentation of suspended sediments occurs, together with associated adsorption and precipitation processes. This result in general improvement of water quality with only Ba and Pb concentrations remaining above the WHO recommended values for drinking water. Increase in concentration of metals Al, Ba, K, Pb and Sr occurring in the Chicamba Dam is likely to be due to input to the dam of water from rivers which cross the Granite-gneiss Complex. Geochemical speciation modelling using MINTEQA2 program suggests that the behaviour of metals Cr, Al, Mn and Fe is controlled by redox and precipitation reactions while the behaviour of As, Cd, Zn, Cu, Ni, Pb, Ba and Ca is controlled by adsorption on the sediment surfaces. Changes in environmental conditions, such as pH and dissolved organic matter (DOM) could result in metals being released back into the water. Modelling the effect of a change in pH and variation in DOM indicate that adsorption and precipitation would decrease with decreasing pH values and with increasing DOM. The chemical form of dissolved metals, the type of interactive processes (adsorption and precipitation) and concentration of particulate matter gives the distribution of pollutants while the transport process affect the fate of pollutants in the Revuè river water.

PREFACE

The study described in this dissertation was carried out in the School of Geological and Computer Sciences, University of Natal, Durban from July 1997 to February 2000, under the supervision of Dr. Carol A. Marsh.

The dissertation is about the impact of alluvial gold mining on surface water quality in the Revuè basin, Manica District, Mozambique and is divided in seven chapters. The first, the introduction, defines the problem to be solved, describes the physical environment, the research aims and the methods of investigation used, including their limitations. Chapter two reviews the geology of the Manica alluvial gold deposits, their geologic setting and genesis, tectonism, size and mineralogy of the deposits. Chapter three describes the alluvial gold mining methods used in Manica, starting with brief historical notes and then the traditional gold mining methods used by the local people and ending with the mining methods used by small scale mining companies. Chapter four focuses on water quality in the Revuè basin and is organised to reflect the physical and chemical characteristics of surface waters in three areas: upstream of the mining area (natural background water quality), within the mining area and downstream of the mining area. Particular attention is given to the concentration of metals. Descriptions of each determinand behaviour and spatial distribution graphs down the Revuè river are presented. Chapter five examines the distribution and fate of pollutants by making use of the geochemical speciation computer model MINTEQA2. The chapter begins with a short review of aspects linked to the distribution and fate of pollutants, progresses through a review of the MINTEQA2 program and ends with Revuè water modelling procedure and results. In chapter six, the point sources and non-point sources of water pollution along the Revuè river are discussed as well as the water treatment strategies. Discussion and conclusions of the study are presented in the chapter seven.

Durban, February 2000

Enoque Mendes Vicente

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CHAPTER ONE

1. INTRODUCTION

1.1 PROBLEM FRAMING

The upper part of the Revuè basin is located in a mountainous area underlain by rocks of the Manica greenstone belt. The Manica greenstone belt has alluvial gold deposits concentrated in the Revuè river and some of its tributaries, namely Chua and Zambuzi (Fig. 1.1).

Alluvial gold in the Manica District has been mined from pre-colonial times up to the present by small scale mining companies and by local people using traditional mining methods (panning). During this period, mining activity has played an important role in the economy of the region and to the survival of the indigenous people. These mining activities are not environmentally friendly and they have caused large alterations of the surface water quality in the Revuè basin as well as other physico-environmental degradation and disturbance namely pits, trenches, holes, tailings and river diversions. Because of the mining activities it is generally assumed that the water quality has been impaired.

Within and downstream of the mining area, the water is cloudy and is brown to reddish-brown in colour due to suspended clay and silt particles that enter the water during the mining process. The suspended sediment load of the Revuè river is deposited in the Chicamba Dam which is situated on the Revuè river approximately 62 km downstream from the mining area. The increased rate of sedimentation due to suspended sediments being carried from the mining area could affect the life expectance of the reservoir. Data from EDM (Electricidade de Moçambique), the company which manages the Chicamba Dam, indicate that the rate of sedimentation in the reservoir is approximately 5 mm/year. Such sediments can have both a direct effect on aquatic life through damage to organisms and their habitat (Walling & Webb, 1992) and an indirect effect through its influence on turbidity and light penetration. Furthermore,

suspended sediments have been demonstrated to be the main transport pathway of various trace metals (Lacerda & Salomons, 1991) due to their high sorptive capacity for many chemicals.

The turbidity of Revuè river water causes serious problems for the local people, as they can not use the river water directly. To obtain clear water the local people dig small holes in the riverbanks (1-2 m from the rivers). This water probably has the same chemical composition as the river water but is free of suspended sediments.

Since 1996 the Chicamba Dam has been the source of potable water for Chimoio City, located 35 km NE from the dam (Fig. 1.1). It was constructed for the potential generation of hydroelectric power. Impaired water quality could have implications for the health of people and for the corrosion of turbines.

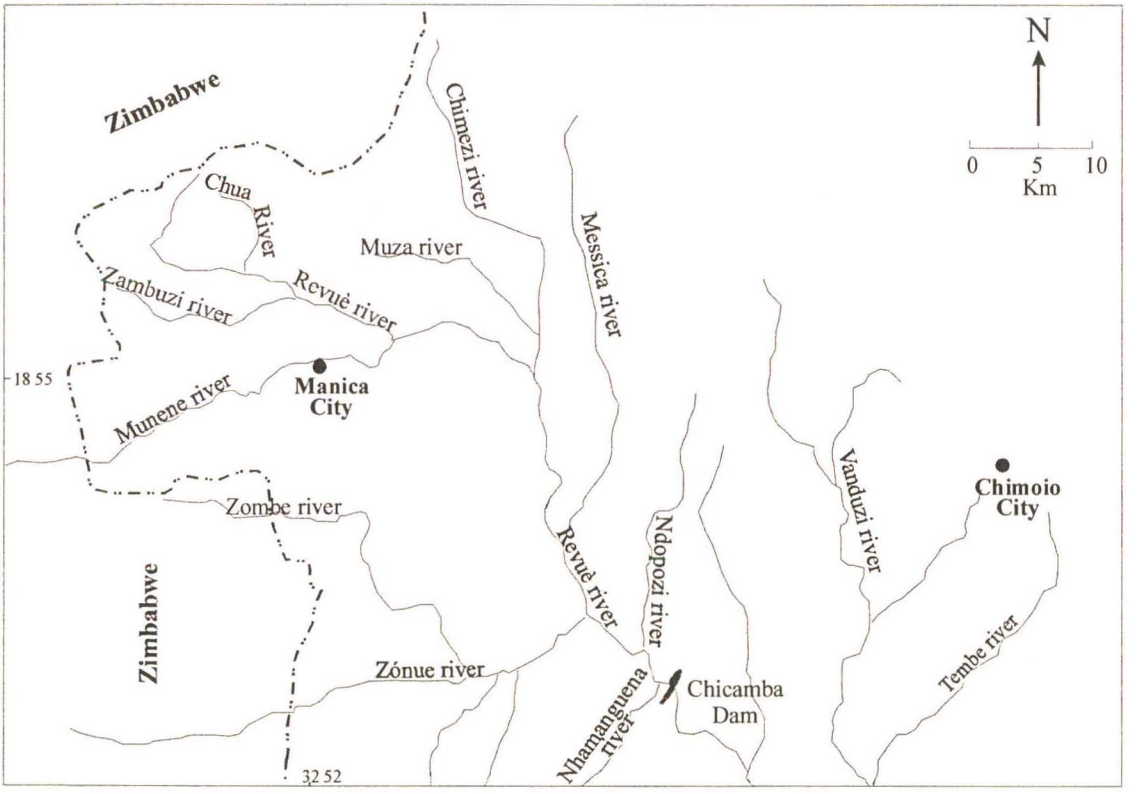


Fig. 1.1 - Area map of the upper part of the Revuè hydrographic basin. Manica greenstone belt covers the part between Munene river and North border with Zimbabwe and the western part of Chimezi river.

1.2 THE PHYSICAL ENVIRONMENT

Manica District is situated in the west central part of Mozambique between the co-ordinates 19° 08' and 19° 20' latitude South and 33° 17' and 32° 41' longitude East, and is part of the Revuè hydrographic basin (Fig. 1.1), that covers an area of 8350 km^2. The Revuè river rises in the

Penhalonga mountains in Manica District, close to the border with the Republic of Zimbabwe, at an approximate altitude of 1750 m, and flows for 234 km before discharging into the Búzi river (Manzanares, 1957). It runs in a NW-SE direction and develops 60% of its total length between the altitude of 800 and 500 m. It has therefore characteristics of a tableland river (Manzanares, 1957). The main tributaries of the Revuè river in the study area are the Chua, Zambuzi, Inhamazonga, Messica, Nhamanguena and Zónue rivers. Alluvial gold mining occurs along the Chua and Zambuzi rivers.

Three zones are distinguished within the Revuè basin based on river gradient. Zone 1 is a mountain reach zone with altitudes between 1750 and 800 m and a gradient of 34.7. It is 6 km in length and contains the headwaters that flow to the Revuè river. This zone is characterised by steep, narrow and shallow channels. Presently the width of the channel varies between 3 to 4 m. The water is clear and turbulent. Zone 2, with an altitude between 800 and 150 m and gradient of 1.7, is a vast tableland where the river descends only 130 m in 100 km. As a result the river channel is flat, deep and wide. As the river approaches the Chicamba Dam the water velocity is reduced and the impounded water start to influence the channel which becomes larger and deeper. The mean width of the river channel increases from 10 m to more than 100 m close to Chicamba Dam. The change in gradient from zone 1 to 2 is not due to changes in lithology, because it occurs within the greenstone belt, but rather is due to the geomorphological change from mountainous to tableland terrain. The marked change in the lithology from the greenstone belt to granite gneiss complex which occurs within the zone 2 is not reflected in a gradient change. Zone 3 has an altitude of between 150 and 50 m and a gradient of less than 1.7% (Manzanares, 1957). The change in the gradient from zone 2 to 3 is a result of the change of lithology from igneous to flat lying sedimentary rocks. The river in this zone is more than 100m wide. The mean depth of the Revuè river is 50 cm in zone 1 but this increases downstream due to both the impounded water in the Chicamba Dam and the channel geomorphology.

The study area extends from the source of the Revuè river within the Manica greenstone belt (zone 1) to the Chicamba Dam (in zone 2), 84 km downstream and includes the downstream part of the main affluents. The discharge of the Revuè river is nowadays very small due to climatic changes which in the late 80's and in the early 90's have caused severe droughts in Southern Africa. The Revuè river is not a big river but is the most important in the region.

In the late 60's two dams, Chicamba and Mavúzi, were built for the potential generation of hydroelectric power for all cities along the Beira Corridor including Mutare City in the Republic

of Zimbabwe. Since 1996, the Chicamba Dam has been supplying potable water to Chimoio City located 35 km NE from the dam (Fig. 1.1).

The climate of Manica is temperate humid with dry winter, following the Köppen classification (Faria & Gonçalves, 1968) which takes into account two fundamentals climatic elements; the air temperature and the quantity of precipitation. The mean annual temperature of Manica is 21.1°C, the relative humidity ranges from 65 to 70 % and the mean annual precipitation is 1109.6 mm (FAO, 1980). During the severe droughts in the region in 1980 and 1991-92, the lowest mean annual precipitation of 110.9 mm (1980) and 367.2 mm (1991) were recorded. After the last drought period the normal precipitation has never return to previous levels and some rivers are still dry. There is a marked seasonal variation in rainfall. The rainy season has a duration of 5 months, from October to March, with January as the rainy month (230 mm). The driest month is July with 9 mm. The mean annual evaporation is 1290 mm, with 150 and 140 mm in October and November respectively, reducing to 58 mm during June.

Land in the upper part of the Revuè river basin is used for subsistence agriculture, pasture and mining activities. Many conflicts were reported in the area between mining companies and the local people, as the fertile land used for agriculture lies within the alluvial gold mining area. Compensation for loss of land use, paid to the local community has in most of the cases not been satisfactory (Local community, 1998, Interviews).

The occupations of the population of Manica are mainly rural farming in the rainy season and alluvial gold mining activity during the dry season. However, a large portion of the population at present engages only in the artisanal mining activity.

The soils of the Revuè basin are fertile and there is no reference to the use of any kind of fertilisers to increase the yield. The forests are characterised by dense indigenous vegetation and plantations of some exotic species, such as eucalyptus and pine-tree used for the production of wood.

1.3 RESEARCH AIMS

This research aims to assess the effect of alluvial gold mining in the Manica greenstone belt on surface water quality in the Revuè basin. The specific objectives of this study are:

- to determine the physical and chemical characteristics of surface water, upstream of, within and downstream of the alluvial gold mining area.

- to characterise unpolluted upstream water quality background levels with reference to lithological type.

- to identify possible point sources of water pollution within the mining area.

- to identify any possible non-point sources of water pollution along the Revuè river.

- to examine the distribution and fate of pollutants using geochemical speciation computer models such as MINTEQA2.

- to suggest possible water treatment strategies to ameliorate any dissolved pollutant species in Chicamba Dam.

1.4 METHODS OF INVESTIGATION

To address the research aims listed above, several methods were used.

1.4.1 Sample Collection

Water samples were collected at several points within the study area for laboratory analysis. The distribution of sampling points is shown in Fig. 1.2. Generally sample points upstream of and within the mining area were approximately 2 km apart, while sample points downstream of the mining area were located approximately 5 km apart. Samples were also collected in Chicamba Dam and within the affluents before their confluence with the Revuè river.

In total 19 water samples were collected and care was taken to obtain a representative and homogeneous sample. The homogeneity of a stream at a cross section is determined by such physical factors as proximity of inflows and turbulence in the channel (Hem, 1985). The samples were taken as near as possible to the centre of the stream. Each sample was then filtered twice, first using filter paper (Whatmans n° 1) to remove coarse suspended particulate matter and then by Millipore membrane filter 0.45μm to remove colloidal and possible biological fractions, which would influence analytical results. Colloidal material would sorb significant quantities of metals due to their large specific surface areas (Filella *et al.*, 1995). After filtering, the samples were placed in 100 ml polyethylene bottles and 0.5 ml (equivalent to 5 ml/l) of 1:1 HNO_3 were added to the sample to lower the pH to less than 2, thus keeping the metal ions in solution (Parr *et al.*, 1988). The low pH also reduces or inhibits the precipitation of trace elements as hydroxides or hydrated oxides and avoids any adsorption by the surface of polyethylene.

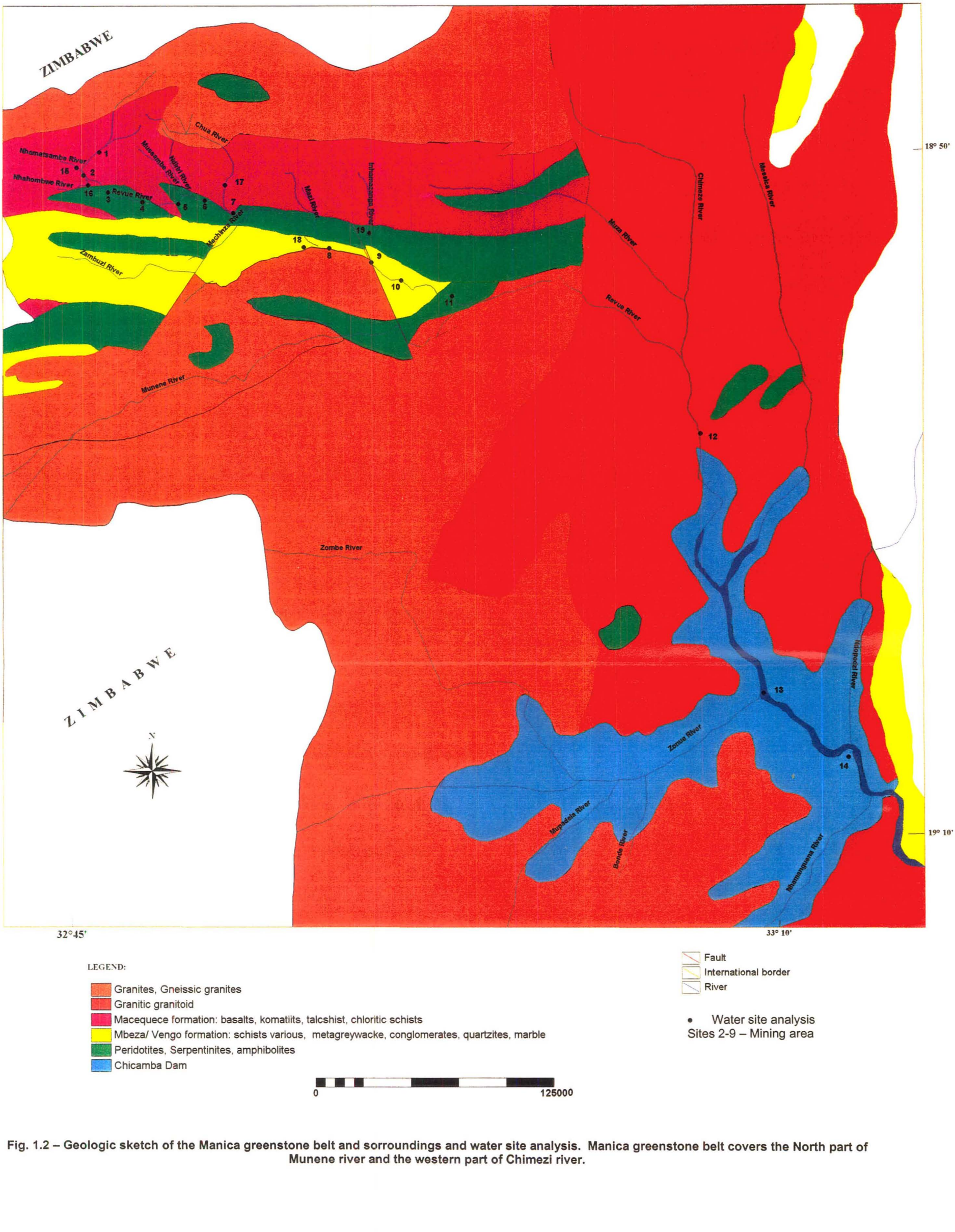


Fig. 1.2 – Geologic sketch of the Manica greenstone belt and sorroundings and water site analysis. Manica greenstone belt covers the North part of Munene river and the western part of Chimezi river.

1.4.2 Field Analysis

There are certain parameters of water quality that must be measured in the field, particularly those that define the carbonate system and oxygen regime. Thus, electrical conductivity, TDS (Total Dissolved Solids) and turbidity were measured at each sampling point (Fig. 1.2) using the HACH conductivity meter model CO150 and the portable turbidimeter model 2100P. The pH and temperature were measured by HACH EC10 portable pH/mV/Temperature meter model 50050 while alkalinity was obtained using a portable HACH Datalogging Spectrophotometer model DR/2010. This instrument is pre-programmed to perform tests for more than 120 parameters. For each parameter a portion of the water sample is inserted in the instrument together with the prescribed chemicals and the result is displayed on the screen. The field parameters were measured before sample preservation with HNO_3.

Field data and samples were collected during the dry season to avoid the rainfall that causes major seasonal changes in water quality. The rain can have a diluting effect or a concentrating effect, if erosion occurs. The salt load of water is dependent on discharge and concentration. Thus, in the dry season when discharge is low, high concentrations of elements or dissolved compounds are found. These data correspond to the worst case scenario situation that can be expected in the Revuè river water.

1.4.3 Laboratory Analysis

The collected water samples were analysed in the Department of Applied Chemistry, University of Natal, Durban to determine the concentration of major, minor and trace metals. The following elements were determined in the laboratory:

- major metals: Ca, Mg and Na.
- minor metals: Al, Fe, K and Sr.
- trace metals: As, Ba, Cd, Co, Cr, Cu, Mn, Mo, Ni, Pb, and Zn.

The metals Na and K were determined by FES (Flame Emission Spectrometry) method which uses the chemical flame for bringing about atomic excitation and the analytical parameters measured are the emitted visible ultra-violet radiation.

The total concentrations of all other elements were analysed by ICP-AES (Inductively Coupled Plasma) method. The instrument used is the Jobin-Yvon JY 24 sequential ICP spectrometer for

multielement analysis, developed and manufactured by the JOBIN-YVON Division of INSTRUMENTS S.A.

1.4.4 Limitations

The selection of sampling and analytical methods used in this investigation took into account the sampling conditions, the sample preservation techniques and transport available to the author as well as the available laboratory techniques. However, the investigation methods used had their limitations both in analytical methods and in the field investigation.

The major limitation of the analytical methods was the impossibility of analysing for mercury that is presumed to be present at high concentrations in the Revuè water as it is used to recover alluvial gold. Mercury was excluded from the group of trace metals to be analysed because of water samples for the determination of mercury in the laboratory need to be cooled at temperatures of 4° C. This was not possible because of field conditions, the available preservation techniques and the distance between the sampling area and the laboratory.

The investigation method is limited by the fact that this study has been done with water analysis of only one season (the dry season). Thus comment on the behaviour of the river water quality during the rainy season can not be made. It is known that the rain causes major seasonal changes in the water quality. The data presented, thus, represents a snapshot of the water quality in the Revuè river during July 1998.

A further limitation is that no attempt was made to assess the total load of metals transported by the river. Calculations of total metals would require analysis of suspended sediment together with calculations of total dissolved salt load. Salt load requires knowledge of river discharge as well as concentration values. No river discharge values were available.

CHAPTER TWO

2. GEOLOGY OF MANICA ALLUVIAL GOLD DEPOSITS

2.1 GEOLOGIC SETTING OF MANICA

The Manica greenstone belt is situated on the eastern margin of the Zimbabwe craton and covers the part between the Munene river and the North border with Zimbabwe and the Western part of the Chimezi river (Fig. 1.1, p. 2). It has a length of 35 km and width of 10-15 km. The Manica greenstone belt represents one synclinorium within a volcano-sedimentary formation and is one of many greenstones occurring in the Zimbabwe craton.

Lithostratigraphically the Manica greenstone belt is subdivided into three major units (Fig. 1.2, p. 6):

Lower Macequece Formation

The lower Macequece Formation is correlated with Bulawaian Formation of the Zimbabwe craton and is a unit of massive and generally grey-greenish greenstones. It consists of metamorphic rocks, intrusive, extrusive and sedimentary in origin, which crop out in the South and North of the Manica greenstone belt. Ultramafic volcano-sedimentary metamorphites that include massive serpentinite, talc schists, actinolite schists, komatiites and basalts have been transformed to amphibolites, chloritic schists, tremolitic schists and talc schists as a result of regional metamorphism of the ultramafic source rocks. These rocks are associated with peridotites, picritic basalts, epidiorites and chlorite schists (Oberholzer, 1964). Serpentinite with pillow lava structures, and rocks with spinifex texture formed as a result of fast crystallisation of ultramafic magma also occur.

Intercalated in the greenstone rocks are metasedimentary material which is irregularly distributed in lenticular lens and discontinous layers as striped quartzite and represents metamorphosed sandy deposits.

Upper M'beza/Vengo Formation

The upper M'beza/Vengo Formation is correlated with the Shamvaian Formation of the Zimbabwe craton. It is comprised of metasediments, which are divided into three units:

a) A lower Quartzitic unit composed of grey quartzites, sericitic quartzites, quartzites with epidote and zoizite and marble with magnetite and ferruginous quartzite (Manuel, 1992).

b) The middle M'beza unit is a metamorphosed sedimentary unit, which consists of a basal conglomerate followed by argillite, fine metagreywacke and arkoses. The greywackes are found as continuous irregular beds (Manuel, 1992). The basal conglomerates, located in Zambuzi valley are monomictic or polymictic (in the central part of the greenstone belt). They are composed of clasts of serpentinite, komatiite and ferruginous quartzite.

c) The upper Vengo unit is made up of conglomerates, meta sedimentary rocks, black schists argillaceous schists, sericiteous schists, chloritic schists, quartzitic schists, carbonaceous schists and ferruginous schists, argillaceous phyllite, argillite, conglomerate and breccia.

Intrusive Rocks

Later Precambrian intrusive rocks are composed of gneissic granites, granites and micro granite intrusions, quartz veins, gabbro and diabases. Dolerites dikes, oriented NW-SE, are widespread in the Manica greenstone belt.

The Manica greenstone belt is one large E-W synclinorium (Manuel, 1992). The area has been affected by seven deformation phases distributed in three main deformation categories: ductile, transitional and fragile or brittle (Matos, 1996). The earliest phase of deformation, ductile deformation category, is characterised by folding and formation of different types of foliation. This was followed by the transitional category, which is characterised by the appearance of kink folds. The last phase of deformation, the brittle category is marked by the appearance of different kinds of fractures such as strike slip faults, thrust faults and joints.

Folding accompanied by green-schist facies metamorphism together with the emplacement of granite stocks is believed to have played an important role in the subsequent remobilization of gold (Hutchison, 1983). The plutons acted as heat centres that drove large-scale circulation of brine through the volcano-sedimentary pile, depositing gold in fissures created during the folding of the greenstone belt.

2.2 GEOLOGY OF THE MANICA ALLUVIUM

Alluvial gold deposits in the Manica greenstone belt occur in the Revuè river and some of its tributaries. These rivers are part of the Revuè hydrographic basin, the headwaters of which arise in the Manica greenstone belt (Fig. 1.1, p. 2). As detailed in section 1.2, three zones are distinguished within the Revuè hydrographic basin based on river gradient. The alluvial gold deposits are found in the downstream part of Zone 1 and in the upper part of Zone 2. Gold accumulated in these zones as a result of changes in the river gradient.

Revuè basin alluvium can be divided into lower, middle, and upper terraces. The lower terrace is composed mainly of gravel that accumulated below the present average river height. The middle terrace is also composed of gravel and is found above the present average river height. The upper terrace is represented by soils.

The lower terrace of the Manica alluvium is the only gold bearing unit and is composed of four layers (Fig. 2.1). Vicente (1996) describes these layers as:

1 - an upper soil layer normally covered with vegetation. It is dark brown in colour and 15 to 85 cm thick.

2 - an interbeded clayey sand or sandy clay that is light brown in colour and 1.15 to 9.00 m thick.

3 - an auriferous gravel which is light brown yellowish in colour and 1 to 5 m thick.

4 - a basal layer of highly weathered bedrock derived from the Manica greenstone belt.

Thickness of the layers is variable as a function of the channel morphology and reflects the concentration and calibre of sediment moving down the channel.

The lower terrace shows an upward decrease in grain size and increasing clay content. Gold is only concentrated in gravels overlying bedrock. The distribution and thickness of Manica gold deposits are very irregular. These irregularities are associated with the geomorphologic conditions of the surface during the alluvial gold accumulation in Manica.

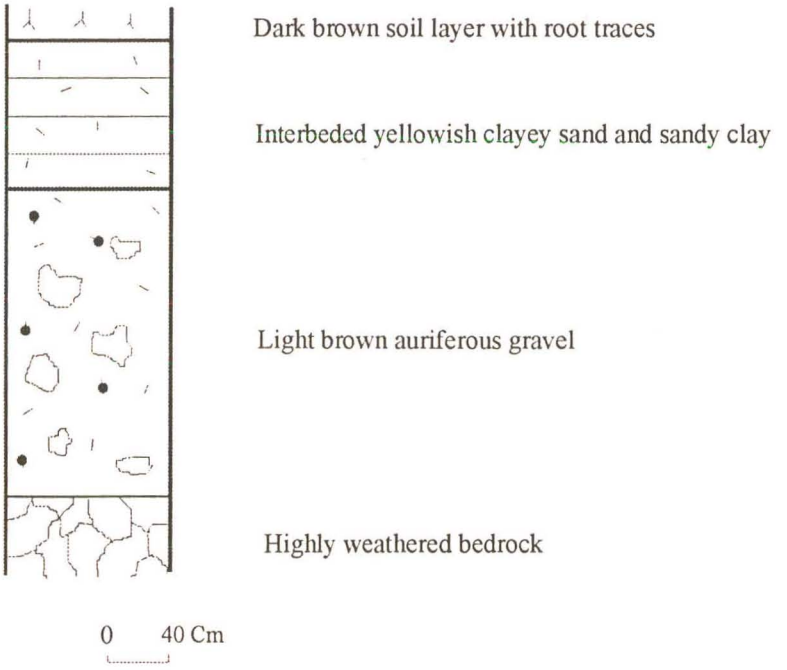


Fig. 2.1 - Simple geologic profile of a lower terrace of the Manica alluvial deposits (Modified from Vicente, 1996).

2.2.1 Genesis

The source of gold in the Manica alluvium is the granite-greenstone rocks. The granite intrusions favoured the formation of syngenetic gold deposits (formed at the same time as the enclosing rock). It includes volcanogenic stratabound massive sulphides, volcanogenic-stratiform subaqueous exhalative, plutonic stocks and sills (Fig. 2.2) (Hutchison, 1983). Epigenetic deposits containing high grade gold formed after its host rocks. These epigenetic deposits are due to gold mobilisation during the metamorphism of the rocks of Manica greenstone belt (Manuel, 1992). The gold mobilisation occurred along fractures (Afonso & Marques, 1993) formed by folding of the greenstone belt.

Rivers eroded the granite-greenstone source rocks and the gravel was deposited along the Revuè hydrographic basin within the Manica greenstone belt. In the Revuè river gold can be found from 4.5 km to 22 km from its source (Fig. 1.2, p. 6). Mineralization coincides with a marked decrease in river gradient allowing alluvial gold accumulation.

In the Chua river (tributary of the Revuè river) the main gold deposit was recovered from a feature interpreted as a pothole. A pothole is a circular deep hole in the bed of a river formed by abrasion and grinding effect on the bed rock of pebbles whirled round by eddies (Monkhouse, 1970).

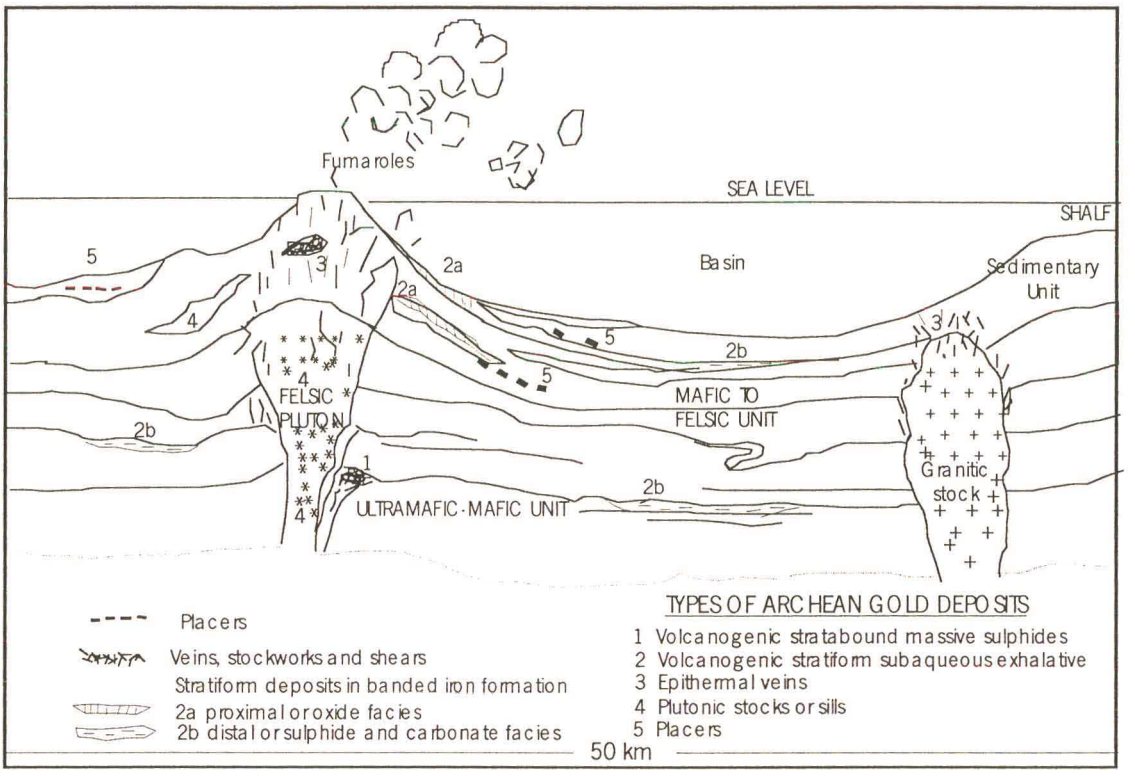


Fig. 2.2 - Schematics diagram of an Archaean Vulcan-sedimentary greenstone belt basin showing the possible relation of mineralization to the volcanic-exhalative activity (From Hutchison, 1983).

The potholes are dominated by centrifugal action of the water ejecting particles and produced in conditions of turbulent flow. This theory is used by Bache (1989) to suggest that gold can not accumulate in a pothole. However, the ridge of mountains (Vengo with 1767 m height) exists next to the pothole may have hindered the normal flow of water carrying gold. The reduction of turbulent flow favoured the accumulation of gold.

2.2.2 Tectonic Setting

The geomorphologic evolution of the Manica greenstone belt contributes towards understanding modern alluvial gold deposits.

The deformation phases refered to in section 2.1. (Folding and faulting), played an important role in the tectonic setting of Manica. As a result of tectonic movements mountainous regions formed. These mountains have altitudes varying from 1500 to 1920 m, and contain the Revuè river and its tributaries.

The Revuè river rises at an approximate altitude of 1750 m. The first 6 km of the river has strong declives (within the mountainous relief). Both the formations of mountains and very strong declives from there could have facilitated the erosion of beds containing gold.

2.2.3 Size and Mineralogy

The Manica greenstone belt is very small in areal extent reducing the possibility of forming a large alluvial gold deposit. The present alluvial gold production is very low and the remaining gold grades are also low.

Gold in Manica is found as particles of 0.1-2.5 mm in size and seldom as nuggets. Its size distribution follows sediment size distribution, with coarser particles being formed in the upstream sections. Gold in Manica alluvial gold deposits is accompanied by heavy minerals such as magnetite, titano-magnetite, ilmenite, calcopyrite and copper.

CHAPTER THREE

3. ALLUVIAL GOLD MINING METHODS

3.1 HISTORICAL NOTES

Alluvial gold mining in Manica is undertaken by mining companies using small scale methods, and by indigenous people using several traditional mining methods (panning). The mining of alluvial gold deposits in Manica started centuries ago, probably in the time of the State of Zimbabwe (1250-1450) and of the Empire of Monomotapa (1325-1600). Rounded pits (50-75 cm in diameter and 3-7 m deep) were excavated in the lower terrace of Revuè river (Galiläer *et al.*, 1980).

In the XVI century the Portuguese temporarily occupied the Manica mining area and is estimated that up till that time 500 kg of gold had been produced. In the XVII and XVIII centuries the Portuguese transported large and non-specified quantities of gold to Lisbon. With the development of the mining industry in the world in later XIX century, the demand of gold increased and in 1889 the "Comissariado de Minas" was created in Manica (Manuel, 1986). At this time 23 mining companies were registered and another 140 companies asked for concessions (Galiläer *et al.*, 1980), and started the scientific exploration by the English and Portuguese. There are records of 30 companies that mined quartz veins and 7 that mined deposits in ferruginous quartzites and quartzitic veins (Sheeran, 1987).

In this century, dredge mining in the lower terrace of the Revuè and Chua rivers was started by several companies. Between 1914 and 1949 about 6456 kg of gold were produced by dredge method but production declined in the following 3 decades with only a few kilograms of gold extracted per year. In 1990 a new phase of gold mining in Manica was started by ALMA (Aluviões de Manica) and small scale mining companies. In 1994 it was estimated that about 11000 kg of gold has been produced in Manica from all known sources (MIREM, 1990-1994).

3.2 TRADITIONAL GOLD MINING

Gold panning is a very old tradition in Manica District. It has been used from pre-colonial times up to the present. In the late 80's and early 90's, due to drought and civil war in Mozambique, panning was used extensively and represented a survival activity to a large part of the local people who had no other source of income.

This traditional gold mining activity is not controlled by the state. In a small plot of land, hundreds of people can be found working the deposit.

Traditional gold mining in Manica is undertaken by local people using low technology mining methods. The mining methods used differ depending upon both the morphological and geological conditions of the mining site and the kind of auriferous material. If the gold-rich layer is located at depth, pits are opened, even on river beds, or else material is taken from the tailings.

Pits ranging from 3 to 10 m in depth are opened to expose the auriferous gravel layer at the base of the lower terrace. Most of these pits are opened in the form of benches and large quantities of overburden are removed to expose only a small area of auriferous gravel. The auriferous gravel is brought to the surface with buckets fastened to ropes and is then washed directly in the river water to produce gold-rich gravitic concentrate. In some situations, the auriferous layer is followed horizontally producing small galleries of 2-10 m length and approximately 1 m diameter. Due to the low technology of the mining method many cases of pit collapse causing injuries and deaths have been reported. The pits are normally abandoned without any rehabilitation resulting in changes to the topography of the area and reducing the beauty and the security of the landscape.

In other cases the river is diverted so that the river bed can be excavated to remove auriferous material. Rerouting also occurs where the pits to the auriferous layer are located far from the river bank and the river is diverted so that water can be directed to gold washing points. This river rerouting changes only small portions of the basin causing local variations in erosion, transport and sedimentation processes.

Dredge mining used by mining companies between 1914 and 1949 resulted in low recovery of gold. Significant quantities of gold remain dispersed in tailings. The local miners remine this tailing material and wash it again to recover the remaining particles of gold. In the tailings the gold is distributed randomly within the detritical sediments of fine and medium size.

Regardless of the method used, the final stage is washing of the gold with the river water (Fig. 3.1). The gold rich material is submitted to the panning process to produce a gold-rich gravitic concentrate. A rounded pan, 50 cm in diameter and 10 cm in height is commonly used, or if not available metal or plastic basins are substituted. A small quantity of gold-rich material is placed in the pan, and alternatively immersed and removed form the river water. This is accompanied by rotation of the pan. In this way light material is washed out which increases the turbidity in the Revuè river water and, due to its high density, the gold and other heavy minerals which also occur in the alluvial gold deposits are retained within the pan and form a gold-rich gravitic concentrate.

The large gold grains in the concentrate are selected by hand. The remaining fine fraction of gold is put in rounded pans and a few grams of liquid mercury and a small quantity of water are added. The pan is stirred to facilitate the adherence of gold to the mercury. The mercury-gold amalgam is squeezed in a piece of tissue to remove excess mercury which is recycled to the next batch. The amalgamation process takes place in open air, thus releasing part of the mercury content of the amalgam directly to the atmosphere.

The tools commonly used in the traditional mining are hoes, shovels, sacks, buckets, pans, wheelbarrow, motor water pump and ropes. These tools are used to remove the overburden layer, draining the water, extraction of the auriferous material and the panning process.

Fig. 3.1 – Local people processing gold in the river water.

3.3 SMALL SCALE GOLD MINING

The alluvial gold mining methods used by small scale mining companies consists of several steps. The first step consists of removal of the topsoil and storing it in a safe place. In the Manica alluvium the topsoil is about 15 to 85 cm thick. The intention is to reuse the top soil to rehabilitate the landscape so that the adverse effects of mining on the environment are eliminated or reduced. However, in most cases this does not happen.

Following the removal of the top soil, the interbeded clayey sand and sandy clay which comprises the overburden to the auriferous gravel is removed. This material is light brown in colour and 1.15 to 9.0 m thick. Small pebbles are distributed randomly. This material is deposited as tailings.

Once the auriferous gravel layer is reached it is sent to the processing plant. There it is fed through a grizzly. The oversize material is discarded and the fine material is fed to a scrubber. In the scrubber the gravel is washed and sorted by running water. This results in density separation and the light fraction is dumped in the river margins.

The water used in the auriferous gravel washing process is deposited in a small settling pond intended to allow sediment precipitation, but because of the high volume throughput, sedimentation is limited and the water which is returned to the river has a high sediment load.

The denser material from the scrubber passes to the gig plant. Here the material is separated into three categories accordingly to grain size. Particles with diameter of more than 0.5 cm are retained by the primary gig. Particles with diameter between 0.2 and 0.5 cm are retained by the secondary gig. Particles with diameter less than 0.2 cm are retained by the tertiary gig.

Any nuggets of gold retained in the primary gig are selected by hand and the remaining material is dumped. In the secondary gig, small grains of gold are collected and the remaining material is mixed with that retained in the tertiary gig.

The mixture of material from the secondary and tertiary gigs is taken to the "Gemine table" (vibration table) where the heavy minerals including gold are collected. This concentrate is moved to the amalgamation cylinder. After a gravimetric preconcentration step of the heavy fraction of the auriferous gold-containing material, liquid mercury is added to the cylinder. The amalgamation cylinder is rotated and the gold particles form an amalgam with the mercury. The remaining material is discarded. The mercury-gold amalgam is then squeezed to remove excess

mercury and then taken to a retort for roasting. The amalgamation process is done in the laboratory, thus the risk of releasing mercury to the atmosphere is reduced.

The gold particles recovered are liquefied at 1000° C temperature to produce gold bars with approximately 98% gold and 2% of impurities.

CHAPTER FOUR

4. WATER QUALITY IN THE REVUÈ BASIN

To assess the water quality of the Revuè basin several physical and chemical parameters were determined in the field as well as in the laboratory. For the chemical parameters total soluble concentrations were determined. However, total concentration provides no information concerning the particular behaviour of an element in terms of its interaction with sediments, its ability to cross biological membranes (bioavailibility), or its resultant toxicity (Christie, 1995). Förstner (1990) started that the particular behaviour of trace metals is determined by their specific form rather than by their total concentration. Therefore, any changes in speciation may dramatically affect the toxicity of a metal. The chemical speciation of the elements in the Revuè river water is the main subject of Chapter 5. Table 4.1 shows the water quality data measured in the Revuè river. The distribution of each determinand along the Revuè river is described below and graphs are drawn for each determinand to show its spatial change down the river. These changes are related to proximity to inputs of affluents, sites and intensity of mining activity and lithology. As there are no geochemical data available on the rocks of the Manica greenstone belt, references to lithology are based on the typical concentrations of heavy metals in the earth's crust and in major types of igneous and sedimentary rocks (Table 4.2).

In order to determine the impact of the alluvial gold mining on surface water quality, the study area was divided in three parts; upstream of, within and downstream of the mining area. The water quality data from these areas were compared to see the evolution of water quality down the Revuè river. The analytical data of water collected in site 1 in the Revuè river were used as a background reference value because this site is in a pristine area far from the influence of mining activity.

The Chicamba Dam situated downstream of the mining area is the source of potable water for Chimoio city. In order to quantify the impact of mining on the quality of water entering the dam, water quality data were compared to the 1996 WHO (World Health Organisation) recommended values for drinking water.

Table 4.1 – Water quality data measured along the Revuè river water and the 1996 WHO recommended values for drinking water.

Determinands	Upstream of the mining area		Mining area							Downstream of the mining area					Min Value	Max Value	1996 WHO standards
	1	2	3	4	5	6	7	8	9	10	11	12	13	14			
Temp (° C)	18.9	20.8	21.7	17.9	17.6	21.6	21.5	19	17.3	19.2	17.8	18	19	19.2	17.3	21.7	25
TDS (mg/l)	74.34	79.65	90.27	95.58	106.2	106.2	116.82	191.16	138.06	143.37	148.68	111.51	116.82	106.2	74.34	191.16	....
Condutivity (µS/cm)	155.3	164.0	179.9	199.3	219.2	220.2	236.59	308.65	285.6	291.8	298.9	222.3	235.6	218.2	155.3	308.65	....
Turbidity (NTU)	7.28	14.4	16.9	10.9	8.41	23.6	14.7	59.1	142	92.2	84	10.4	1.56	1.42	1.42	142	< 5
Alkalinity (mg/l) *	32.4	32.8	47.6	24.8	50.8	41.2	43.6	52	61.6	58.4	56.2	42	39.8	32.2	24.8	61.6	NS
pH	7.3	7.3	7.7	7.6	7.8	7.5	7.1	7.6	7.5	7.3	7.5	7.4	7.5	7.6	7.1	7.8	6.5 – 8.5
Ca (mg/l)	3.8	4.1	4.3	4.9	5.3	5.5	5.8	6.9	7.2	7	7.1	5.6	5.2	5.2	3.8	7.2	< 200
Mg (mg/l)	3.1	3.2	4.5	4.9	5.6	5.7	6.4	7.5	7.6	7.6	7.7	3.9	3.5	3.5	3.1	7.7	< 150
Na (mg/l)	4.1	4	3.3	3.4	3.45	3.3	3.3	4.75	5.2	3.8	5.85	5	5.3	4.8	3.3	5.85	< 120
K (mg/l)	0.3957	0.3867	0.5036	0.4856	0.4676	0.7014	0.4766	0.6745	0.7644	1.0612	1.0432	2.5899	2.5629	2.5989	0.3867	2.5989	< 10
Al (mg/l)	0.04	0.03	0.1	0.07	0.08	0.06	0.11	0.06	0.06	0.08	0.02	0.09	0.14	0.13	0.02	0.14	< 0.2
Fe (mg/l)	0.02	0.02	0.05	0.09	0.26	0.27	0.18	0.07	0.05	0.06	0.06	0.05	0	0.03	0	0.27	< 0.3
Mn (mg/l)	0.024	0.026	0.044	0.094	0.13	0.132	0.14	0.18	0.2	0.18	0.11	0.0042	0	0	0	0.2	< 0.02
Sr (mg/l)	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.04	0.04	0.04	0.04	0.05	0.05	0.05	0.02	0.05	NS
As (mg/l)	0.011	0	0.012	0.007	0.0095	0.0058	0.025	0.0084	0.004	0.015	0.03	0.0047	0.042	0	0	0.042	< 0.05
Ba (mg/l)	0.09	0.08	0.08	0.1	0.1	0.1	0.1	0.14	0.17	0.17	0.16	0.18	0.19	0.19	0.08	0.19	< 0.1
Ni (mg/l)	0.0018	0.0069	0.00061	0.0004	0.0015	0	0.00042	0.00058	0	0.0023	0	0	0	0.0011	0	0.0069	< 0.02
Co (mg/l)	0.0024	0	0.011	0.0073	0.0059	0	0.0056	0.0039	0.024	0.023	0.0098	0.006	0.0051	0.0038	0	0.024	NS
Cu (mg/l)	0	0.01	0	0	0.05	0	0.01	0	0	0	0.02	0.03	0	0.02	0	0.05	< 1-2
Cr (mg/l)	0.0064	0.0069	0.0051	0.0076	0.0084	0.0072	0.0068	0.0077	0.0047	0.0062	0.0048	0.0032	0.0015	0.0024	0.0015	0.0084	< 0.05
Cd (mg/l)	0.0027	0.0016	0.0021	0.00045	0.0017	0.00023	0.002	0.00001	0.00032	0.0018	0.0014	0.0022	0	0.00053	0	0.0027	< 0.005
Mo (mg/l)	0.0065	0.0018	0.00096	0.0061	0.006	0.00081	0.005	0.0025	0.0055	0.0081	0.0054	0.0033	0.0013	0	0	0.0081	< 0.05
Pb (mg/l)	0.0096	0.01	0.0088	0.019	0.0055	0.005	0.025	0.053	0.027	0.026	0.028	0.017	0.025	0.037	0.005	0.053	< 0.01
Zn (mg/l)	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0.02	0	0.02	< 3

* Alkalinity as $CaCO_3$

Table 4.2 - Typical concentrations of heavy metals in the earth's crust and major types of igneous and sedimentary rocks in ppm (from Alloway & Ayres, 1993; Drever, 1997).

Elements	Earth's crust	Igneous rocks			Sedimentary rocks		
		Ultramafic	Mafic	Granitic	Limestone	Sandstone	Shales/clays
Ag	0.07	0.06	0.01	0.04	0.12	0.25	0.07
As	1.5	1	1.5	1.5	1	1	13
Au	0.004	0.003	0.003	0.002	0.002	0.003	0.0025
Ba	...	...	330	600	10	193	580
Cd	0.1	0.12	0.13	0.09	0.028	0.05	0.22
Co	20	110	35	1	0.1	0.3	19
Cr	100	2980	200	4	11	35	39
Cu	50	42	90	13	5.5	30	39
Hg	0.005	0.004	0.01	0.08	0.16	0.29	0.18
Mn	950	1040	1500	400	620	460	850
Mo	1.5	0.3	1	2	0.16	0.2	2.6
Ni	80	2000	150	0.5	7	9	68
Pb	14	14	3	24	5.7	10	23
Sb	0.2	0.1	0.2	0.2	0.3	0.05	1.5
Se	0.05	0.13	0.05	0.05	0.03	0.01	0.5
Sn	2.2	0.5	1.5	3.5	0.5	0.5	6
Ti	0.6	0.0005	0.08	1.1	0.14	0.36	1.2
U	2.4	0.03	0.43	4.4	2.2	0.45	3.7
V	160	40	250	72	45	20	130
W	1	0.1	0.36	1.5	0.56	1.6	1.9
Zn	75	58	100	52	20	30	120

4.1 NATURAL BACKGROUND WATER QUALITY

In the catchment area of the Revuè basin, the water crosses a variety of rocks of the Manica greenstone belt. Epidiorite, metagabbro, anorthosite, dolerite, quartz porphyry schist, actinolite chlorite schist, metafelsite, and komatiite metabasalt has been described by Passela (1996). These rocks are composed of minerals such as plagioclase, augite, epidote, clinozoisite, quartz, chlorite, feldspar, biotite, muscovite, magnetite, and actinolite. Dissolution of these minerals results in metals such as Ca, Al, Fe, Si, Na, Mg and K being present in the Revuè basin water. The presence of these metals in the chemical composition of water cannot be considered evidence of pollution in the strict sense of definition. A widely used definition of pollution is "the change in the physical, chemical, radiological or biological quality of the resource (air, land or water) caused by man or due to man's activities that is liable to cause hazards to human health, harm to ecological systems, damage to structures or amenity and is injurious to existing, intended or potential uses of the resource" (Holdgate, 1979; Novotny, 1995).

To characterise the natural background water quality in the Revuè basin, the analytical data of water collected at site 1 in the Revuè river was selected (Fig. 1.2, p. 6). This site is in a pristine area far from the influence of the mining activity and represents the water quality upstream of the mining area. Water quality at this site can be used as base level against which the impact of mining can be judged.

The electrical conductivity of water in this site is 155.3 µS/cm, TDS 74.34 mg/l, alkalinity 32.4 mg/l and turbidity 7.28 NTU (Table 4.1). The suspended sediment concentration in this site is very low as reflected in the clearness of the water.

Trace metals present in the minerals will also be dissolved in the Revuè river water. The content of metals and other determinands in the water upstream of the mining area is generally small, except Cd and Ni, when compared with other two parts of the study area (Figures 4.1 to 4.21 and Table 4.1). Table 4.1 includes the 1996 WHO recommended values for drinking water. In this upstream area, the concentrations of all metals are lower than the WHO standards for drinking water. In the case of Ba, Pb and Mn the concentrations are close to the recommended limit while Al, As, Ca, Cd, Co, Cr, Cu Fe, K, Mg, Mo, Na, Ni, Sr and Zn are markedly lower. Water quality problems are not cause of concern upstream of the alluvial gold mining area in the Revuè basin. This water is therefore of suitable quality to be used as potable water.

4.2 WATER QUALITY PARAMETERS

4.2.1 Physical Parameters

i) TDS and Electrical Conductivity

Electrical conductivity (EC) is the capacity of a substance to conduct electricity. Chemically pure water has very low electrical conductivity. Small quantities of dissolved ions are enough to increase the electrical conductivity of water. The more ions present in the water, the higher the electrical conductivity will be. Therefore, electrical conductivity is proportional to the Total Dissolved Solids (TDS). In the Revuè river the electrical conductivity ranges from 155.3 to 308.65 µS/cm while the concentration of total dissolved solids ranges from 74.34 to 191.16 mg/l. The lowest values of these two determinands are observed upstream of the mining area. Values rise gradually until site 8 where there is a marked increase in the both TDS and electrical conductivity values (Fig. 4.1). At this locality, mining activity by a considerable number of artisanal miners is very intense and large quantities of substances enter the river water from the

gold washing process. This results in the highest electrical conductivity and TDS along the river being recorded at this locality. Similar high values are recorded at sites 9, 10 and 11. From site 12 to site 14 there is a decrease in both TDS and electrical conductivity, reflecting a reduction of metal concentrations in the dam water.

High TDS in potable water may lead to salt overload in sensitive individuals, e.g. those with impaired renal function or those with immature kidneys (Sherman, 1998).

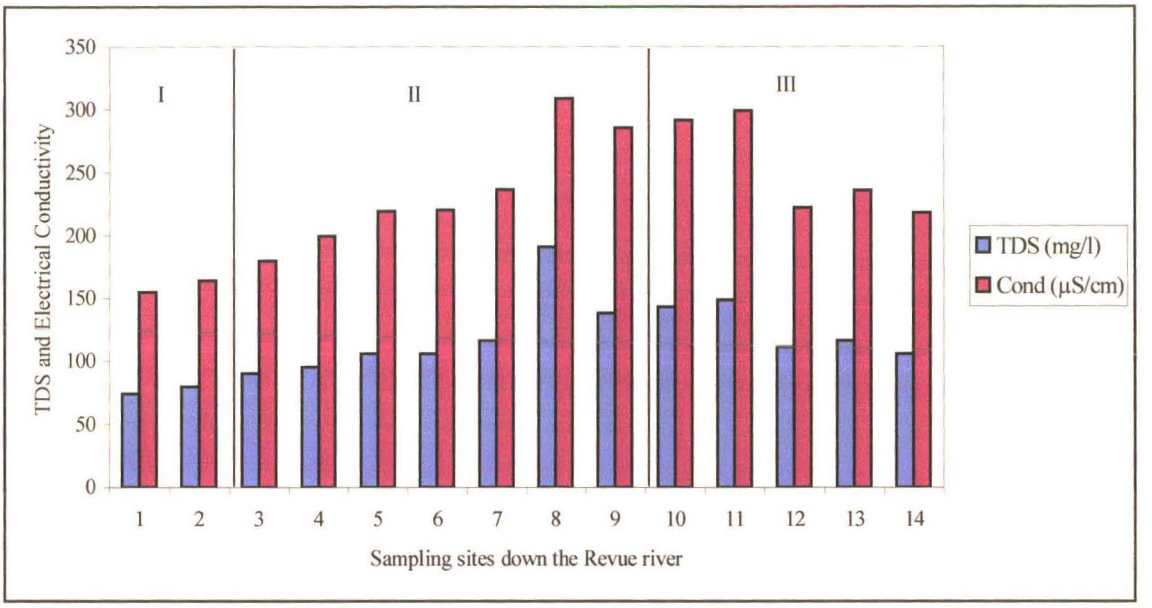


Fig. 4.1 – Spatial distribution of TDS and Electrical Conductivity down the Revuè river. I – Upstream of the mining area; II – Within the mining area; III – Downstream of the mining area.

ii) Turbidity

Turbidity is the state, condition or quality of opaqueness or reduced clarity of a fluid, due to the presence of suspended matter (Jackson, 1997). Water turbidity is a normal function of nature but can be influenced by human activities. Turbid water contains particles that are too small to be seen without magnification, but the particles produce effects that can be detected with the human eye because they scatter light. The particles that cause turbidity are those that are about the same size as wavelengths of visible light (or smaller), described as colloidal size. Colloids are so small that they never settle, even gravity doesn't affect them (Everpure, 1999). Clay and silt particles can also be maintained in suspension for a long time in a turbulent flux due to their small size and also contribute to turbidity. Turbidity is measured in Nephelometric Turbidity Units (NTU).

The maximum value of turbidity allowed in drinking water by the WHO is 5 NTU. In the Revuè river water turbidity values of between 1.42 and 142 NTU were measured (Fig. 4.2). Turbidity starts to increase immediately after the first mining site (site 3) and reaches a maximum at site 9. This is due to washing the auriferous gravel directly in the river water (Chapter 3). Clay and silt particles are held in suspension in the water which becomes brown to reddish-brown in colour. Turbidity values are influenced by the intensity of mining activities as the more mining sites that are crossed by the river water, the higher the turbidity will be. For example, mining activity is intense between site 8 and 9 and this is reflected in high turbidity value of 142 NTU measured at site 9. Furthermore, the number of local miners at a site will also influences the turbidity as there is a direct relationship between the number of miners and the volume of material removed and washed. Along the Revuè river and the Chua and the Zambuzi affluents (Fig. 1.1, p. 2) there are areas where more than one hundred artisanal miners can be found in a small site. Within the mining area, all sample sites have turbidity values that exceed the WHO recommended values set at 5 NTU.

Downstream of the mining area the turbity drops to values of 1.42 NTU and 1.56 NTU in the Chicamba Dam. This reflects settling of clay and silt particles in the impounded water and consequently the turbidity drops.

The water turbidity in the Revuè river basin causes different negative effects:

- transportation and accumulation of clay and silt particles accelerates the reduction in depth of the Chicamba Dam.
- water quality for domestic use is impaired.
- the high level of water turbidity prevents animals from drinking river water.
- aquatic flora and fauna habitats are disturbed.
- the reduction of light penetration in the water can affect the photosynthesis of aquatic plants.
- suspended particles causing turbidity adsorb other dissolved water contaminants and carry them through the system.

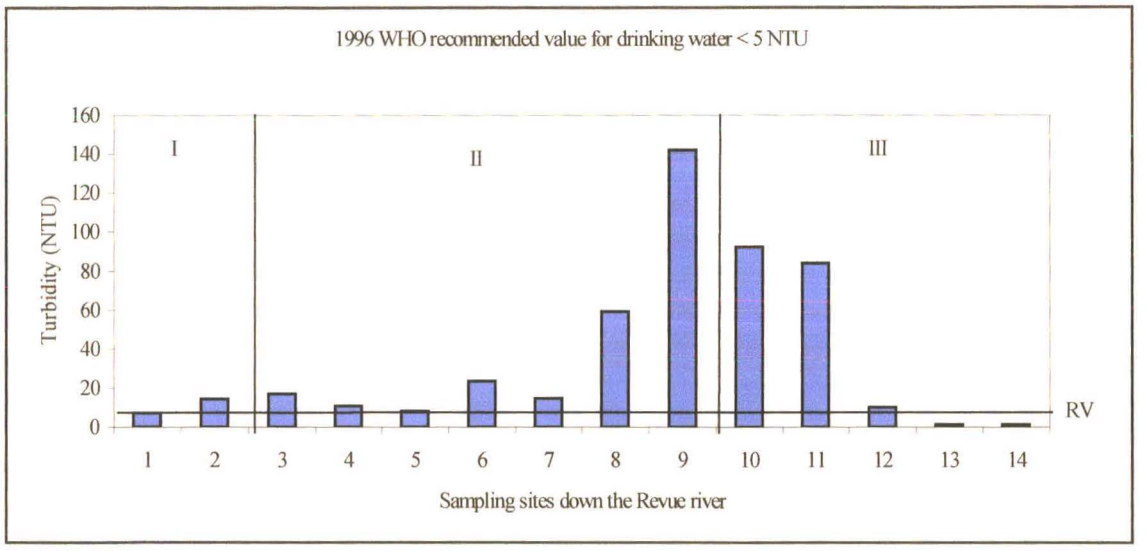


Fig. 4.2 – Spatial distribution Turbidity down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

4.2.2 Chemical Parameters

i) pH

pH expresses the concentration of free hydrogen ions in water. The relative concentration of hydrogen ion in water indicates whether it will act as weak acid or as an alkaline solution. In most natural waters the pH is controlled by reactions involving the carbonate system. These reactions produce H^+ and influence the pH of the solution. The equilibrium reactions are:

$$CO_2\ (aq) + H_2O\ (l) = H_2CO_3\ (aq)$$

$$H_2CO_3\ (aq) = H^+ + HCO_3^-$$

$$HCO_3^- = H^+ + CO_3^{2-}$$

River water in areas not influenced by pollution generally has a pH in the range 6.5 to 8.5. The pH of natural water is useful index of status of equilibrium reactions in which the water participates. In low pH water (acidic), metals generally tend to be more soluble.

In the Revuè river water, pH values of between 7.1 to 7.9 were measured, i.e. within the normal values for natural waters.

ii) Alkalinity

The alkalinity of a solution is defined as the capacity for solutes it contained to react with and neutralize acid. The property of alkalinity must be determined by titration with a strong acid,

and the end point of the titration is the pH at which virtually all solutes contributing to alkalinity have reacted (Hem, 1980). The alkalinity titration is an important analytical procedure in natural water chemistry. The titration curve also provides insights into pH stability and buffering.

Alkalinity is caused by different types of solutes and in almost all natural water the alkalinity is produced by dissolved carbon dioxide species, bicarbonate and carbonate. The important non-carbonate contributors to alkalinity include hydroxide, silicate, borate and organic ligands, especially acetate and propionate (Hem, 1980). The principal source of carbon dioxide species that produce alkalinity in surface or ground water is the CO_2 gas fraction of the atmosphere or the atmospheric gases present in the soil.

In the Revuè river the alkalinity concentrations measured are between 24.8 and 61.6 mg/l as $CaCO_3$. In a general manner the alkalinity values rises gradually from upstream of the mining area with some small oscillations. Fig. 4.3 shows that the highest alkalinity is observed within the mining area at site 9 with 61.6 mg/l as $CaCO_3$. This site is underlain by carbonate rocks. Downstream of the mining area the alkalinity starts to drop gradually until the Chicamba Dam at site 14. Chemical precipitation of Ca and Mg carbonates which occurs in the water column to form particles and colloids can be the cause of the reduction (Fillela *et al.*, 1995).

The WHO does not establish the maximum alkalinity value in drinking water.

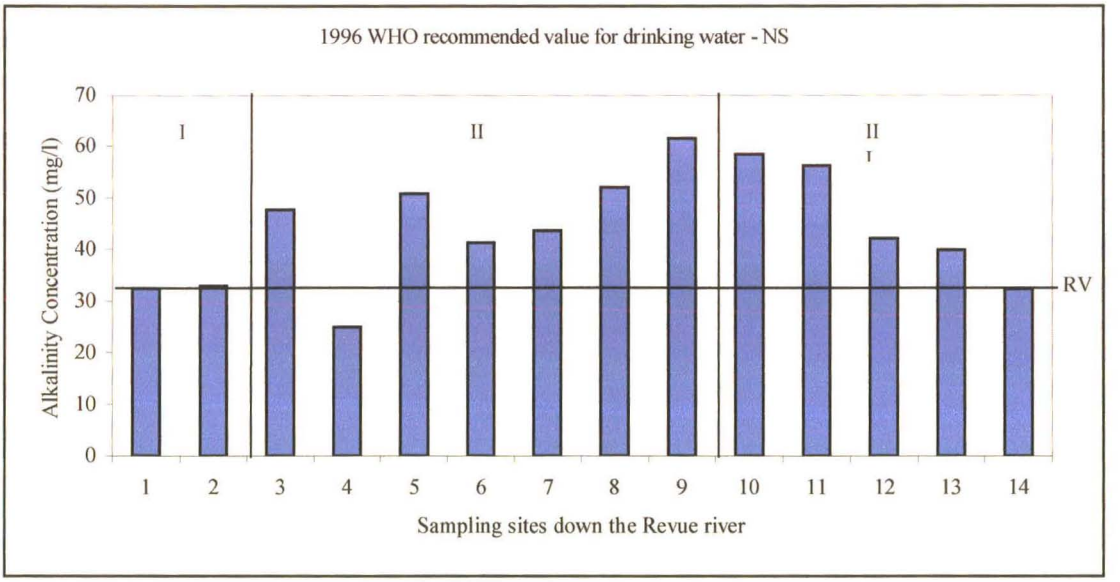


Fig. 4.3 – Spatial distribution of Alkalinity down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

4.2.2.1 Major metals

i) Calcium

Calcium is the most abundant of the alkaline-earth metals and is a major component of the solutes in most natural waters. The sources of calcium are the sedimentary rocks where Ca is found as carbonates and as calcareous cement between particles. In igneous rocks plagioclase feldspars are a major source of calcium but calcium is also present in pyroxenes, amphiboles and in other silicate minerals produced by metamorphism.

Calcium has only one oxidation state, Ca^{2+}, and generally it is a predominant cation in river water. The behaviour of calcium in natural aqueous systems is generally governed by the availability of the more soluble calcium-containing solids and by solution and gas-phase equilibria that involve carbon dioxide species (Hem, 1980).

In the Revuè river the calcium concentrations range between 3.8 and 7.2 mg/l. The lowest values are found at site 1. Here the possible sources of calcium are the pyroxinites and amphibolites. The highest concentrations of Calcium are observed, at the site 9, within the mining area, where the river crosses carbonate rocks as marble which is found within the Manica greenstone belt.

Downstream of the mining area at sites 12 to 14 the calcium concentration drops gradually until the Chicamba Dam (Fig. 4.4). When river water is impounded in a storage reservoir, changes may occur in calcium content as a result of calcium carbonate precipitation (Hem 1980). The increased pH near the water surface, caused by algae and plankton, may bring about supersaturation, and precipitation can occur on solid surfaces around the edges of the water.

All sites sampled in the Revuè river are well below 200 mg/l, the recommended maximum calcium concentration for drinking water.

ii) Magnesium

Magnesium is an alkaline-earth metal together with calcium ions contributes to the property of water hardness. Magnesium is derived from different sources. In igneous rocks, magnesium is typically a major constituent of ferromagnesian minerals such as olivine, pyroxenes, amphiboles and biotite. In metamorphic rocks magnesian mineral species such as chlorite and serpentine occur. In sedimentary rocks it is found in magnesite and hydromagnesite, the hydroxide brucite, limestone and dolomite (Hem, 1980).

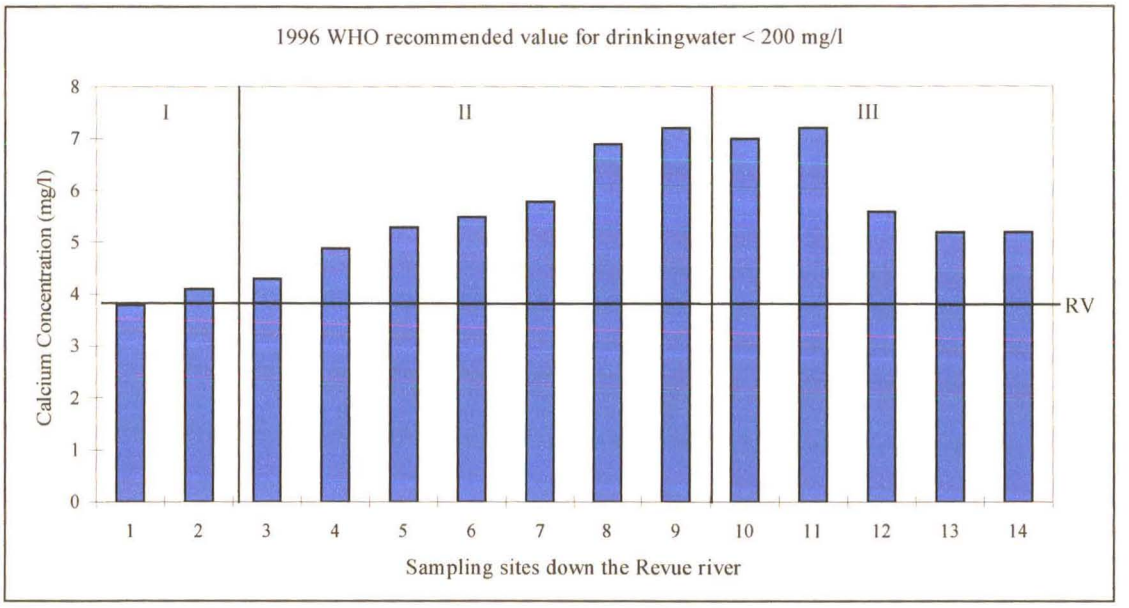


Fig. 4.4 – Spatial distribution of Calcium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

Magnesium has only one oxidation state of significance in water chemistry, Mg^{2+}. The magnesium ion, Mg^{2+}, will normally be the predominant form of magnesium in solution in natural water. Other magnesium forms in solution are the ion complexes $MgOH^{+}$ formed at pH >10 and the neutral ion pair $MgSO_{4\,(aq)}$ (Hem, 1980).

The concentrations of magnesium measured in the Revuè river range between 3.1 and 7.7 mg/l. The distribution of magnesium down the Revuè river is similar to that reported for calcium. The smallest concentrations are found upstream the mining area (Fig. 4.5). The magnesium concentration rises within the mining area reaching a peak at sites 8 and 9. This coincides with the change in lithology to carbonates rocks (marble). Similar concentrations are found at sites 10 and 11. Downstream of the mining area the magnesium concentration drops until the Chicamba Dam. This may be due to the chemical precipitation of calcium and magnesium carbonates in the water column to form particles and colloids (Fillela *et al.*, 1995) or to dilution by other river waters flowing in the Chicamba Dam. In this area the water is quiescent which would aid settlement of suspended material.

Magnesium is a common element and is essential to plant and animal nutrition. The maximum recommended concentration in drinking water is 150 mg/l which is higher than the observed concentrations in the Revuè river.

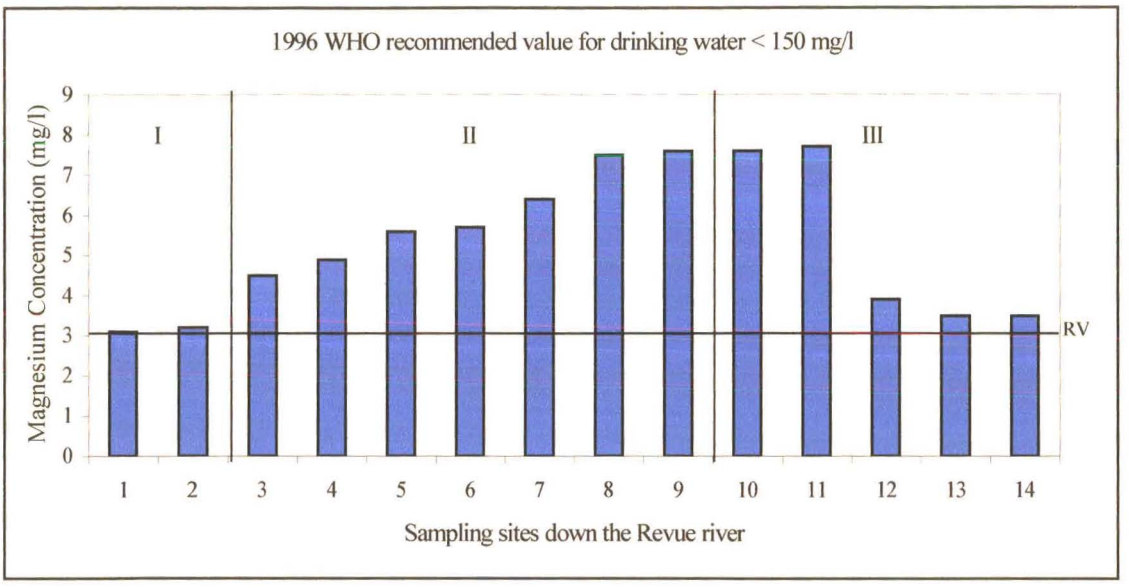


Fig. 4.5 - Spatial distribution of Magnesium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

iii) Sodium

Sodium is economically the most important and abundant member of the alkali metal group of the periodic table. It occurs in igneous, sedimentary and evaporite rocks. Sodium is found in plagioclase minerals ranging in composition from albite ($NaAlSi_3O_8$) to anorthite ($CaAlSi_2O_8$). These plagioclases are susceptible to weathering and form clay minerals (kaolinite, illite or montmorillonite). The sodium occurs in the Na^+ oxidation state and does not participate in redox processes (Hem, 1980). When it is in solution, it tends to remain as sodium ions and does not readily participate in precipitation reactions.

The sodium ion Na^+ predominates in waters with TDS below 1000 mg/l. In more concentrated solutions the complex ions and ion pairs $NaCO_3^-$, $NaHCO_{3\,(aq)}$ and $NaSO_4^-$ are possible.

Natural water can have a very wide range of sodium concentration from less than 1 mg/l in rain water and dilute stream runoff to more than 100 g/l in brines associated with evaporites. In the Revuè river water concentrations of 3.3 to 5.85 mg/l of sodium were measured (Fig. 4.6).

There is a close correlation between sodium concentration and lithology, for example, sites 1 and 2 situated on basalts, komatiites, talschists and chloritic schists have similar sodium concentrations. Likewise, sites 3 to 7 situated on peridotites, serpentinites and amphibolites, also have similar sodium concentrations. Generally the highest sodium concentrations in the Revuè river are associated with granitic lithologies.

Minor variation in concentration along the river, may possibly be attributed to adsorption by clay minerals, as at site 10 or dissolution of igneous rocks, as at site 11.

High sodium concentrations can be of concern in infants as the infant kidney is less effective than the adult at sodium elimination. If sodium is present in excess in drinking water given to infants hypernatraemia may result. However, the concentrations along the river are well bellow recommended WHO value of 120 mg/l.

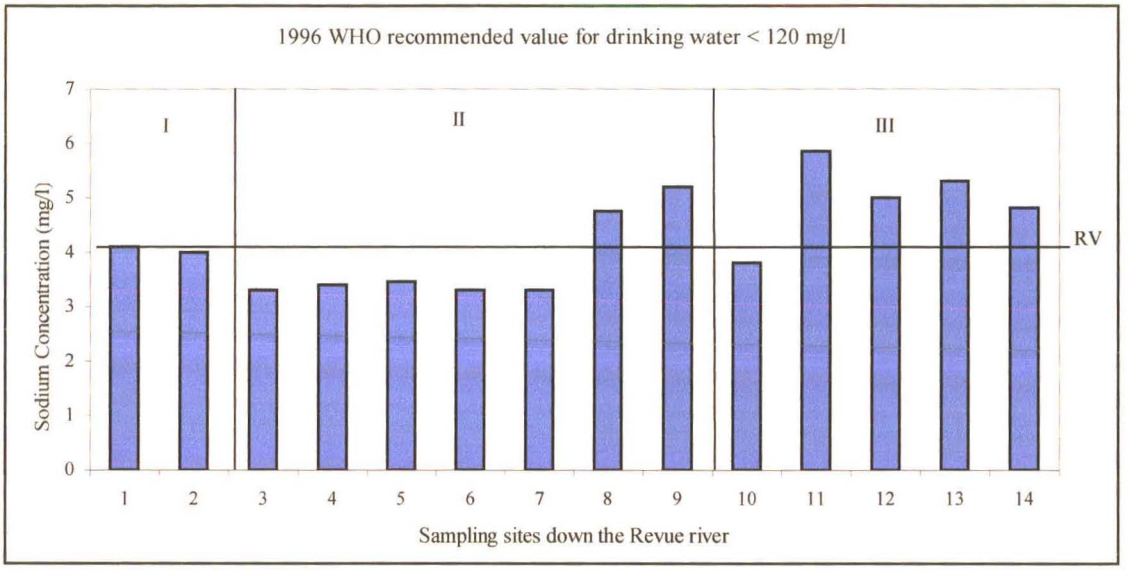


Fig. 4.6 - Spatial distribution of Sodium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

4.2.2.2 Minor metals

i) Aluminium

Aluminium is the third most common element in the earth's crust. It rarely occurs in solution in natural water in concentrations greater than few tenths or hundredths of a milligram per liter (Hem, 1980). Aluminium is considered to be non-essential element for human health and development, as no substantiating evidence has been found to indicate that it fulfils any vital biological function.

Aluminium is a major compound in a large number of silicate igneous rock minerals like feldspars, feldspathoids, micas and amphiboles, and in clays. At neutral pH the aqueous concentration of aluminium is low in subsoil water, lakes, rivers and seawater, due to the formation of secondary hydroxo phases (Hem, 1980). At high and low pH levels the solubility increases substantially.

Aluminium is trivalent and the cation Al^{3+} predominates in many solutions in which the pH is less than 4.0. Above neutral pH, the predominant dissolved form of aluminium is the anion $Al(OH)_4^-$. In the presence of few tenths of a milligram per liter to a few milligrams per liter of fluoride the ions AlF^{2+} and AlF^+_2 appear to be most likely in natural water. The sulfate complex $AlSO^+_4$ may predominate in acid solutions in which much sulfate is present (Hem, 1980).

The median concentration of aluminium in rivers range from 0.01 to 40 mg/kg (Frech & Cedergren, 1992). The aluminium values measured in the Revuè river are of 0.02 to 0.14 mg/l. In a general manner the aluminium concentration rises gradually from upstream to downstream of the mining area with some small oscillations (Fig. 4.7). The presence of granitic rocks at sites 13 and 14 coincides with the highest Al^{3+} concentrations found in the area.

Possible toxic effects due to high aluminium concentration in water are the development of neurological diseases such as Alzheimer's senile and pre-senile dementia, amyotropic lateral sclerosis, and Parkinson's dementia as well as dialysis encephalopathy (Frech & Cedergren, 1992; Packham, 1993).

The maximum recommended aluminium value for drinking water is 0.2 mg/l. This value is above those observed in the Revuè river.

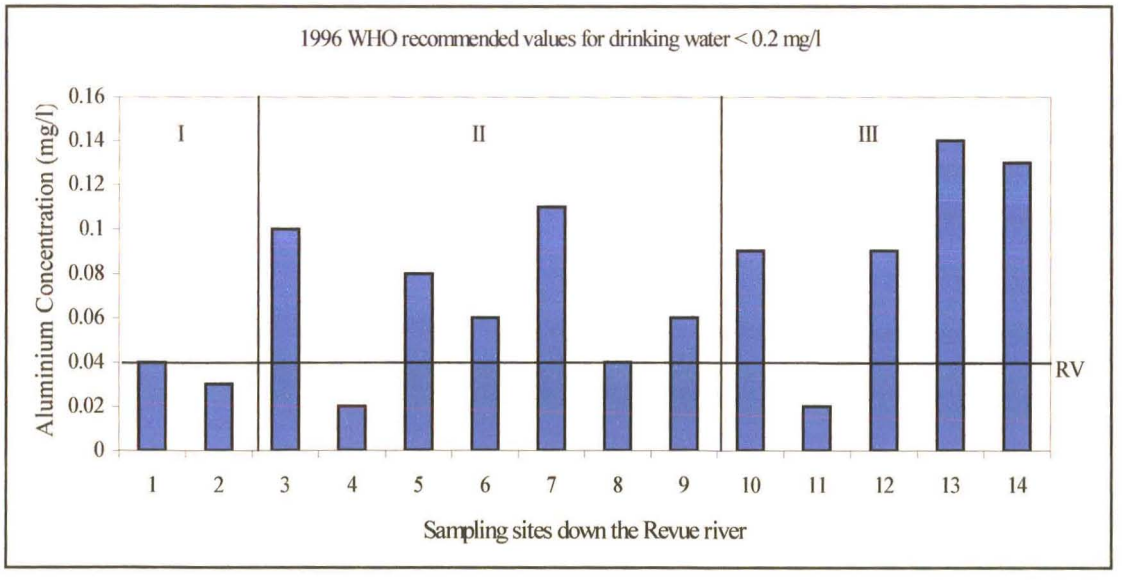


Fig. 4.7 – Spatial distribution of Aluminium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

ii) Iron

Iron, the most important of all metals, is also one of the most abundant in the earth's crust, being second only to aluminium. The most important ores are hematite, Fe_2O_3, magnetite, Fe_3O_4, and siderite, $FeCO_3$. Pyroxenes, amphiboles, biotite and olivine also have relatively high iron contents. Iron in these minerals is in ferrous, Fe^{2+}, oxidation state whereas in magnetite is in the ferric, Fe^{3+} state.

Iron concentrations in water generally are small. Its chemical behaviour and solubility in water depends strongly on the oxidation potential of the system in which it occurs. The iron in aqueous systems can be found as ferrous or ferric ions, anions, monohydroxides and solid ferric oxyhydroxide. Ferric oxyhydroxide surfaces have a substantial adsorption capacity, which may affect the concentration of minor constituents of water associated with such material. Redox co-precipitation process may occur that can control solubilities of other metal ions under some conditions (Hem, 1980).

Water in rivers that is fully aerated should not contain more than a few micrograms per liter of uncomplexed dissolved ferrous iron at equilibrium in the pH range of about 6.5 to 8.5 (Hem, 1980). In the Revuè river concentrations of 0 to 0.27 mg/l were measured. Fig. 4.8 shows that the highest concentrations of iron occur within the mining area. At sites 3 to 7 both the mining activity and lithology have a combined effect in raising the iron concentration. These sites are underlain by the same rock types (peridotites, amphibolites, serpentinites) and the gold washing process increases the releasing of iron to the water. The reduction of iron concentration observed at sites 8 and 9 is possibly due to precipitation of iron as a carbonate as the river flows over marble in the region. Downstream of the mining area the iron concentration continues to drop as the river runs over acid rocks such as granites, gneissic granites and cratonic granitoids. It is believed that the impoundment of water in the Chicamba Dam has also effect on the iron concentration because dilution can occur as well as settling of metal-contaminated solids.

Iron is an essential element in the metabolism of humans, animals and plants. If present in water in excessive amounts it forms red oxyhydroxide precipitates that stain laundry and plumbing fixtures and, therefore, is an objectionable impurity in domestic and industrial water supplies (Hem, 1980). The maximum iron concentration allowed in drinking water is 0.3 mg/l. This value was not recorded in the Revuè river.

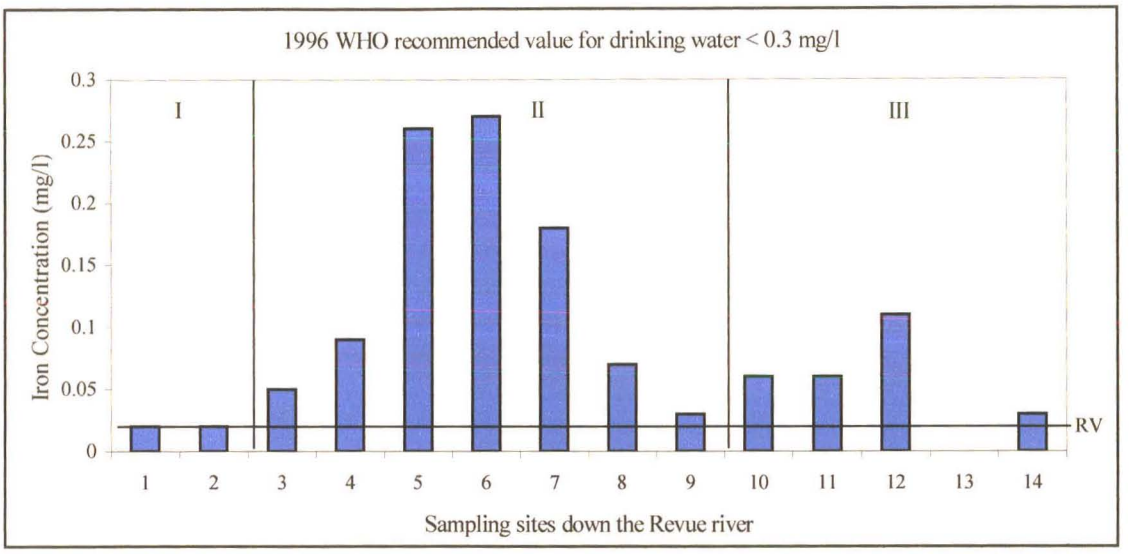


Fig. 4.8 – Spatial distribution of Iron concentration down the Revuè river. I – Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

iii) Potassium

Potassium is the sixth most common element in the earth's crust. Although potassium is an abundant element and its salts are highly soluble, it seldom occurs in high concentrations in natural water. It is slightly less common than sodium in igneous rock but more abundant in all sedimentary rocks (Hem, 1980). Potassium is liberated with greater difficulty from silicate minerals and exhibits a strong tendency to be reincorporated into solid weathering products, especially certain clay minerals (Hem, 1980).

The sources of potassium in silicate rocks are the feldspars orthoclase and microcline ($KAlSi_3O_8$), the micas, and the feldspathoid leucite ($KAlSi_2O_6$). In sediments it is present in unaltered feldspar or mica particles or in illite or other clay minerals.

In dilute natural waters in which the sum of sodium and potassium is less than 10 mg/l, it is not unusual for the potassium concentration to equal or even exceed the sodium concentration (Hem, 1980). This is not the situation observed in the Revuè river where the potassium concentrations of 0.387 to 2.599 mg/l were recorded. There is a little variations in potassium concentration along the river with values below or close to 1 mg/l until site 12 where there is a marked increase in concentration (Fig. 4.9). This increase can be attributed to the granitic lithologies found in the area.

Limits for potassium in drinking water are based on its effect in disturbance of the electrolyte balance of the body (Sherman, 1998). A desirable limit for potassium is 10 mg/l, which is higher than the values observed in the Revuè river.

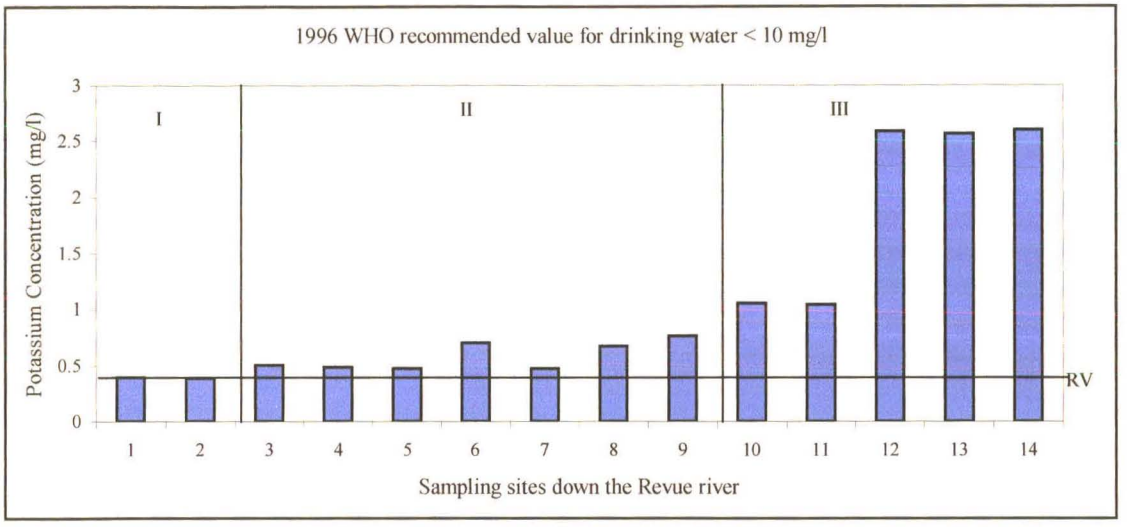


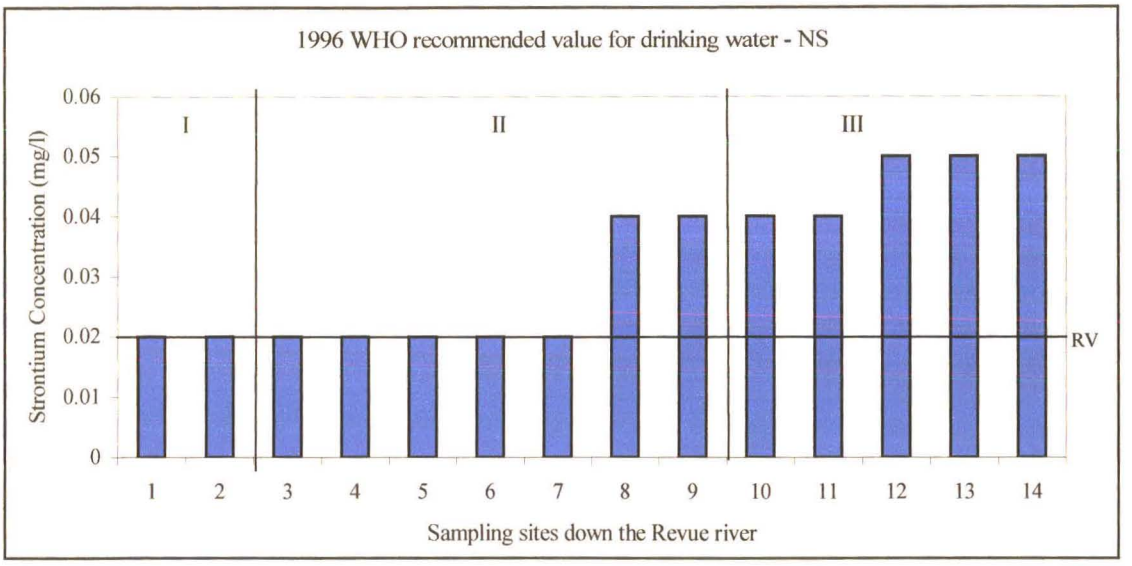
Fig. 4.9 – Spatial distribution of Potassium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III – Downstream of the mining area; RV - Reference Value (Site 1).

iv) Strontium

Strontium is a fairly common element, replacing calcium or potassium in igneous-rock minerals in minor amounts, although apparently favouring those species that are typical of granitic and syenitic rocks rather than ultrabasic rocks (Hem, 1980). Other sources of strontium are strontianite ($SrCO_3$) and celesite ($SrSO_4$) which are common in sediments.

The oxidation state of strontium is +2 and its chemistry is similar to that of calcium. The strontium concentration in most natural waters does not approach the solubility limit of either strontianite or celestite (Hem, 1980). In the Revuè river concentrations of 0.02 to 0.05 mg/l were measured (Fig. 4.10). At site 8, the increase in concentration coincides with the changes in lithology from mafic and ultramafic rocks to metasedimentary and carbonate rocks (quartzites and marble), the latter having higher strontium concentrations than the former. A further increase in strontium concentration occurs at site 12 where the river flows over granitic rocks which have high strontium concentration.

No value was recommended as maximum concentration of strontium in drinking water.



4.10 - Spatial distribution of Strontium concentration down the Revuè river. I - Upstream of the mining area; II - Mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

4.2.2.3 Trace metals

i) Arsenic

Arsenic compounds have been known, at least in impure form, for several millenia. It occurs in the earth's crust at an average of 2-5 ppm (Manahan, 1990). Historical events make it understandable that it is perceived as a life threatening poison (Irgolic, 1992). Arsenic may form metal arsenides in which its oxidation state is negative. Arsenic may also form sulfides and can be present as an accessory element in sulfide ore deposits. Arsenite and arsenate are the most common arsenic compounds in the environment. Arsenite is formed as the weathering product of arsenic-containing sulfide ores and is considered the most toxic among arsenic compounds. Arsenic also occurs with phosphate minerals. In solution in aerobic waters arsenate (As^{5+}) or Arsenite (As^{3+}) oxyanions are the thermodynamically stable forms of inorganic arsenic (Hem, 1980).

The dissolution of the above mentioned sources and the combustion of fossil fuels, particularly coal, introduces large quantities of arsenic into the environment, much of it reaching natural waters (Manahan, 1990). The arsenic concentration values measured in the Revuè river water range from 0 to 0.042 mg/l with the highest value (0.042 mg/l) recorded at site 13 (Fig. 4.11). Examination of Table 4.2 indicates that apart from shales and clays, typical arsenic concentrations in major rock types varies from 1 to 1.5 ppm. Concentrations of arsenic in natural waters can be expected to be lower than the average concentration found in rocks but will be independent of lithology. Within the mining area variations in concentrations may be

the result of adsorption of arsenic by hydrous iron oxide, or co-precipitation, or combination with sulfide in the bottom sediments (Hem, 1980).

Because small amounts of arsenic can be toxic to humans, it is considered a highly undesirable impurity in water supplies. Although, arsenic compounds can have beneficial influences on human and animal life. The recommended arsenic concentration for drinking water set by the WHO in 1996 is less than 0.05 mg/l. This concentration is above the values measured in the Revuè river water.

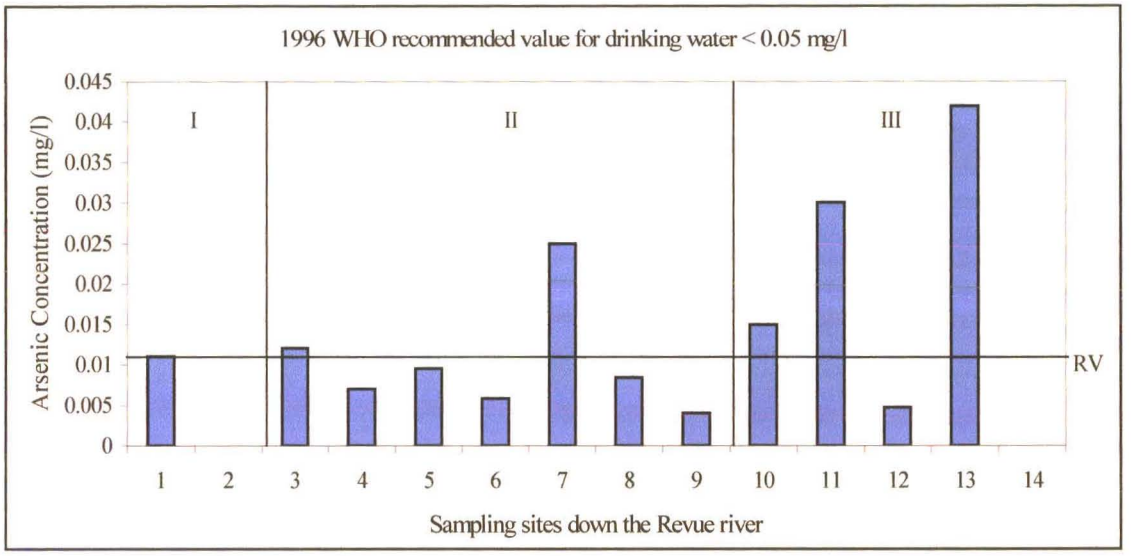


Fig. 4.11 – Spatial distribution of Arsenic concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

ii) Barium

Barium is somewhat more abundant in acid igneous rocks than in basic and ultrabasic. It occurs principally as the mineral barite ($BaSO_4$), which is fairly common mineral. The concentration of barium in natural waters is likely controlled by the solubility of this mineral. This reduces the range between the upper and lower extreme values of barium to be expected in natural waters. Another factor that seems likely to influence the concentration of barium in natural water is adsorption by metal oxides or hydroxides (Hem, 1980).

Barium oxidation state is 2+ and a median concentration of 0.045 mg/l is observed in rivers (Hem, 1980). In Manica barium concentrations of 0.08 to 0.19 mg/l were recorded. The lowest barium concentrations are observed upstream of the mining area (Fig. 4.12). Within the mining area sites 3 to 7 have fairly constant barium concentrations. These sites have similar lithologies of peridotites, serpentinites and amphibolites. The Zambuzi river (also with mining activity),

which flow into the Revuè river between sites 7 and 8 brings high barium content (0.27 mg/l) that increases the barium concentration at site 8. At site 8, the country rocks are carbonatic and metasedimentary (marble, quartzites, metagreywakes). These rock types are likely to contain higher barium concentrations than mafic rocks and also contribute to the higher concentrations at site 8 and 9. The release of barium can be accelerated by the intense mining activity in these sites.

Downstream of the mining area the barium concentration remains fairly constant. The Chicamba Dam (site 14) receives water from other rivers flowing over the granitic gneiss complex and has the highest concentration of barium (0.19 mg/l).

From site 8 downstream to the Chicamba Dam, barium concentrations are higher than the recommended WHO standard for drinking water (0.1 mg/l). Because of the toxicity of barium, it is considered an undesirable impurity in drinking water. Water from Chicamba Dam is pumped to Chimoio City and used as potable water. Apart from desinfection with chlorine, no water treatment is undertaken.

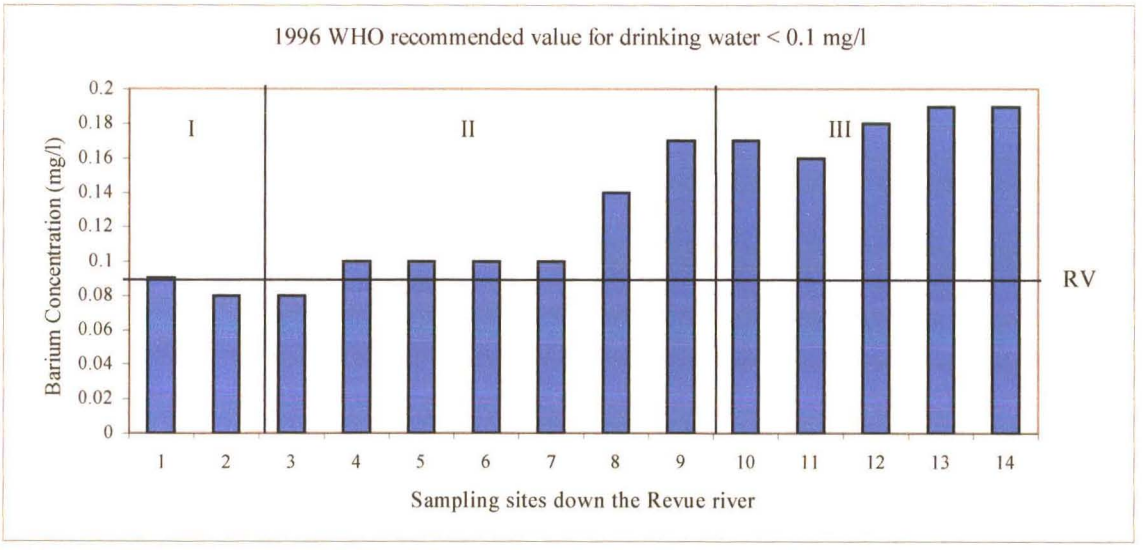


Fig. 4.12 – Spatial distribution of Barium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

iii) Nickel

Nickel is widely distributed in the environment and is the twenty-fourth most abundant element in the earth's crust. It may substitute for iron in ferromagnesian igneous-rock minerals. The source of nickel are ferrous sulfides in which nickel is substituted for part of the iron, and nickel-bearing laterites developed on ultramafic bedrock terranes (Hem, 1980).

Nickel oxidation states are +1, +2 and +3 and the aqueous chemistry is primarily concerned with the Ni^{2+} oxidation state. Important compounds are nickel oxide, nickel hydroxide, nickel sulphate, nickel chloride and nickel subsulfide (Stoeppler & Ostapczuk, 1992).

The median concentration of nickel in river water and probably in most other natural freshwater is somewhat less than 1 to 60 µg/l. In the Revuè river water values between 0 and 0.0069 mg/l (6,9 µg/l) were measured (Fig. 4.13). The highest concentrations were observed in sites underlain by ultramafic and mafic rocks, which have the highest typical concentrations of nickel (Table 4.2, p. 23). The concentrations of nickel in the Revuè river may be a reflection of its natural abundance. Nickel tend to be coprecipitated with iron oxides and especially with manganese oxides (Hem, 1985).

The maximum recommended nickel concentration for drinking water is 0.02 mg/l. Therefore, the concentrations in Revuè water are below the recommended value. Divalent nickel compounds are non-toxic for animals, plants and man at prevalent concentrations in natural waters. In humans beings adverse effects (dermatitis) from inorganic, water-soluble nickel compounds frequently occur following skin contact.

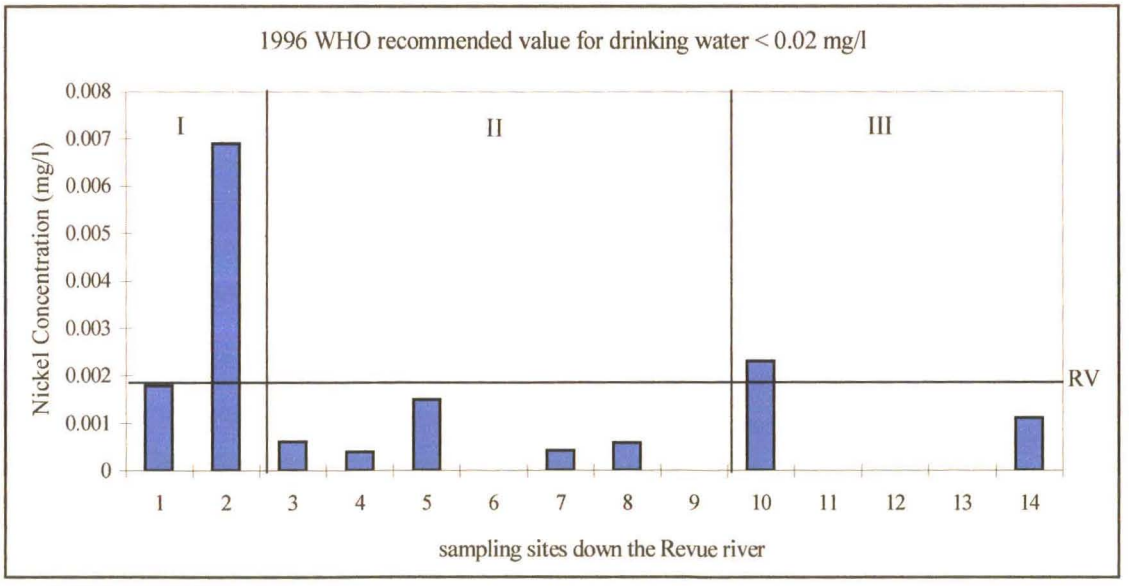


Fig. 4.13 – Spatial distribution of Nickel concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1)

iii) Cobalt

Cobalt is comparatively rare than nickel and is the thirty-second most abundant element in the earth's crust. It can substitute for part of the iron in ferromagnesian rock minerals (Hem, 1985).

Cobalt oxidation states are +2 and +3. Important cobalt compounds are cobalt oxide, cobalt tetraoxide, cobalt chloride, cobalt sulfide and cobalt sulfate (Stoeppler & Ostapczuk, 1992). With the possible exception of certain complex ions, aqueous species of Co^{3+} are not thermodynamically stable under Eh and pH conditions that commonly occur in natural water. (Hem, 1985).

The median concentration of cobalt in river water is between 0.4 to 4 µg/l. In the Revuè river water values between 0 and 0.024 mg/l (24 µg/l) were measured (Fig. 4.14). The first change in the Cobalt concentration is observed at site 3 with the change in lithology from schists to peridotites and serpentinites. The highest concentration is observed in the lower part of the mining area at site 9 which is underlain by metasedimentary and carbonate rocks. The high concentration here may be due to remobilization of the sediments during mining activity. A similar value at site 10, underlain by peridotites and serpentinites, may be a consequence of rock type (Table 4.2, p. 23). Downstream of the mining area the Cobalt concentration drops and returns to values close to those observed upstream of the mining area.

The maximum acceptable concentration of cobalt in drinking water has not been established. Cobalt is a constituent of vitamin B12 and in this form is essential for mammals (i.e. also for human beings) especially for ruminant animals. Extremely low contents in food may lead to deficiency syndromes, which has been especially observed in ruminants. Although, because of its industrial use, cobalt also poses a potential danger in occupational exposure primarily for metal workers (Stoeppler & Ostapczuk, 1992). Exposure to cobalt-containing dust and fumes can cause adverse effects to lungs, heart and skin.

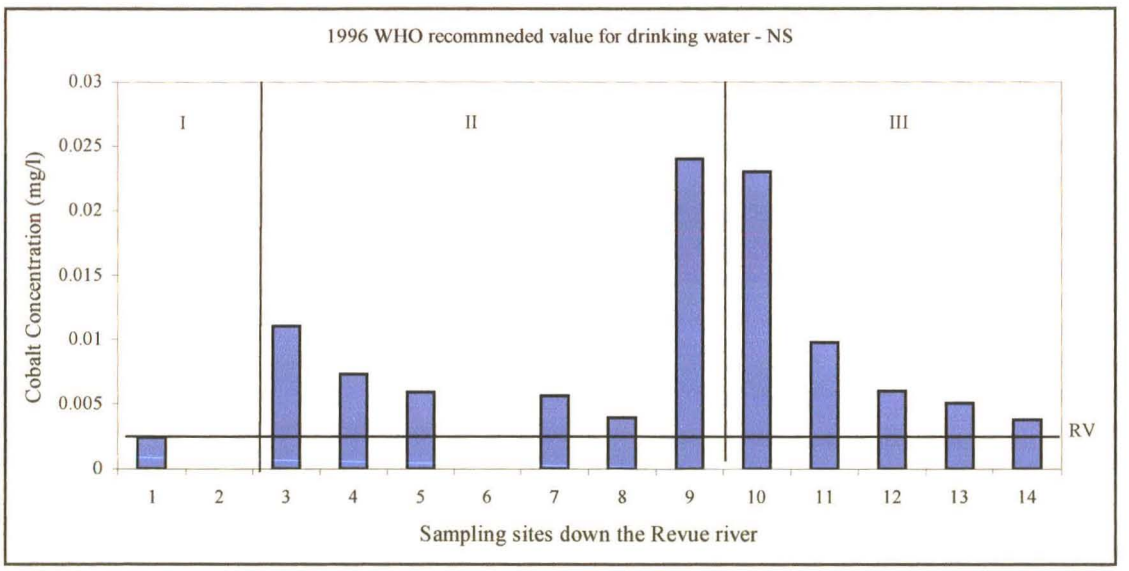


Fig. 4.14 – Spatial distribution of Cobalt concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

iv) Manganese

Manganese is the tenth most abundant element in the earth's crust. Manganese occurs as a minor constituent in igneous and metamorphic minerals. It is not an essential constituent of the more common silicate rock minerals, but it can substitute for iron, magnesium or calcium in silicate structures (Hem, 1985). Manganese is a significant constituent of basalt and many olivines and of pyroxene and amphibole. It is also present in small amounts in dolomites and limestones substituting for calcium.

The chemistry of manganese is somewhat like that of iron, but manganese has three oxidation states, +2, +3 and +4, and can form a wide variety of mixed-valence oxides. The +3 species are unstable. When divalent manganese is released to the aqueous environment during weathering, it is more stable toward oxidation than is ferrous iron (Hem, 1985). Manganese co-precipitates with iron, and other metal ions such as cobalt, lead, zinc, copper, nickel and barium (Alloway & Ayres, 1993). Under conditions in natural waters systems, any dissolved manganese will be in the +2 oxidation state. The ion Mn^{2+} will predominate in most situations. It forms hydroxides, complex ions and ion pairs.

The presence of manganese in a stream water depends on the pH. Acidic streams can have more than 1 mg/l of manganese. In the Revuè river concentrations of 0 to 0.2 mg/l were measured with the highest concentration recorded in the lower part of the mining area (Fig. 4.15). The concentration of manganese increases throughout the mining area, reaching a maximum at site 9 which is underlain by metasedimentary rocks. As high concentrations of manganese are normally associated with mafic rocks, the peak concentration can be attributed to alluvial gold mining activity. Furthermore, between sites 8 and 9 the Revuè river receives water from the Inhamazonga river, a small affluent, which brings water with high manganese concentration (0.33 mg/l). This water also helps to raise the manganese concentration in the Revuè river. Downstream of the mining area manganese concentration drops until zero in the Chicamba Dam as the river runs over acid rocks such as granites, gneissic granites and cratonic granitoids which give a very small input of Mn to the water due to their low Mn concentration. It is believed that the impoundment of water in the Chicamba Dam has also effect on the manganese concentration because dilution can occur as well as settling of metal-contaminated solids. Hem (1985) suggests that manganese takes long time to disappear from solution.

A recommended upper limit for manganese in drinking water is 0.02 mg/l. Fig. 4.15 shows that from site 3 to site 11 Mn exceeds this value. Manganese is an undesirable impurity in water supplies, mainly owing to a tendency to deposit black oxide stains.

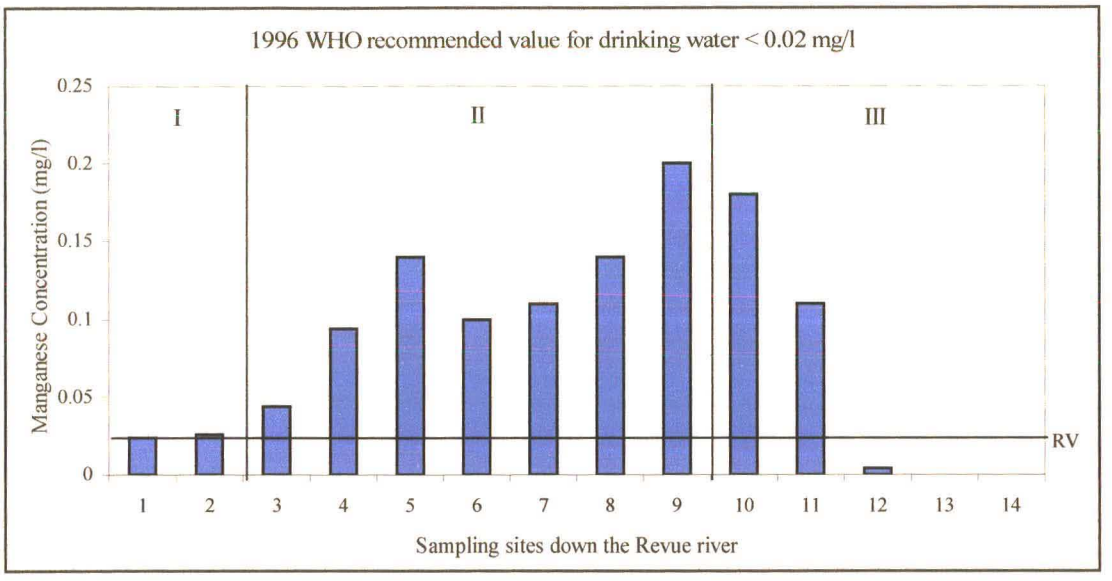


Fig. 4.15 – Spatial distribution of Manganese concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

v) Copper

Copper is by a considerable margin the most noble of the first transition series metals, and it may occur in the earth's crust, as native copper or in Cu^{+} or Cu^{2+} minerals. Copper forms stable sulfide minerals. Common ores are chalcopyrite or copper pyrite, $CuFeS_2$, malachite, $Cu_2(OH)_2(CO_3)$, atacamite, $Cu_2(OH)_3Cl$, and cuprite, Cu_2O (Sharpe, 1986).

Copper may occur in solution in either Cu^{2+} or Cu^{+} oxidation states, but the redox conditions in oxygenated water favour the more oxidised form (Hem, 1985). The species formed in solution are $Cu(OH)_3^{-}$ (above neutral pH) and $CuCO_3(aq)$ in aerated natural water containing dissolved CO_2 species.

Levels of copper near 10 µg/l can be commonly expected in river water. In the Revuè river water 0 to 0.05 mg/l (50 µg/l) of copper were measured. The highest concentration is observed at site 5, within the mining area (Fig. 4.16). There is no clear apparent reason for Cu behaviour along the river.

As with other metals, the copper concentration in river water is also controlled by adsorption on mineral surfaces and co-precipitation with ferric oxyhydroxides. The upper copper limit in drinking water is 1-2 mg/l, well above the concentrations measured in the Revuè river.

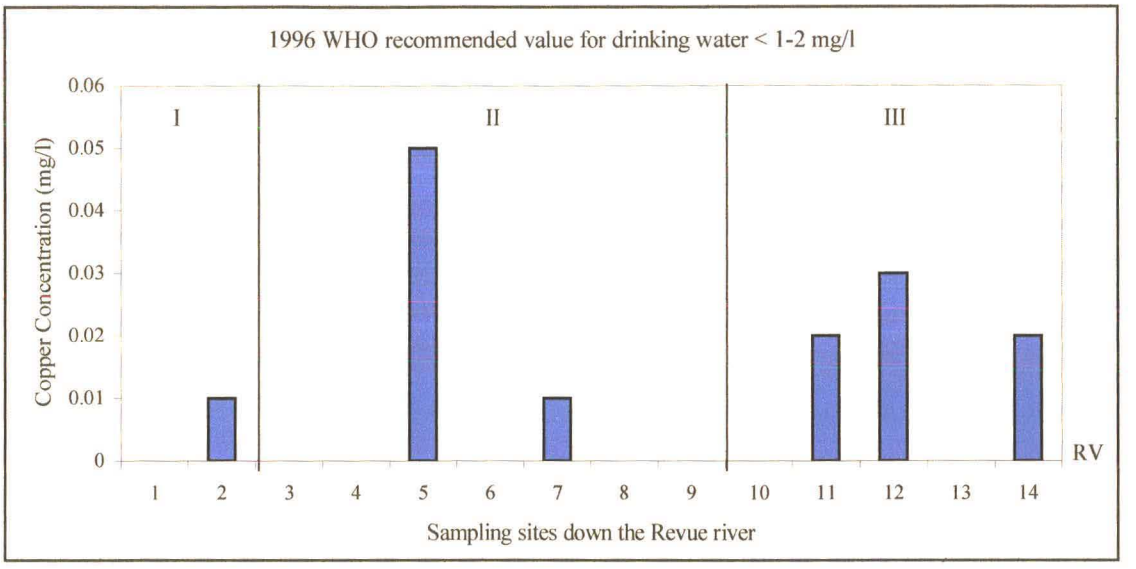


Fig. 4.16 – Spatial distribution of Copper concentration down the Revuè river. I - Upstream of the mining area; II –Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

vii) Chromium

Chromium occurs naturally in the environment and is the twenty-first most abundant element in the earth's crust with an average concentration of 100 µg/g (Miller-Ihli, 1992). Its principal ore is chromite, $FeCr_2O_4$, and elemental chromium is rarely found in nature. Chromium occurs in oxidation states ranging from Cr^{2+} to Cr^{6+}. In minerals the predominant oxidation state is Cr^{3+}. Dissolved chromium, however, may be present as trivalent cations or as anions in which the oxidation state is Cr^{6+} (Hem, 1985).

Concentrations of chromium in natural waters that have not been affected by waste disposal are commonly less than 10 µg/l. Naturally occurring chromium concentrations in water arise from mineral weathering processes, the dissolution of chromium bearing soluble organic species, and adsorption from clays. Chromite, the principal ore of chromium, may be concentrated in lateritic residue overlying ultramafic igneous rocks. These rocks are found in the Manica greenstone belt upstream of and within the mining area and constitute the source of chromium in the Revuè river water. In the Revuè river the chromium concentration ranges from 0.0015 to 0.0084 mg/l (Fig. 4.17). The ultramafic igneous rocks are higher in chromium concentration than other rock types (Table 4.2, p. 23). Downstream of the mining area the concentration of chromium drops gradually until the Chicamba Dam. The chromium concentration in water is largely controlled by precipitation and co-precipitation reactions and by adsorption or co-precipitation with hydrous oxides of iron and manganese (Miller-Ihli, 1992).

Chromium is an element that has several roles in our daily lives. At low concentrations it is an essential micronutrient in human and animal nutrition and at high concentrations it is a known carcinogen when present as chromate. Drinking water recommended value have been set at 0.05 mg/l total chromium because of the toxic effects of Cr (VI) and the possibility of oxidation of Cr (III) to Cr (VI). In the Revuè water the chromium concentrations are lower than this value.

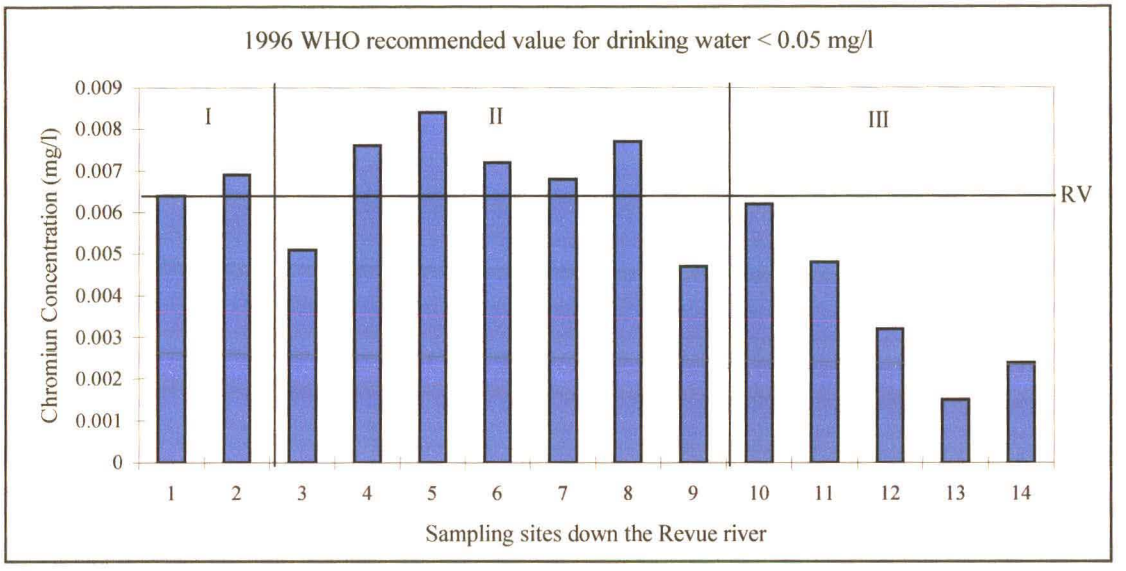


Fig. 4.17 – Spatial distribution of Chromium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

viii) Zinc

Zinc has about the same abundance in crustal rocks as copper or nickel and is fairly common. It is usually recovered from sphalerite, ZnS. Zinc shows a much more restricted range of oxidation state than the other elements, and the chemistry of zinc is confined to that of Zn^{2+} except in so far Zn_2^+ ion has been identified (Sharp, 1986). It tends to be substantially more soluble in most types of natural water than are the other two metals (Hem, 1985).

Zinc concentrations in river water range from 5 to 45 μg/l. The probability of interaction with pre-existing mineral surfaces, through simple adsorption, ion exchange, or co-precipitation processes may inhibit zinc concentration in the river water (Hem, 1985). In the Revuè river, zinc was detected at only two sites; site 8 (0.01 mg/l) and site 14 (0.02 mg/l) (Fig. 4.18).

Zinc is an important element biologically for plants and animals, and occurs in a wide variety of enzymes involved in carbohydrate, lipid and protein metabolism, but is an undesirable

contaminant for some species of aquatic life at much lower concentrations (Hem, 1980; Sharpe, 1986). The upper limit recommended in drinking water set by the WHO is of 3 mg/l because above that limit a significant number of people can detect zinc by taste.

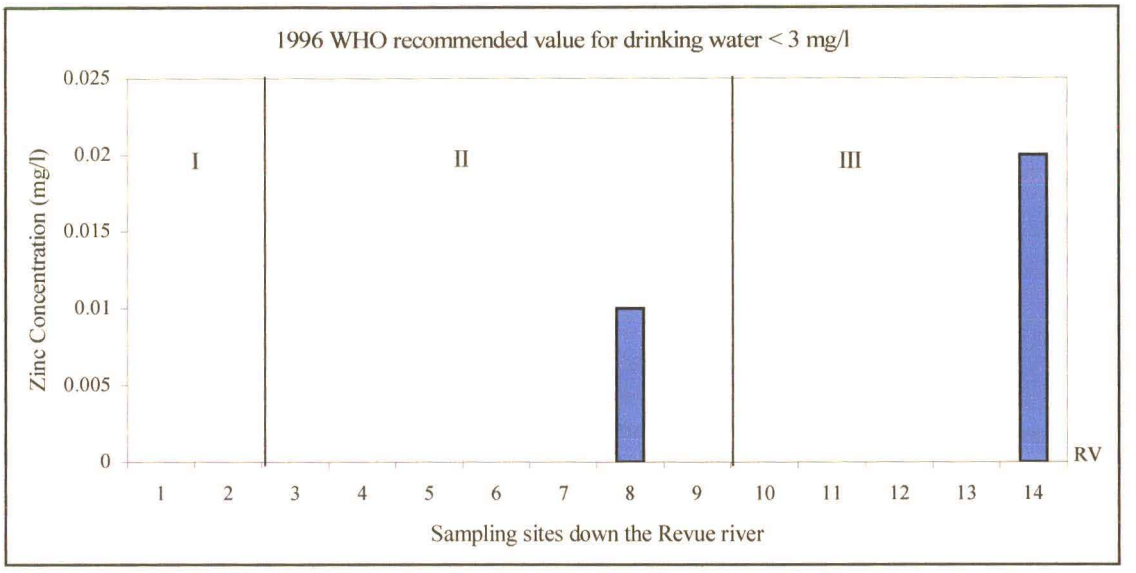


Fig. 4.18 – Spatial distribution of Zinc concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

ix) Cadmium

Cadmium is the sixty-seventh most abundant element in the earth's crust. Generally, cadmium is present in zinc ore minerals such as sphalerite and is recovered from some copper ores during smelting and refining (Hem, 1985). Chemically, cadmium is very similar to zinc, and these metals undergo geochemical processes together. Both metals are found in water in the +2 oxidation state (Manahan, 1990)

The equilibrium solubility of cadmium carbonate was suggested by Hem (1985) as a possible limit for concentrations in natural water. The typical prevalent content for cadmium in river waters, dissolved and particulate bound, is <0.05 - 0.2 μg/l. In the Revuè river water the concentrations of cadmium range from 0 to 0.0027 mg/l (2.7 μg/l) (Fig. 4.19). The distribution of Cadmium appears to be unrelated to mining activity as the highest recorded value occurs at site 1 which was chosen as a background reference value to the pristine nature of the site. Cadmium may be co-precipitated with manganese oxide or adsorbed on mineral surfaces (Stoeppler, 1992) such as calcite (Drever, 1997).

The cadmium recommended value for drinking water set by WHO is 0.005 mg/l. In the Revuè

river cadmium is not a cause of concern. According to present knowledge cadmium is not essential for plants, animals and man. Higher doses of cadmium from ingestion and inhalation can cause toxic effects for humans. Acute effects include high blood pressure, destruction of testicular tissue, destruction of red blood cells and the respiratory and digestive tracts. Cadmium accumulates predominantly in the kidneys with a biological half-life of between ten to twenty years.

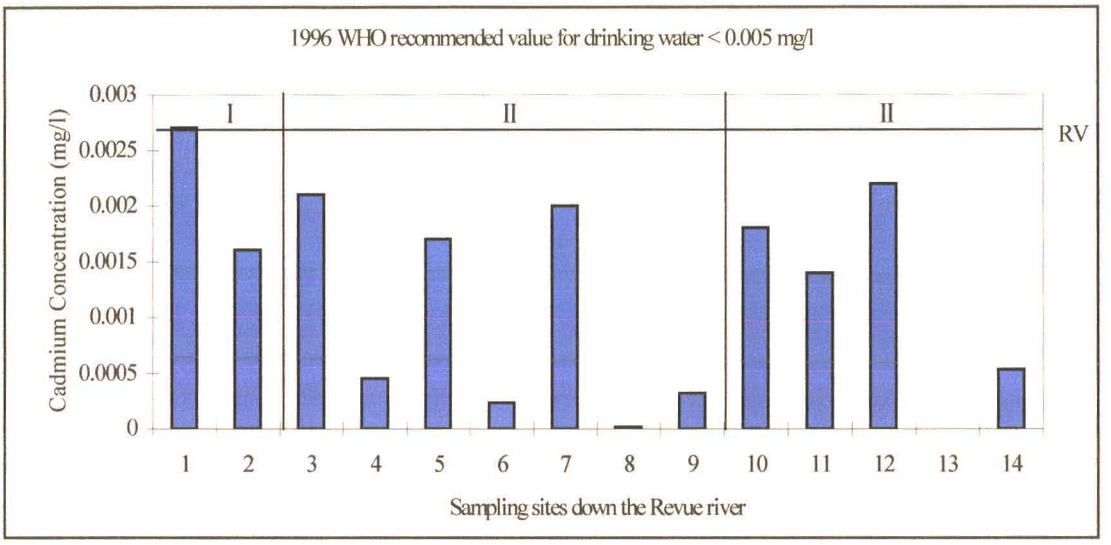


Fig. 4.19 – Spatial distribution of Cadmium concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

x) Molybdenum

Molybdenum is a rather rare element. Its source is sulfide molybdenite, MoS_2 and is an accessory element in many metal ores. Soluble molybdates may be produced in oxidized sectors of these deposits and may appear in detectable concentrations in stream water, sediments, ground water and vegetation at considerable distances from their source. Molybdenum occurs in oxidation states ranging from Mo^{3+} to Mo^{6+}, but the most common solid and aqueous species contain Mo^{4+} and Mo^{6+} (Hem, 1985). In oxidising conditions the predominant oxidation state is Mo^{6+}, which forms molybdate anions in water. Other molybdate species found in water of different pH conditions are H_2MoO_4 (aq) (pH 2), $HMoO_4^-$ (pH 2 to pH 5) and MoO_4^{2-} (above pH 5) (Hem, 1985).

Molybdenum has a relatively high geochemical mobility, i.e., a tendency to enter into solution in water under normal Earth-surface conditions. River water from areas not affected by pollution sources generally have less than 1 μg/l molybdenum (Hem, 1985). In the Revuè river

concentrations of 0 to 0.0081 mg/l were measured. Like cadmium, the distribution of molybdenum appears unrelated to any mining activity as only one site (site 10) exceeds the background reference value. The higher concentration at site 10 is also unrelated to lithology as generally the highest molybdenum values are associated with granitic rocks (Table 4.2) and site 10 is underline by carbonate rocks. The reduction in concentration downstream of site 10 could be related to precipitation and adsorption. Hem (1985) stated that solubility control of molybdenum concentration could include precipitation with common metals as metals molybdates and referenced other authors saying that the downstream attenuation of molybdenum in water and sediment is attributed to adsorption by amorphous ferric oxyhydroxide. Furthermore, Alloway & Ayres (1993) state that molybdenum can be adsorbed and co-precipitated with hydrous oxides of iron in both sediments and soils.

The upper molybdenum concentration limit for drinking water is 0.05 mg/l. Values measured in the Revuè river never exceeded this value.

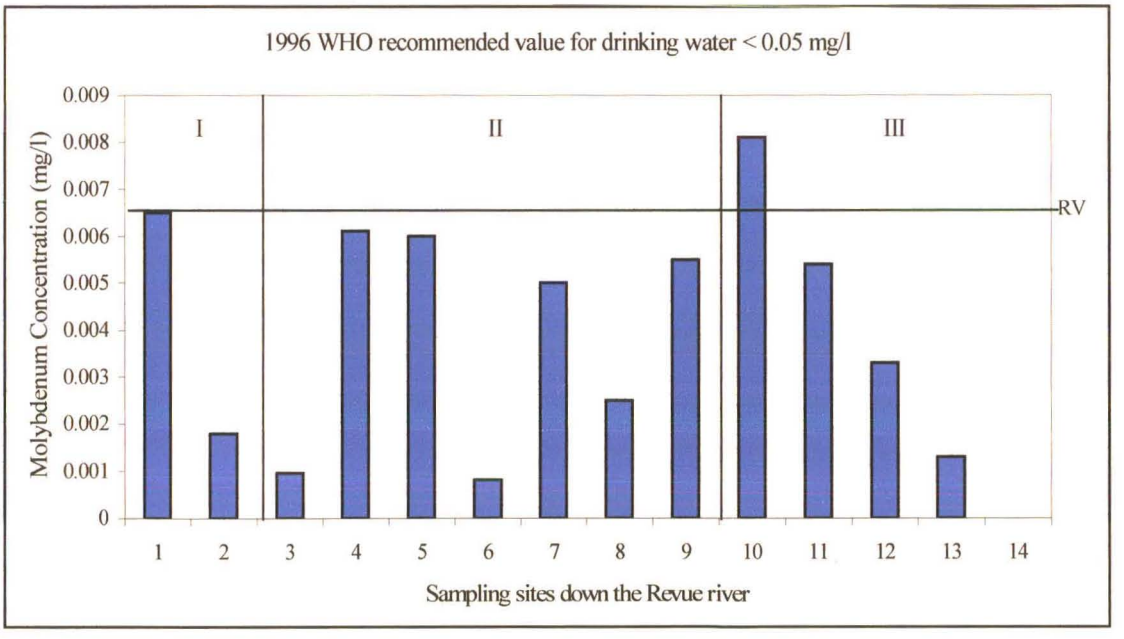


Fig. 4.20 – Spatial distribution of Molybdenum concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

vii) Lead

Although lead rarely occurs naturally in its elemental state, man throughout history has used it. One reason for this is that its principal ore, lead (II) sulphide known as galena, is easily recognised (Hill, 1992). Lead is comparable in abundance to cobalt and is rather widely

dispersed in sedimentary and granitic rocks. Its natural mobility is low, however, owing to the low solubility of lead hydroxy carbonates (Hem, 1985).

The principal dissolved inorganic forms of lead are the free ion Pb^{2+}, hydroxide complexes, and, probably, the carbonate and sulphate ion pairs. Lead from leaded gasoline is a major source of atmospheric and terretial lead and much of this lead eventually enters natural water systems. The dissolved lead concentrations of surface waters depend on the dry fallout and rainout of particulate lead especially in areas of heavy automobile traffic (Hem, 1980; Manahan, 1990). This is not the situation of Manica, therefore the lead concentration in the water comes from the rocks.

The lead values measured in the Revuè river water are between 0.005 and 0.053 mg/l. The lowest concentrations are found upstream of the mining area underlain by ultramafic rocks which have low lead concentrations (Fig. 4.21). At site 8, where the river water crosses metasedimentary rocks, the highest concentration of lead was measured. At this site the most intense artisanal gold mining occurs leading to the disturbance of sediments and releasing clay and silt particles to the water. This can facilitate the dissolution of the metal in the water. Downstream of site 8, the concentration of lead drops slightly as the river flows over basic and ultrabasic rocks. This decrease may be due to co-precipitation of lead with manganese oxide dissolved from the basic and ultrabasic rocks. The lead concentration rises again in the Chicamba Dam. The Chicamba Dam receives water from the Messica, Zonuè and Nhamanguena rivers which run over granitic rocks. As granitic rocks contain relatively high concentrations of lead, dissolution of granite may account for the increase in lead concentration in the dam.

The recommended lead concentration for drinking water set by the WHO in 1996 is of less than 0.01 mg/l. Within and downstream of the mining area the lead concentrations are higher than this value. This water is used as potable water in Chimoio City. Exposure to low concentrations of lead in drinking water leads to detectable increase in blood lead levels. It causes severe dysfunction in the kidneys, reproductive system, liver, and the brain and central nervous system. Possible neurophysiological effects influencing learning ability (mental retardation) and general behaviour in children can occur (Manahan, 1990; Packham, 1993).

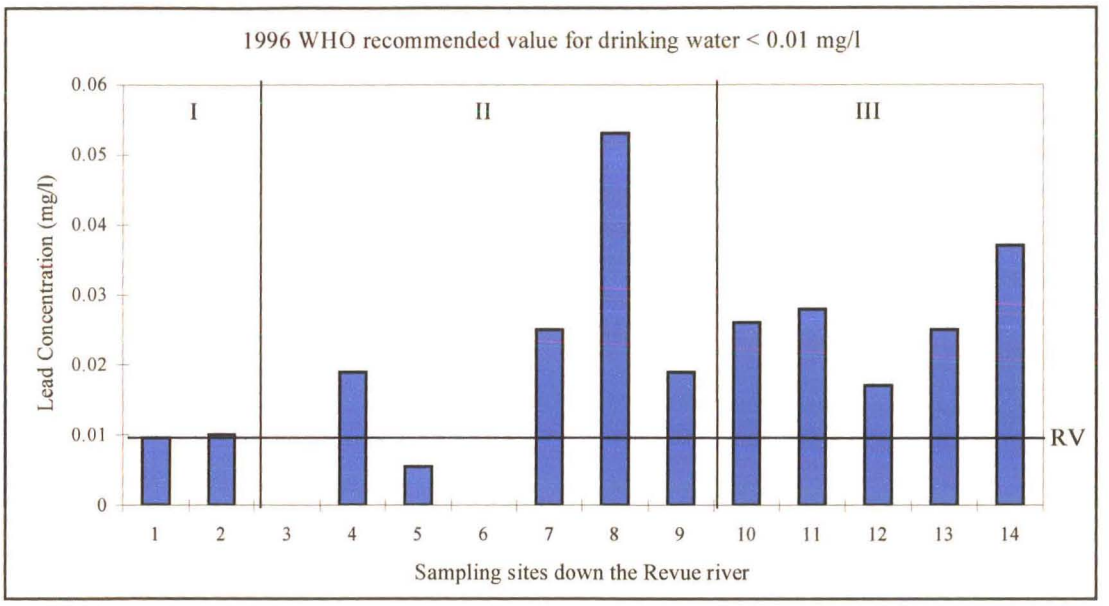


Fig. 4.21 – Spatial distribution of Lead concentration down the Revuè river. I - Upstream of the mining area; II – Within the mining area; III - Downstream of the mining area; RV - Reference Value (Site 1).

4.2 ASSESSMENT OF WATER QUALITY

4.3.1 Water Quality Within the Mining Area

The data collected during this study show that generally the highest concentration of all determinands are found in the lower part of the mining area, i.e., between sites 7 and 9 (Fig. 1.2, p. 6). Figures 4.1 to 4.21 illustrate the spatial changes of the study parameters down the Revuè river and clearly show the sites where the highest inputs, increases and reductions occur.

The highest concentration of TDS and electrical conductivity occur at site 8 with values of 191.16 mg/l and 308,65 µS/cm respectively. Alkalinity is highest at site 9 (61.6 mg/l) reflecting the carbonate nature of rocks at this site. The highest turbidity also occurs at site 9 (142 NTU) (Table 4.1, p. 21). This represents 28 times more the recommended turbidity in the standards for potable water, which is 5 NTU.

The small variations in the total metal concentrations within the mining area can be attributed to sediment loads from the mining sites and the dilution by Revuè river water and affluents and by the adsorption and precipitation capacity of the sediments. According to Bourg (1995) there are three processes that influence metal concentration in rivers:

1 - Dilution. The variations in dissolved metal concentration are given by loads from both diffuse and point sources, and dilution with river water.

2 - Dilution plus sediment transport. The exchange of contaminant sediments due to scour and desorption influences total metal concentration (dissolved+adsorbed) in the water column.

3 - Dilution plus adsorption/desorption equilibria. The application of the previous two approaches is justified if the degradation rate of the metals is negligible and metal concentration are the same in the water and sediment bed and there are no adsorption or desorption.

Between sites 8 and 9 the Revuè river receive water from the Inhamazonga river (Fig. 1.2, p. 6) (Table 4.3), a tributary on which there is no mining activity and which has very clear water. This water has a dilution effect in the Revuè river which is seen in some water parameters, e.g., there is a reduction of conductivity (from 308,65 to 285,6 µS/cm), in TDS (from 191,16 to 138,06 mg/l) and in some metals concentrations (Cr, As, Fe, Ni, Pb and Zn). This breaks the general trend within the mining area of increasing concentrations downstream.

Table 4.3 – Concentration of metals in the main Revuè river affluents immediately before flowing into the Revuè river.

Site	15	16	17	18	19
Al (mg/l)	0,03	0,08	0,04	0,04	0,04
As (mg/l)	0	0,013	0,019	0,028	0,0021
Ba (mg/l)	0,06	0,09	0,12	0,27	0,14
Ca (mg/l)	3,9	5,6	5	9,4	7,7
Cd (mg/l)	0,0022	0,00029	0,0041	0,00076	0,00096
Co (mg/l)	0	0	0,0029	0,023	0,026
Cr (mg/l)	0,0068	0,0094	0,0063	0,0068	0,0078
Cu (mg/l)	0	0,04	0	0,01	0,01
Fe (mg/l)	0,06	0,07	0,11	0,07	0,2
Mg (mg/l)	2,7	5,7	4,6	9,8	7,8
Mn (mg/l)	0,016	0,022	0,21	0,17	0,33
Mo (mg/l)	0,006	0,004	0,0046	0,0031	0
Ni (mg/l)	0,00003	0,0094	0,00032	0	0,0025
Pb (mg/l)	0	0	0,015	0,0099	0,0034
Sr (mg/l)	0,01	0,02	0,02	0,07	0,03
Zn (mg/l)	0	0	0	0	0

Site 15 – Nhamatsambe river; Site 16 – Nhahombwè river; Site 17 – Chua river; Site 18 – Zambuzi river; Site 19 – Inhamazonga river.

In contrast, when the Chua and Zambuzi rivers, both of which have mining activities along their banks, enter the Revuè river, between sites 6 and 8, there is an increase in turbidity (14.7 at site 7 to 59.1 NTU at site 8), in alkalinity (from 43,6 to 52 mg/l), in conductivity (from 236,59 to 308.65 µS/cm), in TDS (from 116,82 to 191,16 mg/l) and in metal concentrations such as Ba, Ca, Cr, K, Mg, Mn, Na, Ni, Pb, Sr and Zn.

Overall it is apparent from Figs. 4.4 to 4.21 that, with the exception of Cd, Ni and Mo, total concentration of all metals are higher within the mining area, than the natural background water quality in the Revuè river (water upstream of the mining area). While changes of lithology along the river and the inputs from affluents may increase the concentration of some elements (Ba, Ca, Cr, Co, As, Cu, Fe, Al, K, Mg, Mn, Na, Pb, Sr and Zn), it is likely that the increase in total metal concentration can be largely attributed to the alluvial gold mining activity. The washing of auriferous gravel can facilitate the dissolution of metals in the water. Table 4.4 shows the percentage difference in metal concentrations at site 9 compared to site 1, site 9 being considered the site most affected by mining. Percentage increases range from 26.8 % for sodium to 900% for cobalt. Within the mining area, the metals are being mobilized at rates greatly exceeding those of natural geologic processes.

Table 4.4 – Comparison of metals concentrations between the reference sites of the three areas of the Revuè river.

Metals	Upstream (I)	Within (II)	Downstream (III)	Variation rate (%)	
	Site 1 (mg/l)	Site 9 (mg/l)	Site 14 (mg/l)	From I to II	From II to III
Al	0,04	0,06	0,13	50	116.67
As	0,011	0,004	0	-63.64	-100
Ba	0,09	0,17	0,19	88.89	11.76
Ca	3,8	7,2	5,2	89.47	-27.78
Cd	0,0027	0,00032	0,00053	-88.15	65.63
Co	0,0024	0,024	0,0038	900	-84.17
Cr	0,0064	0,0047	0,0024	-26.56	-48.94
Cu	0	0	0,02	0	100
Fe	0,02	0,05	0,03	150	-40
K	0,3957	0,7644	2,5989	93.18	239.99
Mg	3,1	7,6	3,5	145.16	-53.95
Mn	0,024	0,2	0	733.33	-100
Mo	0,0065	0,0055	0	-15.38	-100
Na	4,1	5,2	4,8	26.83	-7.69
Ni	0,0018	0	0,0011	-100	100
Pb	0,0096	0,027	0,037	181.25	37.04
Sr	0,02	0,04	0,05	100	25
Zn	0	0	0,02	0	100

Negative signal (-) symbolize the reduction of the concentration.

The alluvial gold mining increases the amount of clay and silt suspended particles in the river water which becomes cloudy. The suspended solid surfaces (particles and colloids) in water have been demonstrated by Lacerda & Salomons (1991) as the main transport pathway of various trace elements and by Filella *et al.*, (1995) as playing a prominent role in controlling the concentration of dissolved trace elements. Suspended clays and silt are, thus, important

components of aquatic systems because they influence the water composition. That is possible because they have a high sorptive capacity for many chemicals.

Cd, As, Cr, Ni and Mo show a percentage decrease at site 9 compared to site 1. The percentage decrease for Cr is misleading as the highest Cr concentrations are found within the mining area. The decrease metals concentration at site 9 could be due to either removal of these elements from the water by precipitation reactions or by adsorption by clay and silt particles. Chemical equilibrium modelling predicts that As and Ni would be removed by adsorption while Cr would be removed by precipitation processes. This will be discussed more fully in Chapter 5. The percentage decrease for Ni and Cd is real, as the highest values of these elements are found upstream of the mining area.

Table 4.4 also shows the percentage difference in total metal concentrations at site 14 (Chicamba Dam) compared to site 9. This will be discussed in Section 4.3.2. Al, Ba, Cd, Cu, K, Ni, Pb, Sr and Zn show a percentage increase compared to the water in the mining area. Most of these increases can be attributed to the acid nature of granite and granitoid rock at site 14. As, Ca, Co, Cr, Fe, Mg, Mn, Mo and Na all show a percentage decrease compared to the water in the mining area.

In the mining area the concentrations of Al, As, Ca, Cd, Cr, Cu, Fe, K, Mg, Mo, Na, Ni, and Zn are lower than the WHO standards for drinking water while Ba, Mn and Pb are higher (Table 4.1, p. 21). The water within the mining area is thus not recommended to be used as potable water, without prior treatment (Chapter 6).

4.3.2 Water Quality Downstream of the Mining Area

Site 14, in the Chicamba Dam was selected as being typical of water quality downstream of the mining area (Figure 1.2, p. 6). Presently this water is used as potable water in Chimoio city. This dam is located 42 km downstream from the mining area and receives large amount of clay and silt sediments released to the water during the gold mining activities. Water from other rivers, such as the Messica, Zónuè and Nhamanguena (Figure 1.2, p. 6) which have no any mining activity along their courses and which run over the Granite-gneiss Complex also enter the dam. The chemical composition of the water in these rivers will differ from the rivers underlain by rocks of the Manica greenstone belt and will influence the water chemistry in the dam.

The impounded water in the Chicamba Dam influences the water flow in the Revuè river, beginning at its confluence with the Messica river. The water flux becomes slow. From this

confluence to the Chicamba Dam the quiescent of water allows the sedimentation of suspended clay and silt particles which is reflected directly in the reduction of turbidity. The sedimentation of suspended material causes accelerated silting and depth reduction of the Chicamba Dam. This has implications for the life expectance of the reservoir (Cook & Doornkamp, 1990). The sediments bury organisms of small dimensions in the river banks and in the Chicamba Dam, eliminating some species, and causing reduction in the biodiversity.

The turbidity of water in the Chicamba Dam, at site 14 is 1.42 NTU, the concentration of TDS is 106.2 mg/l and the electric conductivity is 218.20 µS/cm (Table 4.1, p. 21).

The impoundment of water will also have an effect on metals concentrations. Dilution can occur in the dam and settling of metal-contaminated solids has a much higher likelihood of occurring in the dams than along the river channel itself, both during high flow and low flow periods, as turbulence effects are smaller (Novotny, 1995). Inspection of Figs. 4.4 to 4.21 and Table 4.4 show that the concentration of Ca, As, Co, Cr, Fe, Mg, Mn, Mo and Na drop significantly from site 9 to site 14 in the Chicamba Dam. The percentage decrease for As is misleading as the highest concentrations of As in the area do occur downstream of the mining area (Fig. 4.11). Cd, Ni and Cu show a percentage increase at site 14 compared to site 9. This is also misleading as the highest values of Ni and Cd occur upstream of the mining area (Figs. 4.13 and 4.19). The spatial distribution of copper along the river is erratic (Fig. 4.16).

This reduction in the concentrations of Co, Cr, Cu, Fe, Mn, Mo, Na and Ni may be a result of precipitation and/or adsorption and coprecipitation with hydrous oxides of iron and manganese into sediments. The relative importance of precipitation and adsorption is discussed in Chapter 5. Adsorption occurs when a dissolved ion or molecule becomes attached to the surface of a pre-existing solid substrate generally by complexation with the surface sites. Coprecipitation occurs when a dissolved specie is incorporated as a minor component in a solid phase which itself is being precipitated (Drever, 1997). The extent to which metals are adsorbed depends on the properties of the metal concerned (valency, radius, degree of hydratation and coordination with oxygen), the physico-chemical environment (pH and redox status), the nature of the adsorbent (permanent and pH dependent charge, complex forming ligands), other metals present and their concentrations and the presence of soluble ligands in the surrounding fluids (Alloway & Ayres, 1993).

Alloway & Ayres (1993) report that V, Mn, Ni, Ca, Zn and Mo are believed to co-precipitate with hydrous Fe oxides while Fe, Ca, Ni, Zn and Pb are believed to co-precipitate with Mn oxides. The reductions in metal concentrations in the Chicamba Dam are also consistent with

the work of Rose *et al.* (1979) where it is shown that at pH values of between 6.5 and 8, values found in the Revuè river, large quantities of Ba, Ca, Co, Cu, Mg, Mn, Ni, Sr and Zn can be adsorbed (Fig. 4.22). The reduction of Ca and Mg may be due to chemical precipitation of Ca and Mg carbonates in the water column to form particles and colloids (Filella *et al.*, 1995) while the reduction of Cd may be due to the adsorption by calcite surfaces (Drever, 1997). In this way the elements are removed by sedimentation after incorporation on to or into particles. Particles deposited in this way into water, either react with the constituents of the water or settle to the bottom where they react with sediments (Alloway & Ayres, 1993). The Chicamba Dam therefore acts as a sink for metals, as the particles surfaces deposited in the dam are important scavengers for heavy metal ions in natural water systems because of their ability to compete with soluble complexing agents for metal ions (Bourg, 1988).

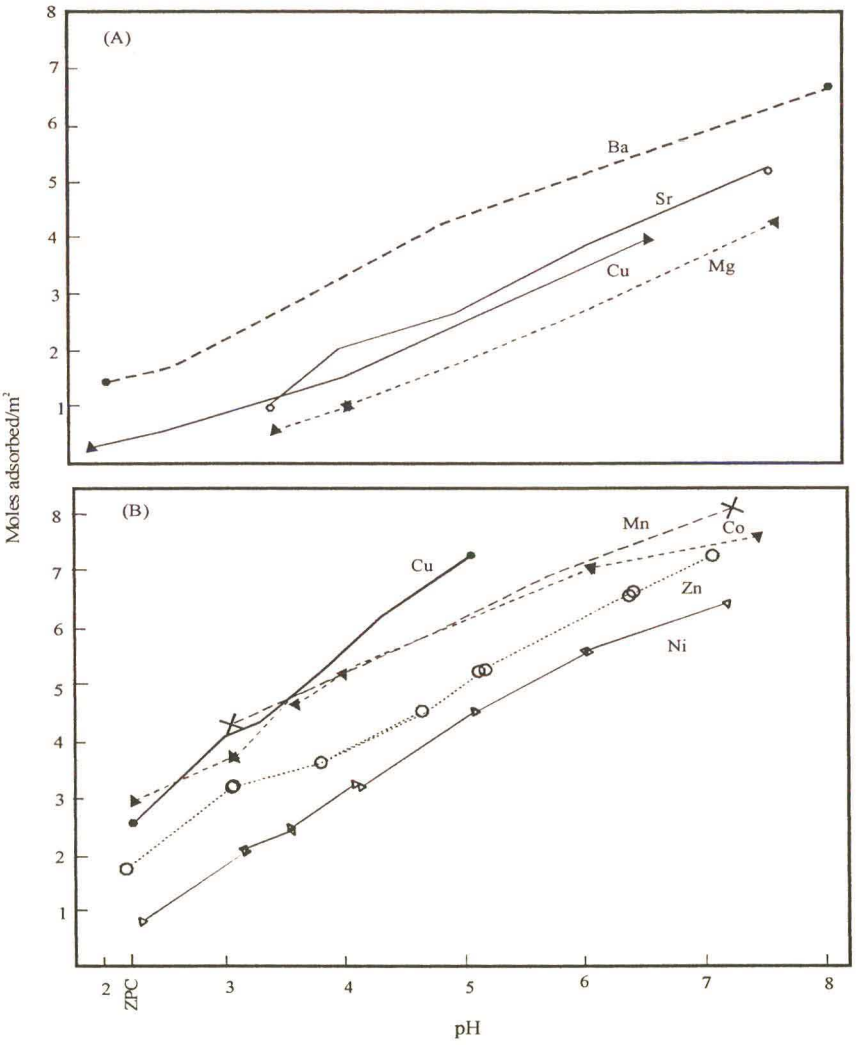


Fig. 4.22 – Adsorption of divalent cations on MnO as a function of pH. (A) alkaline earth; (B) transition metals. Cation concentration = 10^{-3} (From Rose *et al.*; 1979).

The concentrations of Al, Ba, K, Pb and Sr at site 14 (Chicamba Dam) show an increase compared to site 9 within the mining area (Table 4.4). The highest As concentrations of are also found downstream of the mining area but not at site 14. The Chicamba Dam receive water from Messica, Zónuè and Nhamanguena rivers that cross the Granite-gneiss Complex (igneous acid rocks). The increase in concentration of these metals may therefore be a result of the input of water that has crossed these acid rocks. Acid rocks are relatively enriched in these elements compared to basic and ultrabasic rocks which predominantly compose the Manica greenstone belt (Table 4.2, p. 23).

The concentration of Al, As, Ca, Cd, Cu, Cr, Fe, K, Mg, Mo, Mn, Ni, and Zn are lower than the WHO standards for drinking water but Ba and Pb have concentrations higher than these standards (Table 4.1, p. 21). Thus, the water in the Chicamba Dam is not recommended for use as potable water without prior treatment.

CHAPTER FIVE

5. DISTRIBUTION AND FATE OF POLLUTANTS

Natural waters are extremely complex environments. They contain not only most elements in the periodic table, but also dissolved organic matter of largely unknown composition, and colloidal and particulate material, both inanimate and living (Turner, 1993).

The trace metals in the aquatic environment are present in a number of different chemical forms as a result of the interactions between metal ions and other species in solution such as complexing anions and the acidity or redox properties of the system. Some trace metals may be presented in more than one oxidation stage dependent on the redoxpotential. Most trace metals are able to form complexes, which may either be labile or inlabile. Furthermore, the trace metals may be adsorbed to suspended matter and colloids and can form precipitates (Fig. 5.1).

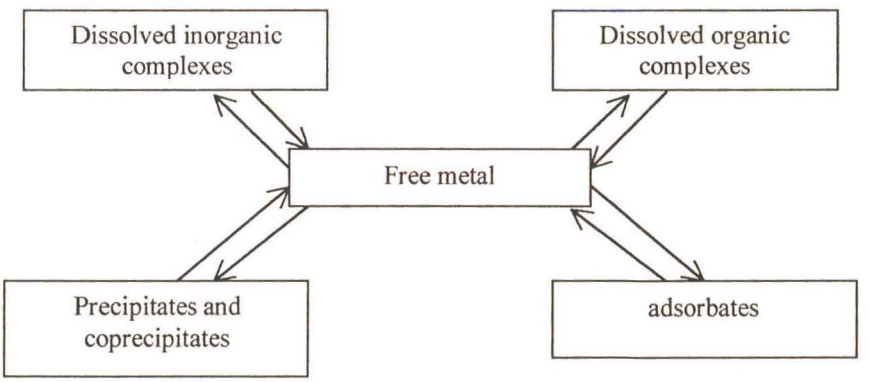


Fig. 5.1 – Geochemical speciation of heavy metals (All of these processes are prone to concurrent reactions with other cations, including H^+) (From Bourg, 1995).

The chemical or physical form in which an element is present is called its speciation (Howard, 1998) which is used in a vague manner both for the operational procedure for determining typical species in environmental samples and for describing the distribution and transformation of such species in various media (Förstner, 1990). Species has been defined as the molecular representation of a specific form of an element. The importance of understanding the speciation

of an element is that the environmental pathway, mobility and toxicity of an element are strongly dependent upon the speciation of the element concerned. The differences in speciation can arise from a number of different causes. An element's speciation is governed by the environment in which it is present. However, any pollutant metal discharged to the aquatic environment enters a complex biogeochemical cycle, and predicting its fate requires multidisciplinary modelling of that biogeochemical cycle and its constituent physical, chemical and biological processes (Turner, 1993). The aim of this chapter is to examine the distribution and fate of pollutants using a geochemical speciation computer model. If all possible physical, chemical and biological processes of trace metal in the aquatic environment should be considered in the development of a model, it would be a very complex model. Jørgensen (1990) suggests that heavy metal pollution may be described by use of 5 submodels: a distribution model, a model of metal speciation, a model for release of metal from sediment, a model related to the metal concentration in biota and an effect model. For this study the metal geochemical speciation computer model MINTEQA2 was used to examine the distribution and fate of pollutants. MINTEQA2 incorporates 3 of the submodels of Jørgensen, namely a distribution model, a model of metal speciation and a model for release of metal from sediment.

5.1 MINTEQA2

MINTEQA2 is a geochemical speciation model based on equilibrium thermodynamics which can calculate the equilibrium composition of dilute aqueous system amongst soluble, solid, adsorbed and gas phases. It was developed by the United States Environmental Protection Agency (USEPA). Calculations can be performed to take into account varied environmental conditions such as pH, ionic strength, temperature and redox conditions. The program also includes an extensive thermodynamic database, for soluble complexes, mineral solubilities, gas solubilities and redox couples. In addition the program contains a database of metal surface complexation constants for the diffuse-double-layer model (DDLM) and also complexation constants for a humic distribution model for metal complexation with dissolved organic matter (DOM). For input of problems the input files can be created interactively with the program PRODEFA2. All the database information can be edited by the user (Lumsdon & Evans, 1995).

To describe the input problem the program uses the concepts of components and species defining the equilibrium problem namely the mass action equations, mass balance equations, the concept of chemical components, the equilibrium problem matrix and the proton balance and electrical neutrality. MINTEQA2 uses a list of current components but the user, however, can also define new components and reaction stoichiometries and change the thermodynamic data. The input of the problem requires total analytical concentrations of the selected components.

Total concentrations of elements (components) from chemical analysis such as ICP and atomic absorption are preferable to methods that only measure some fraction of the total such as selective colorimetric or electrochemical methods. The user defines how the activity coefficients are to be computed (Davis equation or the extended Debye-Huckel), the temperature of the system and whether pH, Eh and ionic strength are to imposed or calculated. Once the total concentrations of the selected components are defined, all possible soluble complexes are automatically selected from the database. At this stage the thermodynamic equilibrium constants supplied with the model may be edited or certain species excluded from the calculation (e.g. species that have slow reaction kinetics). In addition, it is possible for the user to supply constants for specific reactions not included in the database, but care must be taken to make sure the formation equation for the newly defined species is written in such a way as to be compatible with the chemical components used by the rest of the program (Lumsdon & Evans, 1995).

Another useful feature of MINTEQA2 is the range of adsorption models available. These include adsorption isotherm approaches, cation exchange equilibria and three surface complexation models. The surface complexation models are the constant capacitance model (CCM), diffuse-double-layer model (DDLM) and the triple-layer model (TLM).

The results from a MINTEQA2 calculation are read to an output file which can be viewed by a text editor. The format of this file can be preselected to vary the amount of detail given. Multiple output files can be created in which one of the inputs files is systematically varied by selecting the use of the "sweep" option (Lumsdon & Evans, 1995).

5.2 REVUÈ WATER MODELLING PROCEDURE

In order to describe the water quality in the Revuè basin, the study area was divided in three parts; upstream of, within and downstream of the mining area. The same sub divisions have been used to model water quality. Site 1 was selected to represent the water quality upstream of the mining area; site 9 to represent water quality within the mining area; and site 14 located in the Chicamba Dam to represent water quality downstream of the mining area. The composition of the water at these sites is shown in the Table 4.1 (p. 21).

In order to model the water quality was necessary to make some simplifying assumptions:

1 – A chemical equilibrium model is a suitable approximation. The simplest process that might regulate the concentration of a trace element in solution is equilibrium with respect to a solid phase containing the element as a major component (Drever, 1997).

2 – The river water will be in equilibrium with the atmospheric oxygen and carbon dioxide. The turbulence of water facilitates the oxygen dissolution in the water.

3 – The oxidising environment and the introduction of redox pair can lead to precipitation of some trace metals.

4 – For the adsorption, the iron and manganese oxyhydroxides are the adsorbing phases and the FEO-DLM.DBS database will be used as contains surface complexation reactions applicable to diffuse layer model.

The mobility of trace metal pollutants depends on a more or less complex network of interactions between aqueous and heterogeneous chemical reactions as well as particle coagulation and flocculation phenomena. Hydrolysis and dissolved complexation tend to increase the solubility of trace metals while precipitation and adsorption will delay metal availability and transport (Fig. 5.1, p. 61). The distribution of a metal between its various possible species is a result of a series of heterogeneous and dissolved chemical reactions.

For each site four modelling runs were undertaken to allow the program to run without a phase rule violation.

In the first run MINTEQA2 was used as a speciation-saturation program only, with the total concentrations of the water quality variables as the input. This has two purposes: (1) to see which phases are supersaturated and hence are likely to precipitate, and (2) to convert the alkalinity input into total concentration of carbonate species and the concentration of the component H^+ (Drever, 1997). In this initial run the oxidation state of the Fe, Mn and Cr in the analysis was also decided upon. These elements were entered into the program as Fe^{2+}, Mn^{2+} and $Cr(OH)_2$ (reduced species) which are probably their actual form despite that in air saturated fresh waters, all trace elements should be in their maximum oxidation states, because the redox potential of the O_2/H_2O complex is higher than that of any other complex (Lumsdon & Evans, 1995). This water should be in equilibrium with atmospheric oxygen and contain close to the maximum dissolved oxygen possible due to the turbulent flow. The reason for entering these elements in their reduced form was that the water samples were filtered using 0.45 μm Millipore membrane filter. Thus, any oxides or oxyhydroxides of these elements which could have been present in the water as colloidals or suspended solids have been removed. After filtering the samples were also acidified, thus any dissolved Fe, Mg and Cr reported in the chemical analysis are likely to be in reduced state. No post precipitation was noted in the sample bottles. In the initial run the water was specified to be in equilibrium with CO_2 gas phase at partial pressure of 3.10^{-4} atm and O_2 at fixed partial pressure of 0,21 atm.

In the second run the components of the first run were called as a seed file and the total carbonate concentration obtained in the output file of the first run was entered as a component. Saturated solids were allowed to precipitate as it is known that the precipitation limits metal solubility.

In the third run, the redox pairs for Fe and Mn were imposed on the model. With fixed redox ratio imposed, MINTEQA2 calculates the concentration of species present in the reduced and in the oxidised state.

In many aqueous environments the distribution of metals, particularly the trace metals, is regulated by adsorption/desorption reactions occurring at the interface between the aqueous solution and particulate matter such as mineral particles, organic matter or living cells (Fig. 5.2). Thus, in the fourth run the effect of solid surface adsorption was considered, assuming that for natural water systems the binding capacity of sediments is controlled largely by a surface layer of amorphous ferric hydroxide which forms a coating on inorganic support particles (Luoma & Davies, 1983; Kerr 1994)).

Adsorption by iron and manganese oxyhydroxides in particular, is probably the most important process in maintaining the concentrations of trace elements at levels far below those predicted by equilibrium solubility calculations. They have extremely high adsorption capacities and high adsorption affinities for many metals. MINTEQA2 provides a separate database file, FEO-DLM.DBS, which contains surface complexation reactions that are applicable to the diffuse layer model for adsorption of some metals and ligands onto the iron oxide surface (Kerr, 1994).

The properties of the iron hydroxide layer for which the FEO-DLM.DBS database can be attached to the diffuse layer adsorption model are:

Solids concentration of 3,422 g/l and with an amorphous iron concentration of 0,721 mg/g.
Specific surface area = 600 m^2/g.
High energy site density = 1,922. 10^{-4} moles/l.
Low energy site density = 7,690.10^{-3} moles/l.

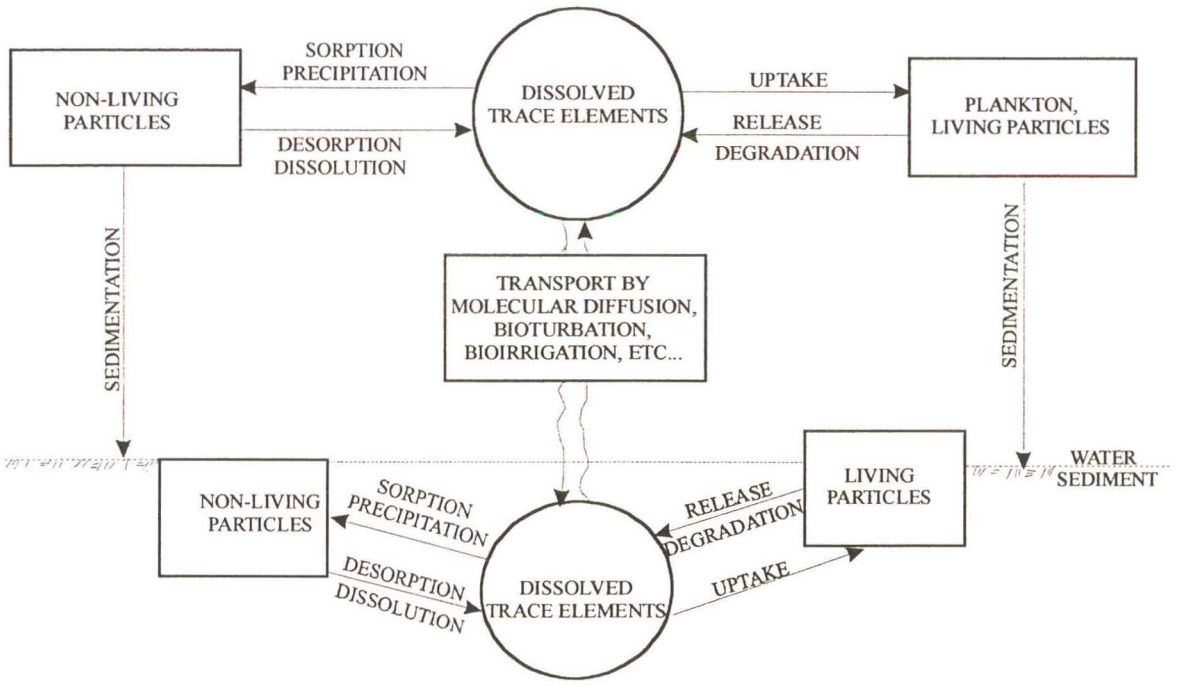


Fig. 5.2 – Schematic representation of internal processes that influence the concentrations of trace elements in a water system (From Tessier *et al.*, 1994).

5.3 REVUÈ WATER MODELLING RESULTS

From the modelling process were obtained large output files. Part of the output files from Run 1 is shown in Table 5.1. As all components are 100 % dissolved in the water in all sites, only the output file of site 14 (Chicamba Dam) is presented as an example. The complete output files of all sites are presented in the Appendix I.

Table 5.1– Output file from the MINTEQA2 for the Site 14 after Run 1(solids not allowed to precipitate). The output file has been condensed for this table. Extended output files are in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	3.060E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	4.818E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.383E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.297E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	4,715E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.790E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
231	Cu+2	3.147E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	5.372E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.874E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.786E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	2.144E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	2.067E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	1.765E-05	100.0	0.000E-01	0.0	0.000E-01	0.0

Parts of the output files from Run 2 are shown in Tables 5.2, 5.3 and 5.4. In all sites MINTEQA2 predicts that the metal Cr should be 100 % precipitated; Al 99,9 % precipitated and Mn more than 95,5 % precipitated. The percentage of Fe predicted to precipitate varies from 2,6 % in the sample from site 14 to 10,4 % in the sample from site 1. The remaining metals are all predicted to be present as dissolved species.

Table 5.2 – Output file from the MINTEQA2 for the Site 1 after Run 2 (solids allowed to precipitate). The output file has been condensed for this table. Extended output is in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.066E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	8.734E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	6.553E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	9.481E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.402E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	6.520E-12	0.0	0.000E-01	0.0	7.436E-08	100.0
600	Pb+2	4.634E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	1.947E-08	4.5	0.000E-01	0.0	4.174E-07	95.5
30	Al+3	2.623E-09	0.2	0.000E-01	0.0	1.480E-06	99.8
1	E-1	-8.655E-11	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.130E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	3.209E-07	89.6	0.000E-01	0.0	3.718E-08	10.4
2	H2O	1.474E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.233E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

Table 5.3 – Output file from the MINTEQA2 for the Site 9 after Run 2 (solids allowed to precipitate). The output file has been condensed for this table. Extended output is in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	3.176E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.238E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.796E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.847E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.441E-12	0.0	0.000E-01	0.0	5.464E-08	100.0
600	Pb+2	1.303E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	8.473E-09	0.2	0.000E-01	0.0	3.632E-06	99.8
30	Al+3	3.333E-09	0.1	0.000E-01	0.0	2.220E-06	99.9
1	E-1	-1.324E-10	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.809E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	8.680E-07	96.9	0.000E-01	0.0	2.732E-08	3.1
2	H2O	2.207E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.911E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

Table 5.4 – Output file from the MINTEQA2 for the Site 14 after Run 2 (solids allowed to precipitate). The output file has been condensed for this table. Extended output is in the Appendix I.

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
950	Zn+2	3.060E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.786E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.383E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.297E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	4.715E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	1.988E-12	0.0	0.000E-01	0.0	2.790E-08	100.0
231	Cu+2	3.147E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.874E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.331E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	2.144E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	5.232E-07	97.4	0.000E-01	0.0	1.395E-08	2.6
2	H2O	8.982E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	2.235E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

The effect of imposing redox pairs on the model is shown in Tables 5.5, 5.6 and 5.7 which represent part of the output files of Run 3. MINTEQA2 predicts that all Iron would be in a ferric state and thus be precipitated. Some Manganese, Mn^{2+} would be converted to Mn^{3+} and be precipitated. Although the concentrations of Manganese in the water is extremely low and unlikely to exert any great control on the water chemistry, they have been included so as to indicate what the likely fate of Manganese would be if Manganese concentrations increase in the future. Chromium is predicted to be between 91,2 to 95,8 % precipitated and Aluminium to be between 99,8 to 99.9 % precipitated. Other metals remain dissolved in the water.

MINTEQA2 predicts that iron would be precipitated as hematite. The kinetics of this reaction are likely to be slow and it is more probable that iron is removed from the water as ferric hydroxide or particularly at site 9 as a carbonate as carbonate rocks are present at this site.

Table 5.5 - Output file from the MINTEQA2 for the Site 1 after Run 3 (Fe and Mn redox pairs included). The output file has been condensed for this table. Extended output is in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
540	Ni+2	3.066E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	8.734E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	6.553E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	9.481E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.402E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	4.634E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	3.157E-09	4.2	0.000E-01	0.0	7.125E-08	95.8
470	Mn+2	4.205E-16	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	2.623E-09	0.2	0.000E-01	0.0	1.480E-06	99.8
140	CO3-2	1.129E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
471	Mn+3	2.468E-27	0.0	0.000E-01	0.0	4.369E-07	100.0
280	Fe+2	5.543E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.396E-15	0.0	0.000E-01	0.0	3.581E-07	100.0
1	E-1	-1.869E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.233E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	1.479E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Table 5.6 – Output file from the MINTEQA2 for the Site 9 after Run 3 (Fe and Mn redox pairs included). The output file has been condensed for this table. Extended output is in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	3.176E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.238E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.796E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.847E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.303E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.835E-09	5.2	0.000E-01	0.0	5.181E-08	94.8
470	Mn+2	9.604E-17	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.333E-09	0.1	0.000E-01	0.0	2.220E-06	99.9
140	CO3-2	1.809E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
471	Mn+3	6.572E-28	0.0	0.000E-01	0.0	3.641E-06	100.0
280	Fe+2	2.139E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.047E-15	0.0	0.000E-01	0.0	8.953E-07	100.0
1	E-1	-1.501E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.911E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	2.183E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Table 5.7 – Output file from the MINTEQA2 for the Site 14 after Run 3 (Fe redox pair included). The output file has been condensed for this table. Extended output is in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.786E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.383E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.297E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	4.715E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.874E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
231	Cu+2	3.147E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	3.060E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.464E-09	8.8	0.000E-01	0.0	2.544E-08	91.2
280	Fe+2	1.448E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.331E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.144E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.495E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.235E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	8.961E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

The effect of adsorption on the water chemistry is shown in Tables 5.8, 5.9 and 5.10 which are part of the output files of Run 4. Cd, Zn, Cu, Pb, Ni and As are predicted to be almost totally removed from the water as adsorbed phases (Fig. 5.3a).

Table 5.8 – Output file from the MINTEQA2 for the Site 1 after Run 4 (adsorption included). The output file has been condensed for this table. Extended output in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	5.682E-11	0.1	8.729E-08	99.9	0.000E-01	0.0
100	Ba+2	3.561E-07	54.3	2.992E-07	45.7	0.000E-01	0.0
150	Ca+2	7.321E-05	77.2	2.160E-05	22.8	0.000E-01	0.0
160	Cd+2	2.421E-11	0.1	2.400E-08	99.9	0.000E-01	0.0
600	Pb+2	6.537E-15	0.0	4.634E-08	100.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	8.239E-11	0.3	3.058E-08	99.7	0.000E-01	0.0
211	Cr(OH)2+	3.156E-09	4.2	0.000E-01	0.0	7.125E-08	95.8
470	Mn+2	4.188E-16	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	2.622E-09	0.2	0.000E-01	0.0	1.480E-06	99.8
140	CO3-2	1.128E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	5.521E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	-1.867E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.394E-15	0.0	0.000E-01	0.0	3.581E-07	100.0
471	Mn+3	2.446E-27	0.0	0.000E-01	0.0	4.369E-07	100.0
330	H+1	1.232E-04	86.7	1.887E-05	13.3	0.000E-01	0.0
2	H2O	1.414E-07	91.2	1.362E-08	8.8	0.000E-01	0.0

Table 5.9 – Output file from the MINTEQA2 for the Site 9 after Run 4 (adsorption included). The output file has been condensed for this table. Extended output in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	2.087E-11	0.1	3.174E-08	99.9	0.000E-01	0.0
100	Ba+2	5.010E-07	40.5	7.368E-07	59.5	0.000E-01	0.0
150	Ca+2	1.175E-04	65.4	6.217E-05	34.6	0.000E-01	0.0
160	Cd+2	1.612E-12	0.1	2.845E-09	99.9	0.000E-01	0.0
600	Pb+2	1.759E-14	0.0	1.303E-07	100.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.833E-09	5.2	0.000E-01	0.0	5.181E-08	94.8
1	E-1	-1.498E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.122E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	9.528E-17	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.331E-09	0.1	0.000E-01	0.0	2.220E-06	99.9
140	CO3-2	1.804E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.044E-15	0.0	0.000E-01	0.0	8.953E-07	100.0
471	Mn+3	6.455E-28	0.0	0.000E-01	0.0	3.641E-06	100.0
330	H+1	1.907E-04	147.8	-6.168E-05	-47.8	0.000E-01	0.0
2	H2O	2.020E-07	66.6	1.014E-07	33.4	0.000E-01	0.0

Table 5.10 – Output file from the MINTEQA2 for the Site 14 after Run 4 (adsorption included). The output file has been condensed for this table. Extended output in the Appendix I.

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
100	Ba+2	4.101E-07	29.6	9.734E-07	70.4	0.000E-01	0.0
150	Ca+2	6.999E-05	53.9	5.975E-05	46.1	0.000E-01	0.0
160	Cd+2	1.689E-12	0.0	4.714E-09	100.0	0.000E-01	0.0
950	Zn+2	3.133E-11	0.0	3.059E-07	100.0	0.000E-01	0.0
231	Cu+2	9.930E-12	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.365E-11	0.2	1.870E-08	99.8	0.000E-01	0.0
600	Pb+2	2.153E-14	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.463E-09	8.8	0.000E-01	0.0	2.544E-08	91.2
30	Al+3	3.327E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.136E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	1.434E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.493E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.235E-04	156.9	-8.101E-05	-56.9	0.000E-01	0.0
2	H2O	2.845E-07	25.7	8.227E-07	74.3	0.000E-01	0.0

The concentrations of Ba and Ca in the water are predicted to be reduced (Fig. 5.3b) with the percentage Ba adsorbed ranging from 45,7 % at site 1 (Table 5.8) to 70,4 % at site 14 (Table 5.10) in the dam and the percentage Ca adsorbed ranging from 22,8 % at site 1 (Table 5.8) to 46,1 % at site 14 (Table 5.10).

Fe, Al, Cr and Mn concentrations are not affected by adsorption modelling and their concentration in the water remains controlled by precipitation processes rather than adsorption (Fig. 5.3c) as indicated by the fact that the percentage of these elements remaining in the water is zero after Run 2 (precipitation only) and/or Run 3 (precipitation and redox).

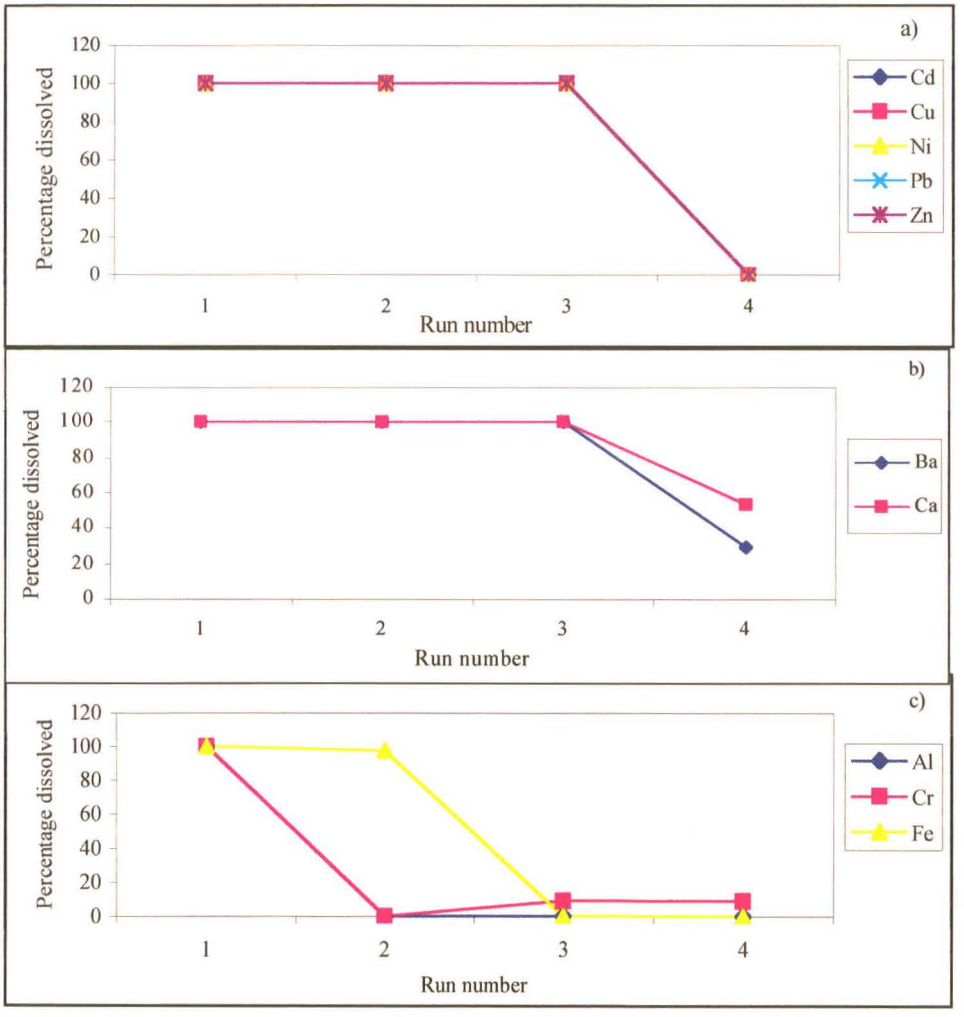


Fig. 5.3 – Elements with same behaviour in the modelling process of water of the site 14 (Chicamba Dam). (a) Predicted reduction in percentage of Cd, Cu, Ni, Pb and Zn dissolved in Chicamba Dam as a result of adsorption. (b) Predicted reduction in percentage of Ba and Ca dissolved in Chicamba Dam as a result of adsorption. (c) Predicted reduction of Al, Fe and Cr concentrations. As the percentage dissolved is zero after Run 2 and 3 the removal of these elements is controlled by precipitation rather than adsorption processes.

Adsorption processes therefore could have a great influence on the chemical composition of water in the Revuè river and have the potential to be responsible for removal of most trace elements from the water.

Comparison of predicted water quality (assuming control on the water chemistry by adsorption processes) and actual water composition (Table 5.11) suggests that adsorption may not be as effective process as predicted. This is particularly true for Ba and Pb, the two elements that are in excess of WHO recommended limits for drinking water. Concentration of other trace metals are negligible and below WHO recommendations.

Table 5.11 – Comparison of predicted water quality by MINTEQA2 with actual water quality in the Chicamba Dam (Site 14).

Metals	Predicted Water		Actual water	
	Mol/kg	mg/l	Mol/kg	mg/l
Ba	4.10E-07	5.60E-02	1.38E-06	1.90E-01
Pb	2.15E-14	4.53E-09	1.78E-07	3.70E-02
Cd	1.69E-12	1.93E-07	4.68E-09	5.30E-04
Zn	3.13E-11	2.07E-06	3.09E-07	2.00E-02
Cu	9.93E-12	6.47E-07	3.16E-07	2.00E-02
Ni	3.37E-11	2.02E-06	1.86E-08	1.10E-03

Förstner (1990) suggests that they are many factors affecting the distribution of trace metals between solution and particulate material in aquatic systems:

- chemical form of dissolved metal input both from natural and antropogenic sources.
- the type of interactive processes, i.e. either sorption/desorption or precipitation/dissolution controlled mechanism. Modelling Runs 2 and 3 indicate that neither Ba nor Pb takes part in precipitation processes.
- concentration and composition of particulate matter, mainly with respect to surface-active phases and grain size distribution. In the case of Ba and Pb the characteristics of the sediment in the Chicamba Dam may not be suitable to Ba and Pb adsorption or differ significantly from the sediments characteristics used by MINTEQA2.

Adsorption of trace metals onto inorganic solid surfaces is often only a temporary condition (Hownslow, 1995). Fluxes of trace elements across the solid-water interface occur in response to changing environmental conditions as they progress toward equilibrium. The remobilization of elements from solid phases (i.e. solubility, mobility desorption and bioavailability) would occur by four majors factors in aquatic environments (Förstner, 1990):

1 – Lowering of pH.

2 – An increase in complexation

3 – Changing redox conditions

4 – Increasing salinity

To investigate the effect of lower pH on the amount of metal predicted to be either adsorbed or precipitated, a series of modelling runs at different pH values were undertaken for the water in the Chicamba Dam (site 14). The output files of the modelling process are in the Appendix II. Table 5.12 and Fig. 5.4 show that at pH 6.5, which is the minimum pH value within the range recommended for drinking water, the adsorbed concentrations of Ba would drop from 70.4 to 2.7 %, Ca from 46.1 to 1.0 % and Ni from 99.8 to 94.4 %, increasing the dissolved metal concentrations. Pb and Cu would remain 100 % adsorbed while Cd and Zn would drop to 96.8 and 99.1 % respectively.

Table 5.12 – Variations in metals percentage adsorbed with pH changes in the Chicamba Dam water (site 14) as predicted by MINTEQA2.

pH	**6**	**6.5**	**7**	**7.6**	**8**	**8.5**
Ni	65.1	94.4	99.3	99.8	99.8	99.8
Pb	100	100	100	100	100	100
Cu	99.9	100	100	100	100	100
Zn	92.2	99.1	99.9	100	100	100
Ba	0.3	2.7	19.2	70.4	90.8	98.6
Ca	0.1	1	7.6	46.1	78.7	96.5
Cd	76.9	96.8	99.6	100	100	100

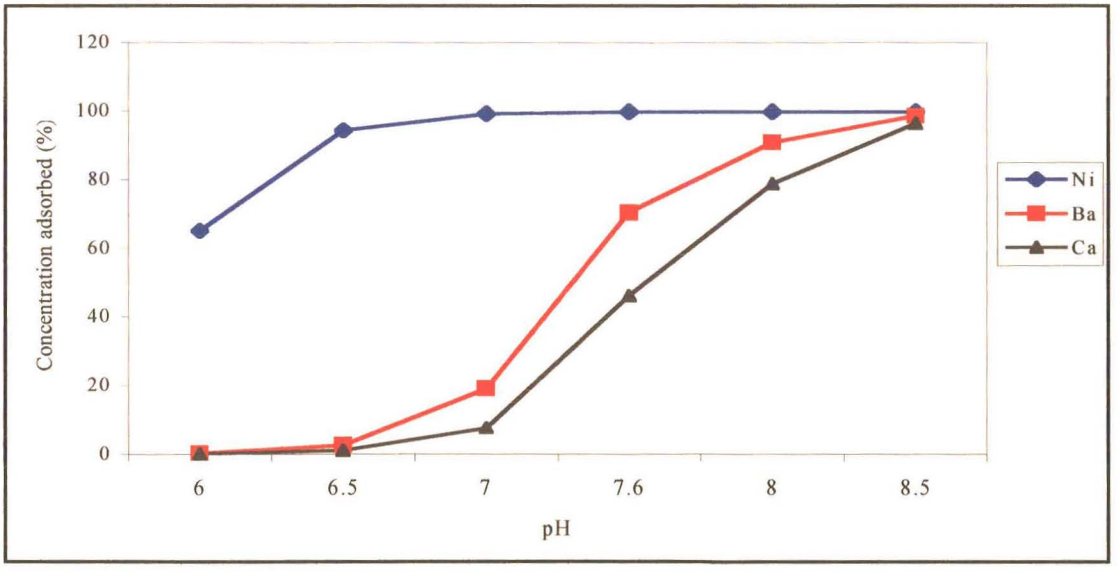


Fig. 5.4 – Variation of Ca, Ba and Ni concentrations adsorbed with changes in pH in the Chicamba Dam (site 14) as predicted by MINTEQA2.

For the metals whose concentrations is controlled by precipitation, i.e., Fe, Al and Cr, MINTEQA2 predicts that only Cr would be strongly influenced by the reduction of pH. Table 5.13 and Fig. 5.5 show that the concentration predicted to precipitate would drop from 91.6 (at pH 7.6) to 60.7 % (at pH 6.5).

Table 5.13 – Variation of Fe, Cr and Al percentage precipitated with pH changes in the Chicamba Dam (site 14) as predicted by MINTEQA2.

pH	6	6.5	7	7.6	8	8.5
Fe	100	100	100	100	100	100
Cr	0	60.7	84	91.2	92.6	93.1
Al	99.9	100	100	99.9	99.9	99.7

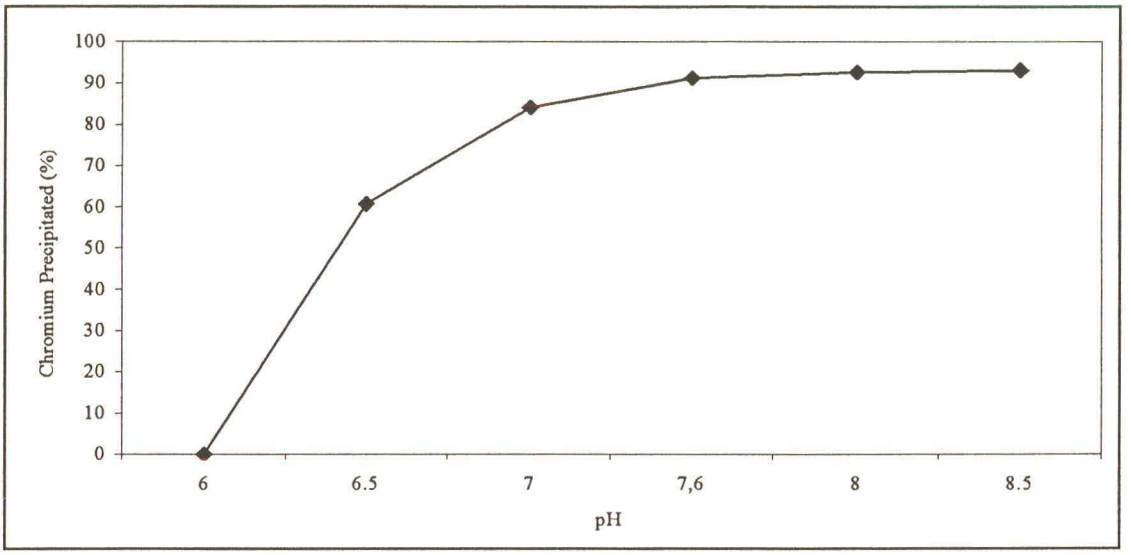


Fig. 5.5 – Influence of different pH values in Cr precipitated concentrations in water for the Chicamba Dam (site 14) as predicted by MINTEQA2.

The redox conditions of any body of water are a function of the amount of dissolved oxygen. This in turn is dependent on the amount of organic matter in the water. The decay of organic matter will place a biological oxygen demand (BOD) on the water and lead to a decrease in dissolved oxygen (Hem, 1985).

The amount of organic matter in the Revuè basin is known to vary with season and therefore the dissolved oxygen content of the water will also vary with season. A decrease in dissolved oxygen could lead to the redistribution of iron and manganese and possibly the release of heavy metals formerly adsorbed on the hydroxides. To simulate the possible effects of changing redox conditions on the predicted percentage adsorbed or precipitated a number of modelling runs were undertaken at increasing dissolved organic matter concentrations. The output files of the modelling process are in the Appendix III. Table 5.14 and Fig. 5.6 show that the more dissolved organic matter present in the water, the lower the adsorbed metal concentrations will be. This is particularly true for Ba and Ca. Table 5.14 and Fig. 5.6 show that the percentage of Ba adsorbed would decrease from 24.5 to 3.6 % while the percentage of Ca adsorbed would decrease from 14.5 to 2 % if dissolved organic matter concentrations increased from 0.001 to 0.005 mol/l.

Table 5.14 - Variations in metals percentage adsorbed with changes in dissolved organic matter (DOM) in the Chicamba Dam (site 14) as predicted by MINTEQA2.

DOM (mol/l)	0.001	0.002	0.003	0.004	0.005
Cd	99.6	99	98.2	97.3	96.3
Ni	99.2	98.1	96.7	95.2	93.6
Pb	100	100	100	100	100
Cu	100	99.9	99.8	99.7	99.5
Zn	99.8	99.5	99.2	98.8	98.3
Ba	24.5	11.6	6.9	4.8	3.6
Ca	14.5	6.6	3.9	2.7	2

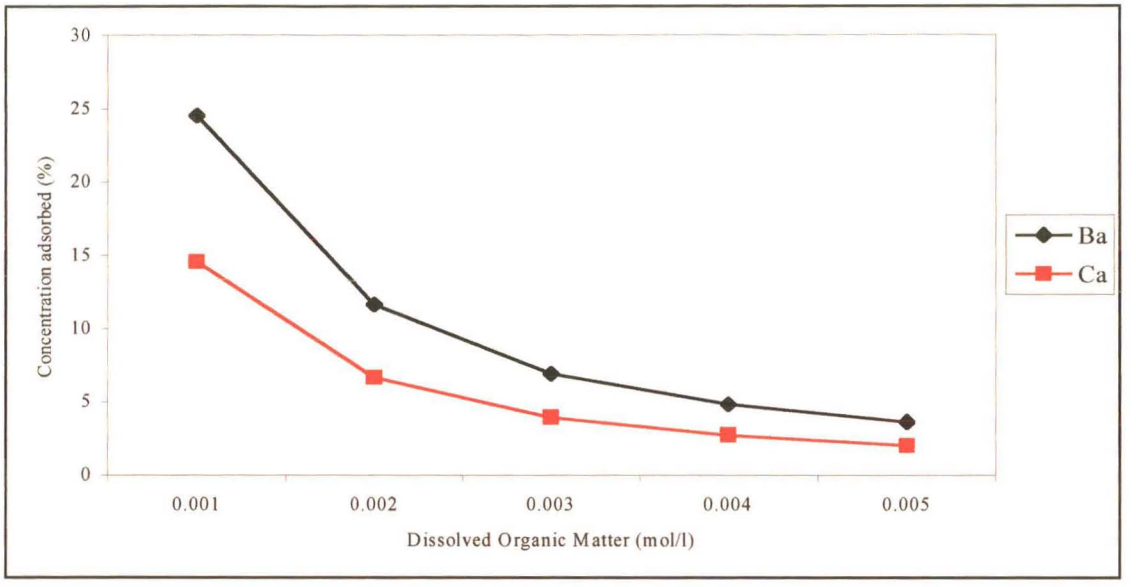


Fig. 5.6 – Influence of DOM changes in Ba and Ca adsorbed concentrations in the Chicamba Dam (site14) as predicted by MINTEQA2.

MINTEQA2 also predicts that the Pb concentration would not be affect by increasing concentrations of dissolved organic matter, and that Pb would remain fully adsorbed. Other metals adsorbed would only show small variations in the adsorbed concentrations. Table 5.15 shows that for metals controlled by precipitation, only Cr would be affected by an increase in dissolved organic matter.

Table 5.15 - Variation of Fe, Cr and Al percentage precipitated with changes in dissolved organic matter (DOM) in the Chicamba Dam (site 14) as predicted by MINTEQA2.

DOM (mol/l)	0.001	0.002	0.003	0.004	0.005
Fe	100	100	100	100	100
Al	99.9	99.9	99.9	99.9	99.9
Cr	91.9	91	90.9	90.8	90.8

Increased inorganic salt concentrations could occur during the dry season, when an increase in the number of local people involved in alluvial gold mining occurs. As samples in this study

were collected during the dry season, it is likely that the total dissolved salt concentration was at a maximum and so further modelling to investigate the effect of increasing salinity on adsorption and precipitation was not attempted. Likewise no modelling was undertaken to investigate the effect of an increase in complexation as the dry season samples are likely to represent the maximum opportunity for complexation.

The main objective of the modelling undertaken in the water quality of the Revuè basin was to know what would be the final behaviour of trace metals in relation to adsorption and precipitation which are some of the factors controlling the distribution of pollutants in natural waters. Novotny (1995) classified the processes affecting the fate of pollutants in the aquatic environment in four main categories:

1 - transport processes (advection, sedimentation and precipitation-dissolution)
2 - transformation processes (biomodification by microbial metabolism)
3 - speciation processes (acid-base equilibria and sorption of inorganic compounds)
4 - bioacumulation (intrusion of nondegradable, nonassimilable compounds in the food chain.

Since metals do not degrade, volatilize or decay by photolysis, their fate in natural waters is mainly controlled by transport processes.

Furthermore, upstream of and within the mining area conditions are not conducive to sedimentation. The influence of precipitation and adsorption factors will not be felt upstream of and within the mining areas due to transport of pollutants by the turbulent flow of water and due to the mining activity which release pollutants to the Revuè river. In contrast, the slow water flow in the impounded water of the Chicamba Dam favours sedimentation. Evidence that the adsorption and precipitation processes occur in the dam is given by the reduction of Ca, Co, Cr, Fe, Mg, Mn, Mo, Na, Cu, Cd and Ni concentrations in the dam water. Where increased metal concentrations were found they can be attributed to lithology (Section 4.3.2).

A summary of the geochemical modelling is given in Table 5.16 which shows the percentage dissolved concentrations as the modelling scenario was made more realistic. The table demonstrates that the dissolved concentration of Al, Fe, Cr and Mn are controlled by precipitation processes while the dissolved concentrations of As, Ba, Ca, Cd, Pb, Ni, Cu and Zn are controlled by adsorption processes. Metals such as Na, Mg, K and Sr, are not predicted to take part in these processes. Co and Mo were not included in the modelling because the program do not contains a database of surface complexation constants for these metals.

Table 5.16 – Comparison of the dissolved percentage of elements in the Revuè river water after each run of the modelling process.

Metals	Site 1				Site 9				Site 14			
	Run 1	**Run 2**	**Run 3**	**Run 4**	**Run 1**	**Run 2**	**Run 3**	**Run 4**	**Run 1**	**Run 2**	**Run 3**	**Run 4**
Al	100	0,2	0,2	0,2	100	0,1	0,1	0,1	100	0,1	0,1	0,1
Fe	100	89,6	0	0	100	96,6	0	0	100	97,4	0	0
Cr	100	0	4,2	4,2	100	0	5,2	5,2	100	0	8,8	8,8
Mn	100	4,5	0	0	100	0,2	0	0	...	...	...	...
As	100	100	100	0,2	100	100	100	0,1	...	...	...	...
Ba	100	100	100	54,3	100	100	100	40,5	100	100	100	29,6
Ca	100	100	100	77,2	100	100	100	65,1	100	100	100	53,9
Cd	100	100	100	0,1	100	100	100	0,1	100	100	100	0
Cu	...	...	...	...	...	...	...	...	100	100	100	0
Ni	100	100	100	0,3	...	...	...	...	100	100	100	0,2
Pb	100	100	100	0	100	100	100	0	100	100	100	0
Zn	...	...	...	...	...	...	...	...	100	100	100	0

Run 1: PCO_2, PO_2, fixed pH, solids not allowed to precipitate.

Run 2: Same as Run 1 but solids allowed to precipitate and CO_3^- as a component.

Run 3: Same as Run 2 and Fe redox pair, Mn redox pair.

Run 4: Same as Run 3 and adsorption.

(...)The total concentration of the metal in the input file is Zero.

CHAPTER SIX

6. SOURCES OF WATER POLLUTION AND WATER TREATMENT

Water, through natural weathering and leaching processes and by dissolving and reacting with rocks, mobilises and incorporates trace elements in its chemical composition (Ward, 1995). The *in situ* chemical and thermodynamic conditions and the factors that control the solubility determine the extent to which these metals are dissolved. The presence of metals incorporated in this way into the chemical composition of water ultimately relates to the lithology occurring in any region.

Following the definition of pollution given by Holgate (1979) and Novotny (1995), the presence of metals, even in high concentrations, can not be considered evidence of pollution in its strict sense. The term pollution of the environment refers to an increase of a element relative to the natural occurrence of that element. In this order to determine the sources of trace element pollution, it is necessary to establish the natural elemental levels and chemical forms of the earth's environment. This situation can be applied to the water upstream of the mining area in the Revuè river where there is no influence of mining activity yet where high concentrations of Ni, Cd and Mo are found. In spite of this, the water in this area meets all WHO recommendations for drinking water.

The mining exploration methods and gold washing process used in the area accelerate the entrance of pollutants in the Revuè river water. These processes have accelerated the dissolution of metals and their entry into the river water causing an increase in concentration above that of the natural background. This is especially true between sites 7 and 9 where the mining activity is very intense. Thus, the mining activity in Manica is the principal point source of pollution in the upper part of the Revuè river basin. Water quality in the mining area has been impaired and Ba, Pb and Mn have concentrations higher than WHO recommended values for drinking water.

Within the impounded water of Chicamba Dam, sedimentation of suspended sediments occurs, together with associated adsorption and precipitation processes. This results in general improvement of water quality with only Ba and Pb exceeding WHO recommended values for potable water.

The upper part of the Revuè river basin is a remote area with no industrial development. There is no production and no emissions of sulphur and nitrogen oxides to the atmosphere. The type of agriculture in the area is subsistence farming. The soils are very fertile and there is no reference to the use of nitrogen-containing fertilisers to increase the yield, which could bring a marked increase in the nitrate content of surface waters. The same can be said to the use of pesticides. Thus the contribution of diffuse sources to the total pollution load is negligible.

By this manner, the common characteristics of this pollution event are identified. Following Alloway & Ayres (1993) all cases of pollution have certain characteristics in common: these involve (i) the pollutant, (ii) the source of pollutant, (iii) the transport medium and (iv) the target or receptor. The pollutants identified are the heavy metals dissolved in the water; the source of the pollutants is the alluvial gold mining activity; the transport medium of pollutants is the Revuè river water and the target are the humans, plants, animals and probably the turbines in the Chicamba Dam.

The water in the Chicamba Dam is used as source of potable water for Chimoio City. The only treatment practiced is disinfection prior to distribution. Because of the toxicity of free Ba and Pb ions this situation is undesirable.

An long accepted method of metal removal from water is addition of lime ($Ca(OH)_2$) to remove metals as hydroxides. Manahan (1990) indicated that Pb can be removed by lime addition followed by activated carbon filtration. This has a reported efficiency of 99.4 %. A drawback of this method is the expense of activated carbon.

Examination of solubility products of Ba and Pb carbonate and sulphates (Table 6.1) show that there are rather insoluble compared to other common carbonates and sulphates.

Table 6.1 – Solubility products of some carbonates and sulphates.

Salts	K_{sp}
$BaCO_3$	$10^{-8.3}$
$BaSO_4$	$10^{-9.96}$
$PbCO_3$	$10^{-13.1}$

This suggests that there is a scope for removal of Ba and Pb by precipitation either as a carbonate or sulphate. Possible sources of carbonate would be limestone, soda ash or CO_2 gas. A possible source of sulphate would be gypsum.

The equilibrium, kinetics of reaction and engineering aspects of possible water treatment processes are outside the scope of this study.

CHAPTER SEVEN

7. DISCUSSION AND CONCLUSIONS

Alluvial gold mining in Manica is undertaken by both small scale and traditional mining methods. The small scale mining utilises fairly standard surface mining methods involving removal of overburden to gain access to the auriferous gravel. The traditional mining methods are haphazard, unorganised and use very low technology. Regardless of the method used the recovery process involves washing of the auriferous gravel with large quantities of water. In the case of traditional mining the washing process occurs in the river bed, while for small scale mining the water is pumped to the washing points and returned directly to the river without any treatment. The quality of water is affected in this process.

This study was carried out with the aim of assessing the effect of alluvial gold mining in the Manica greenstone belt on the surface water quality in the Revuè basin. The dissolved concentrations of major, minor and trace metals as well as other physical and chemical field water quality parameters were determined upstream of, within and downstream of the mining area and in the main tributaries upstream of their confluence with the Revuè river. These data were used to characterise water quality.

Upstream of the mining area the rock types in the Manica greenstone belt are likely to be the only source of metals dissolved in the water. This area is far from the influence of mining activity and the ultimate source of most dissolved ions in water is the mineral assemblage in the surface outcrops. In this area the Revuè river water is clear and there is no sign of pollution. Metal concentrations are generally low, except for Cd, Mo and Ni compared with other areas, and the water is of good quality and can be used as potable water. The higher concentrations of Cd, Mo and Ni in the area can be correlated directly with lithology. In this upstream area the dominant rock types are ultramafic and mafic which contain significant concentrations of these metals. This water represents the natural background water quality in the Revuè river.

Within the mining are there is clear evidence of the negative impacts of alluvial gold mining. Physical degradation of the surface has occurred. Abandoned pits, trenches, holes and tailings are common along the river banks. Disturbance of the sediments at the current working sites has increased the amount of clay and silts particles suspended in the water which has become cloudy.

Exposure of the overburden and the auriferous gravel and the gold washing process itself has facilitated the dissolution of metals in the water. The distribution graphs drawn for each determinand show that the peak of concentrations of most metals are found in the lower part of the mining area (between sites 7 and 9) where the mining activity is very intense. Metal concentrations in this area are, with the exception of Cd, Mo and Ni, higher than in the unpolluted upstream segment of the river. Thus, the alluvial gold mining is directly responsible for elevated metal concentrations in the water and constitutes the major point source of pollution in the Revuè river. Non-point sources are limited to local domestic activities and have a negligible effect on the overall pollution load.

Several metals, Ba, Mn and Pb, have concentrations which exceed the WHO recommended standards for drinking water. Ideally this water should not be used as source of potable water. Local people dislike the cloudiness of the water and dig small holes in the riverbanks to obtain clear water for drinking. This water will probably have the same chemical composition as the river water but is free of suspended sediments.

The suspended sediments in the water, not only impair water clarity but act as a major transport pathway for various trace elements due to they high sorptive capacity.

Downstream of the mining area the impounded water in the Chicamba Dam reduces the water flow in the Revuè river creating conditions for clay and silt sedimentation. The sedimentation process is reflected in the decrease in turbidity and in the concentrations of most total dissolved metals. This results in general auto-purification and improving the water quality with only Ba and Pb exceeding WHO recommended values for drinking water. Geochemical speciation modelling, using MINTEQA2 suggests that the behaviour of most of the metals in the water is controlled by redox, precipitation and adsorption reactions. Modelling indicates that the concentrations of metals Cr, Al, Mn and Fe are controlled by precipitation processes while concentrations of As, Cd, Zn, Cu, Ni, Pb, Ba and Ca are controlled by adsorption on the sediment surfaces. The oxidation of any ferrous iron and the formation of oxyhydroxides of Fe and Mn and their co-precipitation with the settling clay and silt particles is likely to have aided

the adsorption processes by coating the clay and silt particles and thus providing additional adsorption capacity.

As described in Chapter 1, page 8, a major limitation of this work is the lack of data for mercury. Inspection of literature (Holdgate, 1979; Hem, 1985; Lacerda & Salomons, 1991; Alloway & Ayres, 1993; Ward, 1995) indicates that mercury is likely to be found as an adsorbed phase or as organo-mercury complexes. Unfortunately data on the fate and behaviour of mercury in the Revuè river is not available.

The settling sediments act as a sink and scavenger of dissolved metals thus inducing an auto-purification process in the impounded water of Chicamba Dam. Modelling predicts that this process should be capable of removing Ba, Pb, Cd, Zn, Cu and Ni totally from the water. In reality Ba and Pb concentrations remain above the WHO recommended standards for drinking water.

Concentrations of elements such as Al, Ba, K, Pb and Sr show an increase in the Chicamba Dam. This is likely to be due to the input to the dam of water from Zónue, Messica and Nhamanguena rivers which cross the Granite-gneiss complex.

If, as the geochemical modelling suggest, adsorption and precipitation are the major processes by which metals are removed from the water, then this removal may only be temporary. Changes in environmental conditions, such as pH change, could result in metals being released back into the water. Modelling at various pH values indicated that adsorption and precipitation were pH dependent, with percentage adsorption and precipitation decreasing with decreasing pH.

Modelling of the effect of dissolved organic matter on the adsorption process indicated that adsorption would decrease with increasing dissolved organic matter. This could be of concern as changes in the concentrations of dissolved organic matter are likely to be related to season. The extent of any seasonal changes are not known as the data in this study represents only one dry season sampling event.

Ideally the water in Chicamba Dam should undergo water treatment prior to distribution as potable water in Chimoio City to reduce Ba and Pb concentrations to acceptable levels. Currently only disinfection is practiced. Because of the poor economy of the country and lack of trained human resources, any water treatment scheme must need to be relatively inexpensive and be constructed of reliable and proven technology.

Traditional lime treatment followed by active carbon filtration would be suitable but the cost of activated carbon might be prohibitive. Solubility products suggest that a scheme based on precipitation of Ba and Pb as either a carbonate or sulphate might have potential.

The increased sedimentation load due to mining activity in the Revuè river will negatively impact on the Chicamba Dam by reducing the life span of the dam. The sedimentation will also impact on aquatic ecosystems. Rapid sedimentation can cause burial of small organisms, clogging of aquatic flora and eventually a reduction in biodiversity.

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APPENDIX I

OUTPUT FILES OF REVUÈ WATER QUALITY MODELLING WITH THE MINTEQA2 PROGRAM

Extended output files of the Revuè river water quality modelling with the geochemical speciation program MINTEQA2. The output has been reduced. The modelling was undertaken for sites 1, 9 and 14 which represent the areas upstream of, within and downstream of the mining area respectively. For each site four runs were undertaken to allow the program to run without a phase rule violation.

Run 1: PCO_2, PO_2, fixed pH, solids not allowed to precipitate.
Run 2: Same as Run 1 but solids allowed to precipitate.
Run 3: Same as Run 2 and Fe redox pair, Mn redox pair.
Run 4: Same as Run 3 and adsorption.

1 - Modelling of water quality of Site 1

```
                              PART 1 of OUTPUT FILE
Revuè river water-Site 1 - Initial run
Entered alkalinity, PCO2, PO2, fixed pH and solids not allowed to precipitate
-------------------------------------------------------------------------------
 Temperature (Celsius):  18.90
 Units of concentration: MG/L
 Ionic strength to be computed.
 Carbonate concentration represents carbonate alkalinity.
 Do not automatically terminate if charge imbalance exceeds 30%
 Precipitation is allowed only for those solids specified as ALLOWED
   in the input file (if any).
 The maximum number of iterations is: 200
 The method used to compute activity coefficients is: Davies equation
 Intermediate output file
-------------------------------------------------------------------------------

INPUT DATA BEFORE TYPE MODIFICATIONS
   ID        NAME        ACTIVITY GUESS     LOG GUESS    ANAL TOTAL
    330   H+1                 5.012E-08         -7.300     0.000E-01
    140   CO3-2               6.761E-21        -20.170     1.942E+01
     30   Al+3                1.479E-06         -5.830     4.000E-02
     60   H3AsO3              8.710E-08         -7.060     1.100E-02
    100   Ba+2                6.607E-07         -6.180     9.000E-02
    150   Ca+2                9.550E-05         -4.020     3.800E+00
    160   Cd+2                2.399E-08         -7.620     2.700E-03
    211   Cr(OH)2+            7.413E-08         -7.130     6.400E-03
    280   Fe+2                3.548E-07         -6.450     2.000E-02
    410   K+1                 1.023E-05         -4.990     3.957E-01
    460   Mg+2                1.288E-04         -3.890     3.100E+00
    470   Mn+2                4.365E-07         -6.360     2.400E-02
    500   Na+1                1.778E-04         -3.750     4.100E+00
    540   Ni+2                3.090E-08         -7.510     1.800E-03
    600   Pb+2                4.677E-08         -7.330     9.600E-03
    800   Sr+2                2.291E-07         -6.640     2.000E-02
      1   E-1                 1.000E-16        -16.000     0.000E-01
      2   H2O                 1.000E+00          0.000     0.000E-01

     Charge Balance: UNSPECIATED
       Sum of CATIONS=  6.412E-04 Sum of ANIONS =  6.473E-04
       PERCENT DIFFERENCE =  4.698E-01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
```

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	5.152E-08	5.012E-08	-7.30000	0.97284	0.012
140	CO3-2	9.053E-08	8.109E-08	-7.09102	0.89572	0.048
30	Al+3	1.621E-12	1.265E-12	-11.89774	0.78053	0.108
60	H3AsO3	8.651E-08	8.652E-08	-7.06287	1.00014	0.000
100	Ba+2	6.553E-07	5.870E-07	-6.23137	0.89572	0.048
150	Ca+2	9.473E-05	8.485E-05	-4.07134	0.89572	0.048
160	Cd+2	2.336E-08	2.092E-08	-7.67944	0.89572	0.048
211	Cr(OH)2+	3.022E-08	2.940E-08	-7.53168	0.97284	0.012
280	Fe+2	3.568E-07	3.196E-07	-6.49536	0.89572	0.048
410	K+1	1.012E-05	9.845E-06	-5.00678	0.97284	0.012
460	Mg+2	1.274E-04	1.141E-04	-3.94275	0.89572	0.048
470	Mn+2	4.357E-07	3.903E-07	-6.40863	0.89572	0.048
500	Na+1	1.783E-04	1.735E-04	-3.76072	0.97284	0.012
540	Ni+2	1.977E-08	1.770E-08	-7.75192	0.89572	0.048
600	Pb+2	1.727E-08	1.547E-08	-7.81047	0.89572	0.048
800	Sr+2	2.283E-07	2.045E-07	-6.68939	0.89572	0.048

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	4.348E-08	4.348E-08	-7.36169	1.00014	-7.130
2113303	Cr(OH)4-	8.517E-12	8.285E-12	-11.08169	0.97284	-18.138
2113304	CrO2-	2.161E-11	2.102E-11	-10.67728	0.97284	-17.734
3300020	OH-	1.287E-07	1.252E-07	-6.90231	0.97284	-14.190
4603300	MgOH +	2.236E-09	2.175E-09	-8.66251	0.97284	-12.008
4601400	MgCO3 AQ	8.039E-09	8.040E-09	-8.09473	1.00014	2.939
4601401	MgHCO3 +	1.307E-07	1.271E-07	-6.89576	0.97284	11.450
1503300	CaOH +	2.631E-10	2.559E-10	-9.59186	0.97284	-12.809
1501400	CaHCO3 +	7.443E-08	7.241E-08	-7.14020	0.97284	11.334
1501401	CaCO3 AQ	8.625E-09	8.626E-09	-8.06420	1.00014	3.098
5001400	NaCO3 -	1.958E-10	1.905E-10	-9.72016	0.97284	1.144
5001401	NaHCO3 AQ	8.476E-09	8.477E-09	-8.07173	1.00014	10.080
303300	AlOH +2	1.896E-10	1.699E-10	-9.76991	0.89572	-5.124
303301	Al(OH)2 +	4.113E-08	4.002E-08	-7.39775	0.97284	-10.088
303302	Al(OH)4 -	4.362E-07	4.243E-07	-6.37229	0.97284	-23.663
303303	Al(OH)3 AQ	1.005E-06	1.005E-06	-5.99776	1.00014	-16.000
2803300	FeOH +	1.302E-09	1.266E-09	-8.89744	0.97284	-9.690
2803301	FeOH3 -1	8.968E-17	8.725E-17	-16.05925	0.97284	-31.452
2803302	FeOH2 AQ	1.251E-13	1.251E-13	-12.90268	1.00014	-21.007
8003300	SrOH +	1.670E-13	1.624E-13	-12.78930	0.97284	-13.388
1003300	BaOH +	3.101E-13	3.017E-13	-12.52047	0.97284	-13.577
4703300	MnOH +	1.238E-10	1.205E-10	-9.91907	0.97284	-10.798
4703301	Mn(OH)3 -1	5.050E-20	4.913E-20	-19.30865	0.97284	-34.788
4700020	MnO4 -	3.883E-10	3.778E-10	-9.42276	0.97284	-130.516
4700021	MnO4 -2	3.922E-14	3.513E-14	-13.45430	0.89572	-120.689
4701400	MnHCO3 +	6.491E-10	6.315E-10	-9.19965	0.97284	11.612
1601400	Cd(CO3)3-4	2.876E-23	1.851E-23	-22.73250	0.64372	6.411
1603300	CdOH +	2.249E-11	2.188E-11	-10.66000	0.97284	-10.269
1603301	Cd(OH)2 AQ	3.720E-14	3.720E-14	-13.42946	1.00014	-20.350
1603302	Cd(OH)3 -	8.560E-20	8.328E-20	-19.07946	0.97284	-33.288
1603303	Cd(OH)4 -2	1.653E-26	1.481E-26	-25.82947	0.89572	-47.302
1603304	Cd2OH +3	3.104E-18	2.422E-18	-17.61575	0.78053	-9.449
1601400	CdHCO3 +	2.195E-10	2.136E-10	-9.67046	0.97284	12.412
1601401	CdCO3 AQ	4.251E-10	4.251E-10	-9.37146	1.00014	5.399
6001400	Pb(CO3)2-2	4.958E-12	4.441E-12	-11.35251	0.89572	10.688
6003300	PbOH +	6.187E-09	6.019E-09	-8.22047	0.97284	-7.698
6003301	Pb(OH)2 AQ	4.672E-11	4.672E-11	-10.33048	1.00014	-17.120
6003302	Pb(OH)3 -	1.100E-14	1.070E-14	-13.97048	0.97284	-28.048
6003303	Pb2OH +3	2.671E-15	2.085E-15	-14.68094	0.78053	-6.252
6003304	Pb3(OH)4+2	3.394E-19	3.040E-19	-18.51712	0.89572	-24.238
6001401	PbCO3 AQ	2.180E-08	2.180E-08	-7.66149	1.00014	7.240
6003305	Pb(OH)4 -2	5.474E-19	4.904E-19	-18.30949	0.89572	-39.651
6001402	PbHCO3 +	1.024E-09	9.966E-10	-9.00149	0.97284	13.212
5403300	NiOH +	3.235E-11	3.147E-11	-10.50206	0.97284	-10.038
5403301	Ni(OH)2 AQ	7.047E-13	7.048E-13	-12.15193	1.00014	-19.000

5403302	Ni(OH)3 -	1.446E-16	1.406E-16	-15.85193	0.97284	-29.988
5401400	NiHCO3 +	2.183E-10	2.124E-10	-9.67294	0.97284	12.482
5401401	NiCO3 AQ	1.064E-08	1.064E-08	-7.97294	1.00014	6.870
5401402	Ni(CO3)2-2	1.674E-12	1.500E-12	-11.82396	0.89572	10.158
3300600	H2AsO3 -	8.330E-10	8.104E-10	-9.09130	0.97284	-9.316
3300601	HAsO3 -2	1.090E-14	9.767E-15	-14.01025	0.89572	-21.500
3300602	AsO3 -3	7.775E-21	6.069E-21	-20.21688	0.78053	-34.946
3300603	H4AsO3 +	2.208E-15	2.148E-15	-14.66787	0.97284	-0.293
3301400	HCO3 -	1.020E-04	9.925E-05	-4.00326	0.97284	10.400
3301401	H2CO3 AQ	1.058E-05	1.058E-05	-4.97562	1.00014	16.715
2113300	Cr+3	8.022E-13	6.261E-13	-12.20334	0.78053	10.036
2113301	Cr(OH)+2	6.857E-10	6.142E-10	-9.21168	0.89572	5.668

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	2.056E-04	-3.687	0.000	0.000
3300021	O2 (g)	1.670E-04	-3.777	-84.491	133.830
330	H+1	-5.398E-04	-3.268	7.300	0.000
3301403	CO2 (g)	5.447E-04	-3.264	21.691	-0.530

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Pb+2	37.3	PERCENT BOUND IN SPECIES #	600	Pb+2
	13.4	PERCENT BOUND IN SPECIES #	6003300	PbOH +
	47.0	PERCENT BOUND IN SPECIES #	6001401	PbCO3 AQ
	2.2	PERCENT BOUND IN SPECIES #	6001402	PbHCO3 +
Ca+2				
	99.9	PERCENT BOUND IN SPECIES #	150	Ca+2
Mg+2	99.9	PERCENT BOUND IN SPECIES #	460	Mg+2
Na+1	100.0	PERCENT BOUND IN SPECIES #	500	Na+1
K+1	100.0	PERCENT BOUND IN SPECIES #	410	K+1
Al+3	2.8	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
	29.4	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
	67.8	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
Fe+2	99.6	PERCENT BOUND IN SPECIES #	280	Fe+2
Mn+2	99.7	PERCENT BOUND IN SPECIES #	470	Mn+2
Sr+2	100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
H3AsO3	99.0	PERCENT BOUND IN SPECIES #	60	H3AsO3
Ba+2	100.0	PERCENT BOUND IN SPECIES #	100	Ba+2
Ni+2	64.5	PERCENT BOUND IN SPECIES #	540	Ni+2
	34.7	PERCENT BOUND IN SPECIES #	5401401	NiCO3 AQ
Cr(OH)2+	40.6	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
	58.4	PERCENT BOUND IN SPECIES #	2113302	Cr(OH)3 AQ
Cd+2	97.2	PERCENT BOUND IN SPECIES #	160	Cd+2
	1.8	PERCENT BOUND IN SPECIES #	1601401	CdCO3 AQ
CO3-2	90.3	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
	9.4	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ
E-1	100.0	PERCENT BOUND IN SPECIES #	4700020	MnO4 -
H+1	86.2	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
	17.9	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ

H2O	2.6	PERCENT BOUND IN SPECIES	#3300020	OH-
	1.6	PERCENT BOUND IN SPECIES	# 303301	Al(OH)2 +
	34.7	PERCENT BOUND IN SPECIES	# 303302	Al(OH)4 -
	60.0	PERCENT BOUND IN SPECIES	# 303303	Al(OH)3 AQ

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
600	Pb+2	4.634E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	1.483E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	8.734E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	6.553E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	9.481E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.402E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	7.441E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	3.581E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	4.369E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.066E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	-1.942E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.130E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.184E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	5.026E-06	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 6.365E-04 Sum of ANIONS 1.028E-04
PERCENT DIFFERENCE = 7.220E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
NON-CARBONATE ALKALINITY = 7.747E-08
EQUILIBRIUM IONIC STRENGTH (m) = 5.936E-04
EQUILIBRIUM pH = 7.300
EQUILIBRIUM pe = 13.823 or Eh = 800.97 mv

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-0.792	[1.000] 30 [3.000] 2 [-3.000] 30
5015000	ARAGONITE	-2.880	[1.000] 150 [1.000] 140
5046000	ARTINITE	-10.417	[-2.000] 330 [2.000] 460 [1.000] 40 [5.000] 2
2003001	BOEHMITE	0.994	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.530	[1.000] 460 [2.000] 2 [-2.000] 30
5015001	CALCITE	-2.722	[1.000] 150 [1.000] 140
2003002	DIASPORE	2.752	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-5.323	[1.000] 150 [1.000] 460 [2.000] 140
2003003	GIBBSITE (C)	0.883	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-2.976	[2.000] 30 [3.000] 2 [-6.000] 330
5015003	HUNTITE	-14.690	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-25.511	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
5046002	MAGNESITE	-3.099	[1.000] 460 [1.000] 140
3050000	NATRON	-13.060	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.501	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-3.118	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-4.541	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.780	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.732	[1.000] 100 [1.000] 140
3047000	HAUSMANNITE	4.053	[-8.000] 330 [-2.000] 1 [3.000] 470 [4.000] 2
2047003	PYROCROITE	-7.242	[-2.000] 330 [1.000] 470 [2.000] 2
5047000	RHODOCHROSIT	-3.121	[1.000] 470 [1.000] 140
16000	CD METAL	-49.091	[1.000] 160 [2.000] 1
16001	GAMMA CD	-49.193	[1.000] 160 [2.000] 1
5016000	OTAVITE	-1.039	[1.000] 160 [1.000] 140

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2016000 CD(OH)2 (A)     -7.127    [ -2.000] 330  [  1.000] 160  [  2.000]  2
2016001 CD(OH)2 (C)     -6.729    [ -2.000] 330  [  1.000] 160  [  2.000]  2
2016002 MONTEPONITE     -8.579    [ -2.000] 330  [  1.000] 160  [  1.000]  2
  60000 PB METAL       -39.720    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE       -1.697    [  1.000] 600  [  1.000] 140
2060000 MASSICOT        -6.377    [ -2.000] 330  [  1.000] 600  [  1.000]  2
2060001 LITHARGE        -6.181    [ -2.000] 330  [  1.000] 600  [  1.000]  2
2060002 PBO, .3H2O      -6.190    [ -2.000] 330  [  1.000] 600  [  1.330]  2
5060001 PB2OCO3         -7.787    [ -2.000] 330  [  2.000] 600  [  1.000]  2
                                  [  1.000] 140
5060002 PB3O2CO3       -12.747    [ -4.000] 330  [  3.000] 600  [  1.000] 40
                                  [  2.000]   2
2060003 PLATTNERITE     -1.348    [ -4.000] 330  [ -2.000]   1  [  1.000] 00
                                  [  2.000]   2
3060000 PB2O3           -5.215    [ -6.000] 330  [ -2.000]   1  [  2.000]600
                                  [  3.000]   2
3060001 MINIUM         -12.649    [ -8.000] 330  [ -2.000]   1  [  3.000]600
                                  [  4.000]   2
2060004 PB(OH)2 (C)     -1.575    [ -2.000] 330  [  1.000] 600  [  2.000]  2
5060003 HYDCERRUSITE    -5.553    [ -2.000] 330  [  3.000] 600  [  2.000]140
                                  [  2.000]   2
2060005 PB2O(OH)2      -12.621    [ -4.000] 330  [  2.000] 600  [  3.000]  2
5054000 NICO3           -8.155    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2         -3.486    [ -2.000] 330  [  1.000] 540  [  2.000]  2
2054001 BUNSENITE       -5.968    [ -2.000] 330  [  1.000] 540  [  1.000]  2
3006000 ARSENOLITE     -25.231    [  4.000]  60  [ -6.000]   2
3006001 CLAUDETITE     -24.983    [  4.000]  60  [ -6.000]   2
2015000 LIME           -22.977    [ -2.000] 330  [  1.000] 150  [  1.000]  2
2015001 PORTLANDITE    -12.616    [ -2.000] 330  [  1.000] 150  [  2.000]  2
2028000 WUSTITE         -3.618    [ -2.000] 330  [  0.947] 280  [  1.000]  2
2046001 PERICLASE      -11.406    [ -2.000] 330  [  1.000] 460  [  1.000]  2
3028001 HERCYNITE       -0.253    [ -8.000] 330  [  1.000] 280  [  2.000] 30
                                  [  4.000]   2
3046000 SPINEL          -7.035    [ -8.000] 330  [  1.000] 460  [  2.000] 30
                                  [  4.000]   2
3021100 FECR2O4          8.162    [  2.000] 211  [  1.000] 280  [ -4.000]330
3021101 MGCR2O4         -2.496    [  2.000] 211  [  1.000] 460  [ -4.000]330
3021102 CR2O3            2.745    [  2.000] 211  [ -2.000] 330  [ -1.000]  2
2021102 CR(OH)3 (A)      0.518    [  1.000] 211  [  1.000]   2  [ -1.000]330
2021101 CR(OH)3 (C)     -2.041    [  1.000] 211  [  1.000]   2  [ -1.000]330
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PART 1 of OUTPUT FILE

Revuè river water-Site 1 - Run 2

Entered CO_3^{2-}, $PCO2$, P_{O2}, fixed pH, Solids allowed to precipitate

Temperature (Celsius): 18.90
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	5.012E-08	-7.300	0.000E-01
30	Al+3	1.479E-06	-5.830	4.000E-02
60	H3AsO3	8.710E-08	-7.060	1.100E-02
100	Ba+2	6.607E-07	-6.180	9.000E-02
150	Ca+2	9.550E-05	-4.020	3.800E+00
160	Cd+2	2.399E-08	-7.620	2.700E-03
211	Cr(OH)2+	7.413E-08	-7.130	6.400E-03
280	Fe+2	3.548E-07	-6.450	2.000E-02
410	K+1	1.023E-05	-4.990	3.957E-01
460	Mg+2	1.288E-04	-3.890	3.100E+00
470	Mn+2	4.365E-07	-6.360	2.400E-02
500	Na+1	1.778E-04	-3.750	4.100E+00
540	Ni+2	3.090E-08	-7.510	1.800E-03
600	Pb+2	4.677E-08	-7.330	9.600E-03
800	Sr+2	2.291E-07	-6.640	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	4.786E-07	-6.320	6.902E+00
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 6.412E-04 Sum of ANIONS = 2.300E-04
PERCENT DIFFERENCE = 4.719E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	5.152E-08	5.012E-08	-7.30000	0.97287	0.012
30	Al+3	2.868E-15	2.239E-15	-14.64993	0.78072	0.108
60	H3AsO3	8.651E-08	8.652E-08	-7.06288	1.00014	0.000
100	Ba+2	6.553E-07	5.870E-07	-6.23133	0.89582	0.048
150	Ca+2	9.473E-05	8.486E-05	-4.07130	0.89582	0.048
160	Cd+2	2.335E-08	2.092E-08	-7.67941	0.89582	0.048
211	Cr(OH)2+	2.648E-12	2.576E-12	-11.58904	0.97287	0.012
280	Fe+2	3.198E-07	2.865E-07	-6.54293	0.89582	0.048
410	K+1	1.012E-05	9.845E-06	-5.00677	0.97287	0.012
460	Mg+2	1.274E-04	1.141E-04	-3.94271	0.89582	0.048
470	Mn+2	1.942E-08	1.740E-08	-7.75954	0.89582	0.048
500	Na+1	1.783E-04	1.735E-04	-3.76071	0.97287	0.012
540	Ni+2	1.976E-08	1.771E-08	-7.75189	0.89582	0.048
600	Pb+2	1.727E-08	1.547E-08	-7.81045	0.89582	0.048
800	Sr+2	2.283E-07	2.045E-07	-6.68935	0.89582	0.048
140	CO3-2	9.052E-08	8.109E-08	-7.09102	0.89582	0.048

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	3.810E-12	3.810E-12	-11.41905	1.00014	-7.130
2113303	Cr(OH)4-	7.463E-16	7.260E-16	-15.13905	0.97287	-18.138
2113304	CrO2-	1.894E-15	1.842E-15	-14.73464	0.97287	-17.734

3300020	OH-	1.287E-07	1.252E-07	-6.90231	0.97287	-14.190
4603300	MgOH +	2.236E-09	2.175E-09	-8.66246	0.97287	-12.008
4601400	MgCO3 AQ	8.040E-09	8.041E-09	-8.09469	1.00014	2.939
4601401	MgHCO3 +	1.307E-07	1.271E-07	-6.89571	0.97287	11.450
1503300	CaOH +	2.631E-10	2.560E-10	-9.59182	0.97287	-12.809
1501400	CaHCO3 +	7.444E-08	7.242E-08	-7.14016	0.97287	11.334
1501401	CaCO3 AQ	8.625E-09	8.627E-09	-8.06416	1.00014	3.098
5001400	NaCO3 -	1.958E-10	1.905E-10	-9.72015	0.97287	1.144
5001401	NaHCO3 AQ	8.476E-09	8.478E-09	-8.07173	1.00014	10.080
303300	AlOH +2	3.355E-13	3.005E-13	-12.52209	0.89582	-5.124
303301	Al(OH)2 +	7.278E-11	7.081E-11	-10.14993	0.97287	-10.088
303302	Al(OH)4 -	7.718E-10	7.508E-10	-9.12447	0.97287	-23.663
303303	Al(OH)3 AQ	1.778E-09	1.779E-09	-8.74994	1.00014	-16.000
2803300	FeOH +	1.167E-09	1.135E-09	-8.94500	0.97287	-9.690
2803301	FeOH3 -1	8.038E-17	7.820E-17	-16.10681	0.97287	-31.452
2803302	FeOH2 AQ	1.121E-13	1.121E-13	-12.95024	1.00014	-21.007
8003300	SrOH +	1.670E-13	1.625E-13	-12.78926	0.97287	-13.388
1003300	BaOH +	3.101E-13	3.017E-13	-12.52042	0.97287	-13.577
4703300	MnOH +	5.520E-12	5.371E-12	-11.26998	0.97287	-10.798
4703301	Mn(OH)3 -1	2.251E-21	2.190E-21	-20.65955	0.97287	-34.788
4700020	MnO4 -	1.731E-11	1.684E-11	-10.77367	0.97287	-130.516
4700021	MnO4 -2	1.748E-15	1.566E-15	-14.80521	0.89582	-120.689
4701400	MnHCO3 +	2.893E-11	2.815E-11	-10.55056	0.97287	11.612
1601400	Cd(CO3)3-4	2.875E-23	1.852E-23	-22.73246	0.64399	6.411
1603300	CdOH +	2.249E-11	2.188E-11	-10.65996	0.97287	-10.269
1603301	Cd(OH)2 AQ	3.720E-14	3.720E-14	-13.42941	1.00014	-20.350
1603302	Cd(OH)3 -	8.561E-20	8.329E-20	-19.07942	0.97287	-33.288
1603303	Cd(OH)4 -2	1.653E-26	1.481E-26	-25.82942	0.89582	-47.302
1603304	Cd2OH +3	3.103E-18	2.423E-18	-17.61567	0.78072	-9.449
1601400	CdHCO3 +	2.195E-10	2.136E-10	-9.67042	0.97287	12.412
1601401	CdCO3 AQ	4.251E-10	4.252E-10	-9.37142	1.00014	5.399
6001400	Pb(CO3)2-2	4.958E-12	4.441E-12	-11.35249	0.89582	10.688
6003300	PbOH +	6.187E-09	6.019E-09	-8.22046	0.97287	-7.698
6003301	Pb(OH)2 AQ	4.672E-11	4.672E-11	-10.33046	1.00014	-17.120
6003302	Pb(OH)3 -	1.100E-14	1.070E-14	-13.97047	0.97287	-28.048
6003303	Pb2OH +3	2.671E-15	2.085E-15	-14.68091	0.78072	-6.252
6003304	Pb3(OH)4+2	3.394E-19	3.040E-19	-18.51707	0.89582	-24.238
6001401	PbCO3 AQ	2.180E-08	2.180E-08	-7.66147	1.00014	7.240
6003305	Pb(OH)4 -2	5.474E-19	4.904E-19	-18.30947	0.89582	-39.651
6001402	PbHCO3 +	1.024E-09	9.966E-10	-9.00147	0.97287	13.212
5403300	NiOH +	3.235E-11	3.147E-11	-10.50204	0.97287	-10.038
5403301	Ni(OH)2 AQ	7.048E-13	7.049E-13	-12.15190	1.00014	-19.000
5403302	Ni(OH)3 -	1.446E-16	1.406E-16	-15.85191	0.97287	-29.988
5401400	NiHCO3 +	2.183E-10	2.124E-10	-9.67291	0.97287	12.482
5401401	NiCO3 AQ	1.064E-08	1.064E-08	-7.97291	1.00014	6.870
5401402	Ni(CO3)2-2	1.674E-12	1.500E-12	-11.82393	0.89582	10.158
3300600	H2AsO3 -	8.330E-10	8.104E-10	-9.09131	0.97287	-9.316
3300601	HAsO3 -2	1.090E-14	9.767E-15	-14.01025	0.89582	-21.500
3300602	AsO3 -3	7.773E-21	6.069E-21	-20.21689	0.78072	-34.947
3300603	H4AsO3 +	2.208E-15	2.148E-15	-14.66788	0.97287	-0.293
3301400	HCO3 -	1.020E-04	9.925E-05	-4.00326	0.97287	10.400
3301401	H2CO3 AQ	1.058E-05	1.058E-05	-4.97562	1.00014	16.715
2113300	Cr+3	7.027E-17	5.486E-17	-16.26071	0.78072	10.036
2113301	Cr(OH)+2	6.008E-14	5.382E-14	-13.26904	0.89582	5.668

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-1.458E-06	-5.836	0.000	0.000
3300021	O2 (g)	-6.959E-08	-7.157	-84.491	133.830
330	H+1	-1.220E-04	-3.914	7.300	0.000
3301403	CO2 (g)	2.066E-06	-5.685	21.691	-0.530

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.066E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	8.734E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	6.553E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	9.481E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.402E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	6.520E-12	0.0	0.000E-01	0.0	7.436E-08	100.0
600	Pb+2	4.634E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	1.947E-08	4.5	0.000E-01	0.0	4.174E-07	95.5
30	Al+3	2.623E-09	0.2	0.000E-01	0.0	1.480E-06	99.8
1	E-1	-8.655E-11	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.130E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	3.209E-07	89.6	0.000E-01	0.0	3.718E-08	10.4
2	H2O	1.474E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.233E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 6.355E-04 Sum of ANIONS 1.023E-04
PERCENT DIFFERENCE = 7.226E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 5.924E-04
EQUILIBRIUM pH = 7.300
EQUILIBRIUM pe = 13.823 or Eh = 800.97 mv

PART 1 of OUTPUT FILE

Revuè river water-Site 1 - Run 3

Entered CO_3^{2-}, PCO2, PO2, fixed pH, solids allowed to precipitate
Fe redox pair, Mn redox pair

Temperature (Celsius): 18.90
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	5.012E-08	-7.300	0.000E-01
30	Al+3	1.479E-06	-5.830	4.000E-02
60	H3AsO3	8.710E-08	-7.060	1.100E-02
100	Ba+2	6.607E-07	-6.180	9.000E-02
150	Ca+2	9.550E-05	-4.020	3.800E+00
160	Cd+2	2.399E-08	-7.620	2.700E-03
211	Cr(OH)2+	7.413E-08	-7.130	6.400E-03
280	Fe+2	3.548E-07	-6.450	2.000E-02
410	K+1	1.023E-05	-4.990	3.957E-01
460	Mg+2	1.288E-04	-3.890	3.100E+00
470	Mn+2	4.365E-07	-6.360	2.400E-02
500	Na+1	1.778E-04	-3.750	4.100E+00
540	Ni+2	3.090E-08	-7.510	1.800E-03
600	Pb+2	4.677E-08	-7.330	9.600E-03
800	Sr+2	2.291E-07	-6.640	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	4.786E-07	-6.320	6.902E+00
281	Fe+3	1.778E-21	-20.750	0.000E-01
471	Mn+3	1.820E-21	-20.740	0.000E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 6.412E-04 Sum of ANIONS = 2.300E-04
PERCENT DIFFERENCE = 4.719E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	5.152E-08	5.012E-08	-7.30000	0.97288	0.012
30	Al+3	2.868E-15	2.239E-15	-14.64992	0.78082	0.107
60	H3AsO3	8.651E-08	8.652E-08	-7.06288	1.00014	0.000
100	Ba+2	6.553E-07	5.871E-07	-6.23130	0.89587	0.048
150	Ca+2	9.473E-05	8.486E-05	-4.07127	0.89587	0.048
160	Cd+2	2.335E-08	2.092E-08	-7.67938	0.89587	0.048
211	Cr(OH)2+	1.282E-09	1.247E-09	-8.90404	0.97288	0.012
280	Fe+2	5.523E-25	4.948E-25	-24.30556	0.89587	0.048
410	K+1	1.012E-05	9.845E-06	-5.00676	0.97288	0.012
460	Mg+2	1.274E-04	1.141E-04	-3.94269	0.89587	0.048
470	Mn+2	4.194E-16	3.757E-16	-15.42516	0.89587	0.048
500	Na+1	1.783E-04	1.735E-04	-3.76070	0.97288	0.012
540	Ni+2	1.976E-08	1.771E-08	-7.75188	0.89587	0.048
600	Pb+2	1.727E-08	1.547E-08	-7.81044	0.89587	0.048
800	Sr+2	2.283E-07	2.045E-07	-6.68932	0.89587	0.048
471	Mn+3	2.468E-27	1.927E-27	-26.71503	0.78082	0.107
140	CO3-2	9.052E-08	8.109E-08	-7.09102	0.89587	0.048
281	Fe+3	2.751E-24	2.148E-24	-23.66789	0.78082	0.107

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	1.845E-09	1.845E-09	-8.73404	1.00014	-7.130
2113303	Cr(OH)4-	3.613E-13	3.515E-13	-12.45405	0.97288	-18.138
2113304	CrO2-	9.169E-13	8.920E-13	-12.04964	0.97288	-17.734
3300020	OH-	1.287E-07	1.252E-07	-6.90231	0.97288	-14.190
4603300	MgOH +	2.236E-09	2.176E-09	-8.66244	0.97288	-12.008
4601400	MgCO3 AQ	8.040E-09	8.041E-09	-8.09466	1.00014	2.939
4601401	MgHCO3 +	1.307E-07	1.271E-07	-6.89569	0.97288	11.450
1503300	CaOH +	2.631E-10	2.560E-10	-9.59180	0.97288	-12.809
1501400	CaHCO3 +	7.444E-08	7.242E-08	-7.14014	0.97288	11.334
1501401	CaCO3 AQ	8.626E-09	8.627E-09	-8.06413	1.00014	3.098
5001400	NaCO3 -	1.958E-10	1.905E-10	-9.72014	0.97288	1.144
5001401	NaHCO3 AQ	8.477E-09	8.478E-09	-8.07172	1.00014	10.080
303300	AlOH +2	3.355E-13	3.005E-13	-12.52209	0.89587	-5.124
303301	Al(OH)2 +	7.278E-11	7.081E-11	-10.14993	0.97288	-10.088
303302	Al(OH)4 -	7.717E-10	7.508E-10	-9.12447	0.97288	-23.663
303303	Al(OH)3 AQ	1.778E-09	1.779E-09	-8.74994	1.00014	-16.000
2803300	FeOH +	2.015E-27	1.961E-27	-26.70763	0.97288	-9.690
2803301	FeOH3 -1	1.388E-34	1.351E-34	-33.86944	0.97288	-31.452
2803302	FeOH2 AQ	1.937E-31	1.937E-31	-30.71287	1.00014	-21.007
2813300	FeOH +2	2.141E-19	1.918E-19	-18.71709	0.89587	-2.301
2813301	FeOH2 +	1.880E-15	1.829E-15	-14.73790	0.97288	-5.658
2813302	FeOH3 AQ	4.286E-16	4.286E-16	-15.36790	1.00014	-13.600
2813303	FeOH4 -	8.791E-17	8.553E-17	-16.06790	0.97288	-21.588
2813304	Fe2(OH)2+4	1.989E-36	1.281E-36	-35.89246	0.64415	-2.966
2813305	Fe3(OH)4+5	9.459E-49	4.758E-49	-48.32260	0.50296	-6.220
8003300	SrOH +	1.670E-13	1.625E-13	-12.78923	0.97288	-13.388
1003300	BaOH +	3.101E-13	3.017E-13	-12.52040	0.97288	-13.577
4703300	MnOH +	1.192E-19	1.160E-19	-18.93560	0.97288	-10.798
4703301	Mn(OH)3 -1	4.861E-29	4.730E-29	-28.32517	0.97288	-34.788
4700020	MnO4 -	3.738E-19	3.637E-19	-18.43929	0.97288	-130.516
4700021	MnO4 -2	3.775E-23	3.382E-23	-22.47082	0.89587	-120.689
4701400	MnHCO3 +	6.248E-19	6.079E-19	-18.21618	0.97288	11.612
1601400	Cd(CO3)3-4	2.875E-23	1.852E-23	-22.73243	0.64415	6.411
1603300	CdOH +	2.249E-11	2.188E-11	-10.65994	0.97288	-10.269
1603301	Cd(OH)2 AQ	3.720E-14	3.721E-14	-13.42939	1.00014	-20.350
1603302	Cd(OH)3 -	8.561E-20	8.329E-20	-19.07940	0.97288	-33.288
1603303	Cd(OH)4 -2	1.653E-26	1.481E-26	-25.82940	0.89587	-47.302
1603304	Cd2OH +3	3.103E-18	2.423E-18	-17.61562	0.78082	-9.449
1601400	CdHCO3 +	2.196E-10	2.136E-10	-9.67040	0.97288	12.412
1601401	CdCO3 AQ	4.252E-10	4.252E-10	-9.37140	1.00014	5.399
6001400	Pb(CO3)2-2	4.958E-12	4.441E-12	-11.35248	0.89587	10.688
6003300	PbOH +	6.187E-09	6.019E-09	-8.22045	0.97288	-7.698
6003301	Pb(OH)2 AQ	4.672E-11	4.672E-11	-10.33045	1.00014	-17.120
6003302	Pb(OH)3 -	1.100E-14	1.070E-14	-13.97046	0.97288	-28.048
6003303	Pb2OH +3	2.670E-15	2.085E-15	-14.68089	0.78082	-6.253
6003304	Pb3(OH)4+2	3.394E-19	3.041E-19	-18.51704	0.89587	-24.238
6001401	PbCO3 AQ	2.180E-08	2.180E-08	-7.66146	1.00014	7.240
6003305	Pb(OH)4 -2	5.474E-19	4.904E-19	-18.30946	0.89587	-39.651
6001402	PbHCO3 +	1.024E-09	9.966E-10	-9.00146	0.97288	13.212
5403300	NiOH +	3.235E-11	3.148E-11	-10.50202	0.97288	-10.038
5403301	Ni(OH)2 AQ	7.048E-13	7.049E-13	-12.15189	1.00014	-19.000
5403302	Ni(OH)3 -	1.446E-16	1.406E-16	-15.85189	0.97288	-29.988
5401400	NiHCO3 +	2.183E-10	2.124E-10	-9.67290	0.97288	12.482
5401401	NiCO3 AQ	1.064E-08	1.064E-08	-7.97289	1.00014	6.870
5401402	Ni(CO3)2-2	1.674E-12	1.500E-12	-11.82391	0.89587	10.158
3300600	H2AsO3 -	8.330E-10	8.104E-10	-9.09131	0.97288	-9.316
3300601	HAsO3 -2	1.090E-14	9.767E-15	-14.01025	0.89587	-21.500
3300602	AsO3 -3	7.772E-21	6.069E-21	-20.21689	0.78082	-34.947
3300603	H4AsO3 +	2.208E-15	2.148E-15	-14.66788	0.97288	-0.293
3301400	HCO3 -	1.020E-04	9.925E-05	-4.00326	0.97288	10.400
3301401	H2CO3 AQ	1.058E-05	1.058E-05	-4.97562	1.00014	16.715
2113300	Cr+3	3.402E-14	2.656E-14	-13.57570	0.78082	10.036
2113301	Cr(OH)+2	2.909E-11	2.606E-11	-10.58404	0.89587	5.668

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-1.799E-06	-5.745	0.000	0.000
4704710	Mn+2/Mn+3	-4.369E-07	-6.360	25.113	25.760
330	H+1	-1.213E-04	-3.916	7.300	0.000
3301403	CO2 (g)	2.068E-06	-5.684	21.691	-0.530
3300021	O2 (g)	-3.080E-07	-6.511	-84.491	133.830
2802810	Fe+2/Fe+3	-3.581E-07	-6.446	13.185	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	1.791E-07	-6.747	3.536	30.845
2047000	PYROLUSITE	4.369E-07	-6.360	-16.308	29.180
2003002	DIASPORE	1.480E-06	-5.830	-7.250	24.630
3021102	CR2O3	3.563E-08	-7.448	3.208	12.125

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
540	Ni+2	3.066E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	8.734E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	6.553E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	9.481E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.402E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	4.634E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	3.157E-09	4.2	0.000E-01	0.0	7.125E-08	95.8
470	Mn+2	4.205E-16	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	2.623E-09	0.2	0.000E-01	0.0	1.480E-06	99.8
140	CO3-2	1.129E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
471	Mn+3	2.468E-27	0.0	0.000E-01	0.0	4.369E-07	100.0
280	Fe+2	5.543E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.396E-15	0.0	0.000E-01	0.0	3.581E-07	100.0
1	E-1	-1.869E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.233E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	1.479E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 6.348E-04 Sum of ANIONS 1.023E-04
PERCENT DIFFERENCE = 7.224E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 5.917E-04
EQUILIBRIUM pH = 7.300
EQUILIBRIUM pe = 13.823 or Eh = 800.97 mv

PART 1 of OUTPUT FILE

Revuè river water-Site 1 - Run 4

Entered CO_3^{2-}, P_{CO2}, P_{O2}, fixed pH, Fe redox pair, Mn redox pair, solids allowed to precipitate

Adsorption

Temperature (Celsius): 18.90
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	5.012E-08	-7.300	0.000E-01
30	Al+3	1.479E-06	-5.830	4.000E-02
60	H3AsO3	8.710E-08	-7.060	1.100E-02
100	Ba+2	6.607E-07	-6.180	9.000E-02
150	Ca+2	9.550E-05	-4.020	3.800E+00
160	Cd+2	2.399E-08	-7.620	2.700E-03
211	Cr(OH)2+	7.413E-08	-7.130	6.400E-03
280	Fe+2	3.548E-07	-6.450	2.000E-02
410	K+1	1.023E-05	-4.990	3.957E-01
460	Mg+2	1.288E-04	-3.890	3.100E+00
470	Mn+2	4.365E-07	-6.360	2.400E-02
500	Na+1	1.778E-04	-3.750	4.100E+00
540	Ni+2	3.090E-08	-7.510	1.800E-03
600	Pb+2	4.677E-08	-7.330	9.600E-03
800	Sr+2	2.291E-07	-6.640	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	4.786E-07	-6.320	6.902E+00
281	Fe+3	1.778E-21	-20.750	0.000E-01
471	Mn+3	1.820E-21	-20.740	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 6.412E-04 Sum of ANIONS = 2.300E-04
PERCENT DIFFERENCE = 4.719E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	5.146E-08	5.012E-08	-7.30000	0.97387	0.011
30	Al+3	2.842E-15	2.239E-15	-14.64992	0.78796	0.103
60	H3AsO3	5.627E-11	5.628E-11	-10.24964	1.00013	0.000
100	Ba+2	3.561E-07	3.203E-07	-6.49441	0.89950	0.046
150	Ca+2	7.315E-05	6.580E-05	-4.18179	0.89950	0.046
160	Cd+2	2.354E-11	2.117E-11	-10.67420	0.89950	0.046
211	Cr(OH)2+	1.281E-09	1.247E-09	-8.90404	0.97387	0.011
280	Fe+2	5.501E-25	4.948E-25	-24.30555	0.89950	0.046
410	K+1	1.012E-05	9.855E-06	-5.00632	0.97387	0.011
460	Mg+2	1.274E-04	1.146E-04	-3.94093	0.89950	0.046
470	Mn+2	4.177E-16	3.757E-16	-15.42515	0.89950	0.046
500	Na+1	1.783E-04	1.737E-04	-3.76026	0.97387	0.011
540	Ni+2	5.304E-11	4.771E-11	-10.32142	0.89950	0.046
600	Pb+2	2.431E-15	2.187E-15	-14.66022	0.89950	0.046
800	Sr+2	2.283E-07	2.053E-07	-6.68756	0.89950	0.046

811	ADS1TYP1	1.320E-04	1.320E-04	-3.87954	1.00000	0.000
140	CO3-2	9.015E-08	8.109E-08	-7.09102	0.89950	0.046
281	Fe+3	2.727E-24	2.148E-24	-23.66789	0.78796	0.103
471	Mn+3	2.446E-27	1.927E-27	-26.71503	0.78796	0.103
812	ADS1TYP2	5.902E-03	5.902E-03	-2.22903	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8120600	=S2H2AsO3(o)	8.538E-08	8.538E-08	-7.06866	1.00000	5.410
2113302	Cr(OH)3 AQ	1.845E-09	1.845E-09	-8.73404	1.00013	-7.130
2113303	Cr(OH)4-	3.610E-13	3.515E-13	-12.45405	0.97387	-18.139
2113304	CrO2-	9.159E-13	8.920E-13	-12.04964	0.97387	-17.734
3300020	OH-	1.286E-07	1.252E-07	-6.90231	0.97387	-14.191
4603300	MgOH +	2.243E-09	2.184E-09	-8.66068	0.97387	-12.008
4601400	MgCO3 AQ	8.073E-09	8.074E-09	-8.09291	1.00013	2.939
4601401	MgHCO3 +	1.311E-07	1.277E-07	-6.89393	0.97387	11.450
1503300	CaOH +	2.038E-10	1.985E-10	-9.70231	0.97387	-12.809
1501400	CaHCO3 +	5.766E-08	5.615E-08	-7.25065	0.97387	11.334
1501401	CaCO3 AQ	6.688E-09	6.689E-09	-8.17465	1.00013	3.098
5001400	NaCO3 -	1.958E-10	1.907E-10	-9.71970	0.97387	1.143
5001401	NaHCO3 AQ	8.485E-09	8.486E-09	-8.07128	1.00013	10.080
303300	AlOH +2	3.341E-13	3.005E-13	-12.52209	0.89950	-5.126
303301	Al(OH)2 +	7.271E-11	7.081E-11	-10.14993	0.97387	-10.089
303302	Al(OH)4 -	7.710E-10	7.508E-10	-9.12447	0.97387	-23.663
303303	Al(OH)3 AQ	1.778E-09	1.779E-09	-8.74994	1.00013	-16.000
2803300	FeOH +	2.013E-27	1.961E-27	-26.70762	0.97387	-9.691
2803301	FeOH3 -1	1.387E-34	1.351E-34	-33.86944	0.97387	-31.452
2803302	FeOH2 AQ	1.937E-31	1.937E-31	-30.71287	1.00013	-21.007
2813300	FeOH +2	2.133E-19	1.918E-19	-18.71709	0.89950	-2.303
2813301	FeOH2 +	1.878E-15	1.829E-15	-14.73790	0.97387	-5.659
2813302	FeOH3 AQ	4.286E-16	4.286E-16	-15.36790	1.00013	-13.600
2813303	FeOH4 -	8.782E-17	8.553E-17	-16.06790	0.97387	-21.589
2813304	Fe2(OH)2+4	1.957E-36	1.281E-36	-35.89246	0.65464	-2.973
2813305	Fe3(OH)4+5	9.223E-49	4.758E-49	-48.32260	0.51583	-6.231
8003300	SrOH +	1.675E-13	1.631E-13	-12.78747	0.97387	-13.388
1003300	BaOH +	1.690E-13	1.646E-13	-12.78351	0.97387	-13.578
4703300	MnOH +	1.191E-19	1.160E-19	-18.93560	0.97387	-10.799
4703301	Mn(OH)3 -1	4.857E-29	4.730E-29	-28.32517	0.97387	-34.789
4700020	MnO4 -	3.734E-19	3.637E-19	-18.43929	0.97387	-130.516
4700021	MnO4 -2	3.760E-23	3.382E-23	-22.47082	0.89950	-120.691
4701400	MnHCO3 +	6.242E-19	6.079E-19	-18.21617	0.97387	11.611
1601400	Cd(CO3)3-4	2.862E-26	1.874E-26	-25.72725	0.65464	6.404
1603300	CdOH +	2.274E-14	2.214E-14	-13.65476	0.97387	-10.269
1603301	Cd(OH)2 AQ	3.765E-17	3.765E-17	-16.42421	1.00013	-20.350
1603302	Cd(OH)3 -	8.655E-23	8.429E-23	-22.07421	0.97387	-33.289
1603303	Cd(OH)4 -2	1.666E-29	1.499E-29	-28.82422	0.89950	-47.304
1603304	Cd2OH +3	3.149E-24	2.482E-24	-23.60526	0.78796	-9.453
1601400	CdHCO3 +	2.220E-13	2.162E-13	-12.66522	0.97387	12.411
1601401	CdCO3 AQ	4.303E-13	4.303E-13	-12.36622	1.00013	5.399
6001400	Pb(CO3)2-2	6.978E-19	6.277E-19	-18.20226	0.89950	10.686
6003300	PbOH +	8.735E-16	8.507E-16	-15.07023	0.97387	-7.699
6003301	Pb(OH)2 AQ	6.603E-18	6.603E-18	-17.18023	1.00013	-17.120
6003302	Pb(OH)3 -	1.553E-21	1.513E-21	-20.82024	0.97387	-28.049
6003303	Pb2OH +3	5.285E-29	4.164E-29	-28.38045	0.78796	-6.257
6003304	Pb3(OH)4+2	9.541E-40	8.583E-40	-39.06638	0.89950	-24.240
6001401	PbCO3 AQ	3.081E-15	3.081E-15	-14.51124	1.00013	7.240
6003305	Pb(OH)4 -2	7.705E-26	6.930E-26	-25.15924	0.89950	-39.653
6001402	PbHCO3 +	1.446E-16	1.409E-16	-15.85124	0.97387	13.211
5403300	NiOH +	8.708E-14	8.481E-14	-13.07156	0.97387	-10.039
5403301	Ni(OH)2 AQ	1.899E-15	1.899E-15	-14.72143	1.00013	-19.000
5403302	Ni(OH)3 -	3.891E-19	3.789E-19	-18.42143	0.97387	-29.989
5401400	NiHCO3 +	5.876E-13	5.722E-13	-12.24244	0.97387	12.481
5401401	NiCO3 AQ	2.868E-11	2.868E-11	-10.54244	1.00013	6.870
5401402	Ni(CO3)2-2	4.493E-15	4.042E-15	-14.39345	0.89950	10.156
3300600	H2AsO3 -	5.413E-13	5.272E-13	-12.27806	0.97387	-9.317
3300601	HAsO3 -2	7.063E-18	6.353E-18	-17.19701	0.89950	-21.501
3300602	AsO3 -3	5.010E-24	3.948E-24	-23.40365	0.78796	-34.951

3300603	H4AsO3 +	1.435E-18	1.398E-18	-17.85464	0.97387	-0.294
3301400	HCO3 -	1.019E-04	9.925E-05	-4.00326	0.97387	10.399
3301401	H2CO3 AQ	1.058E-05	1.058E-05	-4.97562	1.00013	16.715
2113300	Cr+3	3.371E-14	2.656E-14	-13.57570	0.78796	10.032
2113301	Cr(OH)+2	2.897E-11	2.606E-11	-10.58404	0.89950	5.666
8123301	=SO2-	8.832E-04	8.832E-04	-3.05395	1.00000	-8.930
8123302	=SO2H2+	9.034E-04	9.034E-04	-3.04411	1.00000	7.290
8113301	=SO1-	1.975E-05	1.975E-05	-4.70446	1.00000	-8.930
8113302	=SO1H2+	2.020E-05	2.020E-05	-4.69462	1.00000	7.290
8121600	=SO2Cd+	4.917E-10	4.917E-10	-9.30831	1.00000	-2.900
8111600	=SO1Cd+	2.351E-08	2.351E-08	-7.62882	1.00000	0.430
8115400	=SO1Ni+	2.779E-08	2.779E-08	-7.55604	1.00000	0.150
8125400	=SO2Ni+	2.783E-09	2.783E-09	-8.55553	1.00000	-2.500
8116000	=SO1Pb+	4.625E-08	4.625E-08	-7.33484	1.00000	4.710
8126000	=SO2Pb+	8.048E-11	8.048E-11	-10.09434	1.00000	0.300
8121500	=SO2Ca+	1.714E-06	1.714E-06	-5.76590	1.00000	-5.850
8111500	=SO1HCa++	1.988E-05	1.988E-05	-4.70149	1.00000	4.970
8111000	=SO1HBa++	2.992E-07	2.992E-07	-6.52411	1.00000	5.460
8121000	=SO2Ba+	5.840E-11	5.840E-11	-10.23360	1.00000	-7.200
8110600	=S1H2AsO3(o)	1.909E-09	1.909E-09	-8.71917	1.00000	5.410

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-1.650E-06	-5.782	0.000	0.000
4704710	Mn+2/Mn+3	-4.369E-07	-6.360	25.113	25.760
330	H+1	-1.404E-04	-3.853	7.300	0.000
3301403	CO2 (g)	2.224E-06	-5.653	21.691	-0.530
3300021	O2 (g)	-3.080E-07	-6.511	-84.491	133.830
2802810	Fe+2/Fe+3	-3.581E-07	-6.446	13.185	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	1.791E-07	-6.747	3.536	30.845
2047000	PYROLUSITE	4.369E-07	-6.360	-16.308	29.180
2003002	DIASPORE	1.480E-06	-5.830	-7.250	24.630
3021102	CR2O3	3.563E-08	-7.448	3.208	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1PSIo			
	>1000.	PERCENT BOUND IN SPECIES #8123302	=SO2H2+
	32.1	PERCENT BOUND IN SPECIES #8113302	=SO1H2+
	2.7	PERCENT BOUND IN SPECIES #8121500	=SO2Ca+
	63.3	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++
Ca+2			
	77.2	PERCENT BOUND IN SPECIES # 150	Ca+2
	1.8	PERCENT BOUND IN SPECIES #8121500	=SO2Ca+
	21.0	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++
Mg+2			
	99.9	PERCENT BOUND IN SPECIES # 460	Mg+2
Na+1			
	100.0	PERCENT BOUND IN SPECIES # 500	Na+1
K+1			
	100.0	PERCENT BOUND IN SPECIES # 410	K+1
Pb+2			
	99.8	PERCENT BOUND IN SPECIES #8116000	=SO1Pb+
ADS1TYP1			
	68.7	PERCENT BOUND IN SPECIES # 811	ADS1TYP1
	10.3	PERCENT BOUND IN SPECIES #8113301	=SO1-
	10.5	PERCENT BOUND IN SPECIES #8113302	=SO1H2+
	10.3	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++
ADS1TYP2			
	76.7	PERCENT BOUND IN SPECIES # 812	ADS1TYP2
	11.5	PERCENT BOUND IN SPECIES #8123301	=SO2-
	11.7	PERCENT BOUND IN SPECIES #8123302	=SO2H2+

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Sr+2
              100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
H3AsO3
               97.7     PERCENT BOUND IN SPECIES #8120600   =S2H2AsO3(o)
                2.2     PERCENT BOUND IN SPECIES #8110600   =S1H2AsO3(o)
Ba+2
               54.3     PERCENT BOUND IN SPECIES #    100   Ba+2
               45.6     PERCENT BOUND IN SPECIES #8111000   =SO1HBa++
Ni+2
               90.7     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                9.1     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Cd+2
                2.0     PERCENT BOUND IN SPECIES #8121600   =SO2Cd+
               97.9     PERCENT BOUND IN SPECIES #8111600   =SO1Cd+
Cr(OH)2+
               40.6     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
               58.5     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
Mn+2
               99.7     PERCENT BOUND IN SPECIES #    470   Mn+2
Al+3
                2.8     PERCENT BOUND IN SPECIES # 303301   Al(OH)2 +
               29.4     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
               67.8     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
               90.4     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                9.4     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
               99.6     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
              100.0     PERCENT BOUND IN SPECIES #4700020   MnO4 -
Fe+3
               78.4     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
               17.9     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                3.7     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
Mn+3
              100.0     PERCENT BOUND IN SPECIES #    471   Mn+3
H+1
               71.7     PERCENT BOUND IN SPECIES #3301400   HCO3 -
               14.9     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
              636.0     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
               14.2     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                1.2     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
               82.9     PERCENT BOUND IN SPECIES #3300020   OH-
                1.4     PERCENT BOUND IN SPECIES #4603300   MgOH +
                2.0     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                3.4     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
               15.2     PERCENT BOUND IN SPECIES #8111600   =SO1Cd+
               17.9     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                1.8     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
               29.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	2.283E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	5.682E-11	0.1	8.729E-08	99.9	0.000E-01	0.0
100	Ba+2	3.561E-07	54.3	2.992E-07	45.7	0.000E-01	0.0
150	Ca+2	7.321E-05	77.2	2.160E-05	22.8	0.000E-01	0.0
160	Cd+2	2.421E-11	0.1	2.400E-08	99.9	0.000E-01	0.0
600	Pb+2	6.537E-15	0.0	4.634E-08	100.0	0.000E-01	0.0
410	K+1	1.012E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.275E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.783E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	8.239E-11	0.3	3.058E-08	99.7	0.000E-01	0.0
211	Cr(OH)2+	3.156E-09	4.2	0.000E-01	0.0	7.125E-08	95.8

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470  Mn+2          4.188E-16   100.0    0.000E-01     0.0    0.000E-01     0.0
 30  Al+3          2.622E-09     0.2    0.000E-01     0.0    1.480E-06    99.8
140  CO3-2         1.128E-04   100.0    0.000E-01     0.0    0.000E-01     0.0
280  Fe+2          5.521E-25   100.0    0.000E-01     0.0    0.000E-01     0.0
  1  E-1          -1.867E-18   100.0    0.000E-01     0.0    0.000E-01     0.0
281  Fe+3          2.394E-15     0.0    0.000E-01     0.0    3.581E-07   100.0
471  Mn+3          2.446E-27     0.0    0.000E-01     0.0    4.369E-07   100.0
330  H+1           1.232E-04    86.7    1.887E-05    13.3    0.000E-01     0.0
  2  H2O           1.414E-07    91.2    1.362E-08     8.8    0.000E-01     0.0

     Charge Balance: SPECIATED
       Sum of CATIONS =  1.557E-03 Sum of ANIONS   1.005E-03
       PERCENT DIFFERENCE =   2.153E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
     EQUILIBRIUM IONIC STRENGTH (m) =   5.478E-04
     EQUILIBRIUM pH                 =   7.300
     EQUILIBRIUM pe                 =  13.823   or Eh  =   800.97 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.046652     sig0 = 0.002938
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.544	[1.000] 30 [3.000] 2 [-3.000]330
5015000	ARAGONITE	-2.991	[1.000] 150 [1.000] 140
5046000	ARTINITE	-10.413	[-2.000] 330 [2.000] 460 [1.000]140
			[5.000] 2
2003001	BOEHMITE	-1.759	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.529	[1.000] 460 [2.000] 2 [-2.000]330
5015001	CALCITE	-2.832	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-5.432	[1.000] 150 [1.000] 460 [2.000]140
2028100	FERRIHYDRITE	-6.659	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.463	[-8.000] 330 [2.000] 281 [1.000]280
			[8.000] 2
2003003	GIBBSITE (C)	-1.869	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.480	[2.000] 30 [3.000] 2 [-6.000]330
2028102	GOETHITE	-2.490	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-14.795	[3.000] 460 [1.000] 150 [4.000]140
5046001	HYDRMAGNESIT	-25.502	[5.000] 460 [4.000] 140 [-2.000]330
			[6.000] 2
3028101	MAGHEMITE	-9.922	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-3.097	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.751	[-8.000] 330 [2.000] 281 [1.000]280
			[4.000] 2
3050000	NATRON	-13.060	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.500	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.928	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-4.539	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.779	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.995	[1.000] 100 [1.000] 140
2047000	PYROLUSITE	0.000	[-4.000] 330 [-1.000] 1 [1.000]471
			[2.000] 2
2047001	BIRNESSITE	-1.783	[-4.000] 330 [-1.000] 1 [1.000]471
			[2.000] 2
2047002	NSUTITE	-1.196	[-4.000] 330 [-1.000] 1 [1.000]471
			[2.000] 2
3047100	BIXBYITE	-9.252	[-6.000] 330 [2.000] 471 [3.000] 2
3047000	HAUSMANNITE	-22.997	[-8.000] 330 [-2.000] 1 [3.000]470
			[4.000] 2
2047003	PYROCROITE	-16.259	[-2.000] 330 [1.000] 470 [2.000] 2
2047100	MANGANITE	-4.577	[-3.000] 330 [1.000] 471 [2.000] 2
5047000	RHODOCHROSIT	-12.138	[1.000] 470 [1.000] 140

```
  16000 CD METAL       -52.085    [  1.000] 160  [  2.000]   1
  16001 GAMMA CD       -52.187    [  1.000] 160  [  2.000]   1
5016000 OTAVITE         -4.034    [  1.000] 160  [  1.000] 140
2016000 CD(OH)2 (A)    -10.122    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)     -9.724    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE    -11.573    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL       -46.570    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE       -8.547    [  1.000] 600  [  1.000] 140
2060000 MASSICOT       -13.227    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE       -13.031    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O     -13.040    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3        -21.487    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                  [  1.000] 140
5060002 PB3O2CO3       -33.296    [ -4.000] 330  [  3.000] 600  [  1.000]  40
                                  [  2.000]   2
2060003 PLATTNERITE     -8.198    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                  [  2.000]   2
3060000 PB2O3          -18.915    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                  [  3.000]   2
3060001 MINIUM         -33.198    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                  [  4.000]   2
2060004 PB(OH)2 (C)     -8.424    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE   -26.103    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                  [  2.000]   2
2060005 PB2O(OH)2      -26.320    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3          -10.725    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2         -6.055    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE       -8.538    [ -2.000] 330  [  1.000] 540  [  1.000]   2
3006000 ARSENOLITE     -37.978    [  4.000]  60  [ -6.000]   2
3006001 CLAUDETITE     -37.730    [  4.000]  60  [ -6.000]   2
2015000 LIME           -23.087    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE    -12.727    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE        -20.485    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE      -11.404    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE      -23.567    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                  [  4.000]   2
3046000 SPINEL         -12.538    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                  [  4.000]   2
3046001 MAG-FERRITE    -10.662    [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                  [  4.000]   2
3028102 LEPIDOCROCIT    -3.139    [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021100 FECR2O4        -12.393    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4         -5.239    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3            0.000    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)     -0.854    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)     -3.413    [  1.000] 211  [  1.000]   2  [ -1.000] 330
```

2 - Modelling of water quality of Site 9

PART 1 of OUTPUT FILE

Revuè river water-Site 9 - Initial run

Entered alkalinity, P_{CO2}, P_{O2}, fixed pH, solids not allowed to precipitate

```
 Temperature (Celsius):  17.30
 Units of concentration: MG/L
 Ionic strength to be computed.
 Carbonate concentration represents carbonate alkalinity.
 Do not automatically terminate if charge imbalance exceeds 30%
 Precipitation is allowed only for those solids specified as ALLOWED
   in the input file (if any).
 The maximum number of iterations is: 200
 The method used to compute activity coefficients is: Davies equation
 Intermediate output file
```

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.162E-08	-7.500	0.000E-01
30	Al+3	2.239E-06	-5.650	6.000E-02
60	H3AsO3	3.162E-08	-7.500	4.000E-03
100	Ba+2	1.230E-06	-5.910	1.700E-01
150	Ca+2	1.778E-04	-3.750	7.200E+00
160	Cd+2	2.818E-09	-8.550	3.200E-04
211	Cr(OH)2+	5.495E-08	-7.260	4.700E-03
280	Fe+2	8.913E-07	-6.050	5.000E-02
410	K+1	1.950E-05	-4.710	7.644E-01
460	Mg+2	3.090E-04	-3.510	7.600E+00
470	Mn+2	3.631E-06	-5.440	2.000E-01
500	Na+1	2.239E-04	-3.650	5.200E+00
600	Pb+2	1.288E-07	-6.890	2.700E-02
800	Sr+2	4.571E-07	-6.340	4.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	8.511E-07	-6.070	3.693E+01
2	H2O	1.000E+00	0.000	0.000E-01

```
  Charge Balance: UNSPECIATED
    Sum of CATIONS=  1.250E-03 Sum of ANIONS =  1.231E-03
    PERCENT DIFFERENCE =  7.607E-01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
```

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	3.287E-08	3.162E-08	-7.50000	0.96212	0.017
30	Al+3	6.711E-13	4.740E-13	-12.32419	0.70640	0.151
60	H3AsO3	3.131E-08	3.132E-08	-7.50422	1.00028	0.000
100	Ba+2	1.238E-06	1.061E-06	-5.97441	0.85686	0.067
150	Ca+2	1.794E-04	1.537E-04	-3.81327	0.85686	0.067
160	Cd+2	2.688E-09	2.303E-09	-8.63764	0.85686	0.067
211	Cr(OH)2+	1.670E-08	1.607E-08	-7.79403	0.96212	0.017
280	Fe+2	8.910E-07	7.634E-07	-6.11723	0.85686	0.067
410	K+1	1.955E-05	1.881E-05	-4.72563	0.96212	0.017
460	Mg+2	3.121E-04	2.674E-04	-3.57284	0.85686	0.067
470	Mn+2	3.620E-06	3.102E-06	-5.50842	0.85686	0.067
500	Na+1	2.262E-04	2.176E-04	-3.66231	0.96212	0.017
600	Pb+2	2.794E-08	2.394E-08	-7.62091	0.85686	0.067
800	Sr+2	4.565E-07	3.912E-07	-6.40761	0.85686	0.067
140	CO3-2	2.365E-07	2.027E-07	-6.69321	0.85686	0.067

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	3.766E-08	3.767E-08	-7.42404	1.00028	-7.130
2113303	Cr(OH)4-	1.182E-11	1.138E-11	-10.94405	0.96212	-18.133
2113304	CrO2-	3.000E-11	2.887E-11	-10.53963	0.96212	-17.729
3300020	OH-	1.817E-07	1.749E-07	-6.75732	0.96212	-14.241

4603300	MgOH +	7.260E-09	6.985E-09	-8.15583	0.96212	-12.066
4601400	MgCO3 AQ	4.594E-08	4.595E-08	-7.33769	1.00028	2.928
4601401	MgHCO3 +	5.031E-07	4.841E-07	-6.31509	0.96212	11.468
1503300	CaOH +	6.654E-10	6.402E-10	-9.19371	0.96212	-12.864
1501400	CaHCO3 +	2.127E-07	2.047E-07	-6.68892	0.96212	11.334
1501401	CaCO3 AQ	3.796E-08	3.797E-08	-7.42060	1.00028	3.086
5001400	NaCO3 -	5.703E-10	5.487E-10	-9.26067	0.96212	1.112
5001401	NaHCO3 AQ	1.676E-08	1.677E-08	-7.77552	1.00028	10.080
303300	AlOH +2	1.051E-10	9.007E-11	-10.04541	0.85686	-5.154
303301	Al(OH)2 +	3.913E-08	3.765E-08	-7.42421	0.96212	-10.083
303302	Al(OH)4 -	6.861E-07	6.601E-07	-6.18037	0.96212	-23.839
303303	Al(OH)3 AQ	1.499E-06	1.499E-06	-5.82422	1.00028	-16.000
2803300	FeOH +	4.396E-09	4.229E-09	-8.37371	0.96212	-9.740
2803301	FeOH3 -1	6.468E-16	6.223E-16	-15.20603	0.96212	-31.572
2803302	FeOH2 AQ	5.722E-13	5.724E-13	-12.24230	1.00028	-21.125
8003300	SrOH +	4.462E-13	4.293E-13	-12.36727	0.96212	-13.443
1003300	BaOH +	7.781E-13	7.486E-13	-12.12574	0.96212	-13.635
4703300	MnOH +	1.376E-09	1.324E-09	-8.87822	0.96212	-10.853
4703301	Mn(OH)3 -1	1.616E-18	1.554E-18	-17.80845	0.96212	-34.783
4700020	MnO4 -	1.137E-08	1.094E-08	-7.96102	0.96212	-131.239
4700021	MnO4 -2	1.763E-12	1.511E-12	-11.82083	0.85686	-121.288
4701400	MnHCO3 +	8.225E-09	7.914E-09	-8.10162	0.96212	11.617
1601400	Cd(CO3)3-4	5.903E-23	3.182E-23	-22.49726	0.53907	6.488
1603300	CdOH +	3.504E-12	3.371E-12	-11.47220	0.96212	-10.318
1603301	Cd(OH)2 AQ	1.029E-14	1.029E-14	-13.98766	1.00028	-20.350
1603302	Cd(OH)3 -	3.794E-20	3.650E-20	-19.43767	0.96212	-33.283
1603303	Cd(OH)4 -2	1.201E-26	1.029E-26	-25.98768	0.85686	-47.283
1603304	Cd2OH +3	5.941E-20	4.197E-20	-19.37707	0.70640	-9.451
1601400	CdHCO3 +	3.854E-11	3.708E-11	-10.43085	0.96212	12.417
1601401	CdCO3 AQ	1.170E-10	1.170E-10	-9.93185	1.00028	5.399
6001400	Pb(CO3)2-2	5.009E-11	4.292E-11	-10.36733	0.85686	10.707
6003300	PbOH +	1.534E-08	1.476E-08	-7.83092	0.96212	-7.693
6003301	Pb(OH)2 AQ	1.815E-10	1.816E-10	-9.74093	1.00028	-17.120
6003302	Pb(OH)3 -	6.852E-14	6.593E-14	-13.18094	0.96212	-28.043
6003303	Pb2OH +3	1.120E-14	7.910E-15	-14.10184	0.70640	-6.209
6003304	Pb3(OH)4+2	6.447E-18	5.524E-18	-17.25771	0.85686	-24.328
6001401	PbCO3 AQ	8.429E-08	8.431E-08	-7.07412	1.00028	7.240
6003305	Pb(OH)4 -2	5.586E-18	4.787E-18	-17.31995	0.85686	-39.632
6001402	PbHCO3 +	2.527E-09	2.432E-09	-8.61412	0.96212	13.217
3300600	H2AsO3 -	4.540E-10	4.368E-10	-9.35969	0.96212	-9.339
3300601	HAsO3 -2	9.057E-15	7.760E-15	-14.11013	0.85686	-21.539
3300602	AsO3 -3	1.022E-20	7.216E-21	-20.14171	0.70640	-34.987
3300603	H4AsO3 +	5.100E-16	4.907E-16	-15.30922	0.96212	-0.288
3301400	HCO3 -	1.690E-04	1.626E-04	-3.78877	0.96212	10.421
3301401	H2CO3 AQ	1.075E-05	1.075E-05	-4.96855	1.00028	16.725
2113300	Cr+3	2.335E-13	1.649E-13	-12.78266	0.70640	10.162
2113301	Cr(OH)+2	2.472E-10	2.118E-10	-9.67401	0.85686	5.687

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	1.053E-03	-2.978	0.000	0.000
3300021	O2 (g)	-1.421E-08	-7.847	-85.043	133.830
330	H+1	-2.304E-03	-2.638	7.500	0.000
3301403	CO2 (g)	1.060E-03	-2.975	21.693	-0.530

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Sr+2	100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
Al+3	1.8	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
	30.9	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
	67.4	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
H3AsO3	98.6	PERCENT BOUND IN SPECIES #	60	H3AsO3
	1.4	PERCENT BOUND IN SPECIES #	3300600	H2AsO3 -
Ba+2	100.0	PERCENT BOUND IN SPECIES #	100	Ba+2

Ca+2	99.9	PERCENT BOUND IN SPECIES #	150	Ca+2
Cd+2	94.4	PERCENT BOUND IN SPECIES #	160	Cd+2
	1.4	PERCENT BOUND IN SPECIES #1601400		CdHCO3 +
	4.1	PERCENT BOUND IN SPECIES #1601401		CdCO3 AQ
Cr(OH)2+	30.6	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
	68.9	PERCENT BOUND IN SPECIES #2113302		Cr(OH)3 AQ
Fe+2	99.5	PERCENT BOUND IN SPECIES #	280	Fe+2
K+1	100.0	PERCENT BOUND IN SPECIES #	410	K+1
Mg+2	99.8	PERCENT BOUND IN SPECIES #	460	Mg+2
Mn+2	99.4	PERCENT BOUND IN SPECIES #	470	Mn+2
Na+1	100.0	PERCENT BOUND IN SPECIES #	500	Na+1
Pb+2	21.4	PERCENT BOUND IN SPECIES #	600	Pb+2
	11.8	PERCENT BOUND IN SPECIES #6003300		PbOH +
	64.7	PERCENT BOUND IN SPECIES #6001401		PbCO3 AQ
	1.9	PERCENT BOUND IN SPECIES #6001402		PbHCO3 +
CO3-2	93.4	PERCENT BOUND IN SPECIES #3301400		HCO3 -
	5.9	PERCENT BOUND IN SPECIES #3301401		H2CO3 AQ
E-1	100.0	PERCENT BOUND IN SPECIES #4700020		MnO4 -
H+1	92.0	PERCENT BOUND IN SPECIES #3301400		HCO3 -
	11.7	PERCENT BOUND IN SPECIES #3301401		H2CO3 AQ
H2O	2.4	PERCENT BOUND IN SPECIES #3300020		OH-
	1.0	PERCENT BOUND IN SPECIES # 303301		Al(OH)2 +
	36.1	PERCENT BOUND IN SPECIES # 303302		Al(OH)4 -
	59.1	PERCENT BOUND IN SPECIES # 303303		Al(OH)3 AQ

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	2.224E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	3.176E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.238E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.797E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.847E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	5.465E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	8.954E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	3.641E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.303E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.809E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	-5.686E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.837E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	7.612E-06	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 1.242E-03 Sum of ANIONS 1.704E-04
PERCENT DIFFERENCE = 7.587E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
NON-CARBONATE ALKALINITY = 1.495E-07
EQUILIBRIUM IONIC STRENGTH (m) = 1.204E-03
EQUILIBRIUM pH = 7.500
EQUILIBRIUM pe = 13.761 or Eh = 793.00 mv

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-0.730	[1.000] 30 [3.000] 2 [-3.000]330
5015000	ARAGONITE	-2.238	[1.000] 150 [1.000] 140
5046000	ARTINITE	-8.997	[-2.000] 330 [2.000] 460 [1.000]140
			[5.000] 2
2003001	BOEHMITE	1.051	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-5.867	[1.000] 460 [2.000] 2 [-2.000]330
5015001	CALCITE	-2.074	[1.000] 150 [1.000] 140
2003002	DIASPORE	2.824	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-3.934	[1.000] 150 [1.000] 460 [2.000]140
2003003	GIBBSITE (C)	0.963	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-2.628	[2.000] 30 [3.000] 2 [-6.000]330
5015003	HUNTITE	-11.837	[3.000] 460 [1.000] 150 [4.000]140
5046001	HYDRMAGNESIT	-21.886	[5.000] 460 [4.000] 140 [-2.000]330
			[6.000] 2
5046002	MAGNESITE	-2.357	[1.000] 460 [1.000] 140
3050000	NATRON	-12.401	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-4.758	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-2.364	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.864	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.197	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.076	[1.000] 100 [1.000] 140
3047000	HAUSMANNITE	7.899	[-8.000] 330 [-2.000] 1 [3.000]470
			[4.000] 2
2047003	PYROCROITE	-6.035	[-2.000] 330 [1.000] 470 [2.000] 2
5047000	RHODOCHROSIT	-1.832	[1.000] 470 [1.000] 140
16000	CD METAL	-49.999	[1.000] 160 [2.000] 1
16001	GAMMA CD	-50.101	[1.000] 160 [2.000] 1
5016000	OTAVITE	-1.602	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-7.771	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-7.288	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-9.239	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-39.404	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-1.090	[1.000] 600 [1.000] 140
2060000	MASSICOT	-5.857	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-5.659	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-5.601	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-6.658	[-2.000] 330 [2.000] 600 [1.000] 2
			[1.000] 140
5060002	PB3O2CO3	-11.090	[-4.000] 330 [3.000] 600 [1.000]140
			[2.000] 2
2060003	PLATTNERITE	-0.774	[-4.000] 330 [-2.000] 1 [1.000]600
			[2.000] 2
3060000	PB2O3	-3.761	[-6.000] 330 [-2.000] 1 [2.000]600
			[3.000] 2
3060001	MINIUM	-11.028	[-8.000] 330 [-2.000] 1 [3.000]600
			[4.000] 2
2060004	PB(OH)2 (C)	-1.043	[-2.000] 330 [1.000] 600 [2.000] 2
5060003	HYDCERRUSITE	-3.789	[-2.000] 330 [3.000] 600 [2.000]140
			[2.000] 2
2060005	PB2O(OH)2	-11.442	[-4.000] 330 [2.000] 600 [3.000] 2
3006000	ARSENOLITE	-26.937	[4.000] 60 [-6.000] 2
3006001	CLAUDETITE	-26.694	[4.000] 60 [-6.000] 2
2015000	LIME	-22.509	[-2.000] 330 [1.000] 150 [1.000] 2
2015001	PORTLANDITE	-12.085	[-2.000] 330 [1.000] 150 [2.000] 2
2028000	WUSTITE	-2.963	[-2.000] 330 [0.947] 280 [1.000] 2
2046001	PERICLASE	-10.785	[-2.000] 330 [1.000] 460 [1.000] 2
3028001	HERCYNITE	0.550	[-8.000] 330 [1.000] 280 [2.000] 30
			[4.000] 2
3046000	SPINEL	-6.285	[-8.000] 330 [1.000] 460 [2.000] 30
			[4.000] 2
3021100	FECR2O4	8.713	[2.000] 211 [1.000] 280 [-4.000]330
3021101	MGCR2O4	-2.015	[2.000] 211 [1.000] 460 [-4.000]330
3021102	CR2O3	2.570	[2.000] 211 [-2.000] 330 [-1.000] 2
2021102	CR(OH)3 (A)	0.456	[1.000] 211 [1.000] 2 [-1.000]330
2021101	CR(OH)3 (C)	-2.133	[1.000] 211 [1.000] 2 [-1.000]330

PART 1 of OUTPUT FILE

Revuè river water-Site 9 - Run 2

Entered CO_3^{2-}, P_{CO2}, P_{O2}, fixed pH, Solids allowed to precipitate

Temperature (Celsius): 17.30
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.162E-08	-7.500	0.000E-01
30	Al+3	2.239E-06	-5.650	6.000E-02
60	H3AsO3	3.162E-08	-7.500	4.000E-03
100	Ba+2	1.230E-06	-5.910	1.700E-01
150	Ca+2	1.778E-04	-3.750	7.200E+00
160	Cd+2	2.818E-09	-8.550	3.200E-04
211	Cr(OH)2+	5.495E-08	-7.260	4.700E-03
280	Fe+2	8.913E-07	-6.050	5.000E-02
410	K+1	1.950E-05	-4.710	7.644E-01
460	Mg+2	3.090E-04	-3.510	7.600E+00
470	Mn+2	3.631E-06	-5.440	2.000E-01
500	Na+1	2.239E-04	-3.650	5.200E+00
600	Pb+2	1.288E-07	-6.890	2.700E-02
800	Sr+2	4.571E-07	-6.340	4.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	1.259E-06	-5.900	1.105E+01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 1.250E-03 Sum of ANIONS = 3.683E-04
PERCENT DIFFERENCE = 5.448E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	3.286E-08	3.162E-08	-7.50000	0.96223	0.017
30	Al+3	1.005E-15	7.106E-16	-15.14840	0.70715	0.150
60	H3AsO3	3.131E-08	3.132E-08	-7.50424	1.00028	0.000
100	Ba+2	1.238E-06	1.061E-06	-5.97422	0.85727	0.067
150	Ca+2	1.794E-04	1.538E-04	-3.81307	0.85727	0.067
160	Cd+2	2.688E-09	2.304E-09	-8.63745	0.85727	0.067
211	Cr(OH)2+	7.459E-13	7.178E-13	-12.14402	0.96223	0.017
280	Fe+2	8.637E-07	7.405E-07	-6.13050	0.85727	0.067
410	K+1	1.955E-05	1.881E-05	-4.72559	0.96223	0.017
460	Mg+2	3.121E-04	2.675E-04	-3.57265	0.85727	0.067
470	Mn+2	8.424E-09	7.222E-09	-8.14137	0.85727	0.067
500	Na+1	2.262E-04	2.176E-04	-3.66227	0.96223	0.017
600	Pb+2	2.793E-08	2.394E-08	-7.62088	0.85727	0.067
800	Sr+2	4.565E-07	3.914E-07	-6.40741	0.85727	0.067
140	CO3-2	2.364E-07	2.027E-07	-6.69321	0.85727	0.067

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	1.682E-12	1.683E-12	-11.77403	1.00028	-7.130
2113303	Cr(OH)4-	5.281E-16	5.081E-16	-15.29404	0.96223	-18.133
2113304	CrO2-	1.340E-15	1.289E-15	-14.88962	0.96223	-17.729
3300020	OH-	1.817E-07	1.749E-07	-6.75732	0.96223	-14.241
4603300	MgOH +	7.263E-09	6.988E-09	-8.15563	0.96223	-12.066
4601400	MgCO3 AQ	4.596E-08	4.597E-08	-7.33749	1.00028	2.928

4601401	MgHCO3 +	5.033E-07	4.843E-07	-6.31489	0.96223	11.468
1503300	CaOH +	6.656E-10	6.405E-10	-9.19351	0.96223	-12.864
1501400	CaHCO3 +	2.128E-07	2.048E-07	-6.68873	0.96223	11.334
1501401	CaCO3 AQ	3.797E-08	3.798E-08	-7.42040	1.00028	3.086
5001400	NaCO3 -	5.703E-10	5.487E-10	-9.26063	0.96223	1.112
5001401	NaHCO3 AQ	1.676E-08	1.677E-08	-7.77548	1.00028	10.080
303300	AlOH +2	1.575E-13	1.350E-13	-12.86961	0.85727	-5.154
303301	Al(OH)2 +	5.866E-11	5.644E-11	-10.24841	0.96223	-10.083
303302	Al(OH)4 -	1.028E-09	9.896E-10	-9.00456	0.96223	-23.839
303303	Al(OH)3 AQ	2.246E-09	2.247E-09	-8.64842	1.00028	-16.000
2803300	FeOH +	4.263E-09	4.102E-09	-8.38698	0.96223	-9.740
2803301	FeOH3 -1	6.272E-16	6.036E-16	-15.21928	0.96223	-31.572
2803302	FeOH2 AQ	5.550E-13	5.552E-13	-12.25556	1.00028	-21.125
8003300	SrOH +	4.463E-13	4.295E-13	-12.36708	0.96223	-13.443
1003300	BaOH +	7.784E-13	7.490E-13	-12.12554	0.96223	-13.635
4703300	MnOH +	3.203E-12	3.082E-12	-11.51116	0.96223	-10.853
4703301	Mn(OH)3 -1	3.761E-21	3.619E-21	-20.44139	0.96223	-34.783
4700020	MnO4 -	2.647E-11	2.547E-11	-10.59397	0.96223	-131.239
4700021	MnO4 -2	4.103E-15	3.517E-15	-14.45377	0.85727	-121.288
4701400	MnHCO3 +	1.915E-11	1.843E-11	-10.73457	0.96223	11.617
1601400	Cd(CO3)3-4	5.895E-23	3.184E-23	-22.49707	0.54009	6.488
1603300	CdOH +	3.505E-12	3.373E-12	-11.47201	0.96223	-10.318
1603301	Cd(OH)2 AQ	1.029E-14	1.029E-14	-13.98747	1.00028	-20.350
1603302	Cd(OH)3 -	3.795E-20	3.652E-20	-19.43747	0.96223	-33.283
1603303	Cd(OH)4 -2	1.201E-26	1.029E-26	-25.98748	0.85727	-47.283
1603304	Cd2OH +3	5.940E-20	4.201E-20	-19.37670	0.70715	-9.451
1601400	CdHCO3 +	3.855E-11	3.710E-11	-10.43066	0.96223	12.417
1601401	CdCO3 AQ	1.170E-10	1.170E-10	-9.93166	1.00028	5.399
6001400	Pb(CO3)2-2	5.007E-11	4.293E-11	-10.36729	0.85727	10.707
6003300	PbOH +	1.534E-08	1.476E-08	-7.83088	0.96223	-7.693
6003301	Pb(OH)2 AQ	1.815E-10	1.816E-10	-9.74089	1.00028	-17.120
6003302	Pb(OH)3 -	6.852E-14	6.593E-14	-13.18090	0.96223	-28.043
6003303	Pb2OH +3	1.119E-14	7.911E-15	-14.10176	0.70715	-6.210
6003304	Pb3(OH)4+2	6.446E-18	5.526E-18	-17.25759	0.85727	-24.328
6001401	PbCO3 AQ	8.429E-08	8.432E-08	-7.07408	1.00028	7.240
6003305	Pb(OH)4 -2	5.584E-18	4.787E-18	-17.31990	0.85727	-39.632
6001402	PbHCO3 +	2.527E-09	2.432E-09	-8.61408	0.96223	13.217
3300600	H2AsO3 -	4.540E-10	4.368E-10	-9.35970	0.96223	-9.339
3300601	HAsO3 -2	9.052E-15	7.760E-15	-14.11014	0.85727	-21.539
3300602	AsO3 -3	1.020E-20	7.216E-21	-20.14172	0.70715	-34.987
3300603	H4AsO3 +	5.099E-16	4.906E-16	-15.30924	0.96223	-0.288
3301400	HCO3 -	1.690E-04	1.626E-04	-3.78877	0.96223	10.421
3301401	H2CO3 AQ	1.075E-05	1.075E-05	-4.96854	1.00028	16.725
2113300	Cr+3	1.042E-17	7.368E-18	-17.13266	0.70715	10.162
2113301	Cr(OH)+2	1.104E-14	9.462E-15	-14.02401	0.85727	5.687

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-5.064E-06	-5.296	0.000	0.000
3300021	O2 (g)	-6.054E-07	-6.218	-85.043	133.830
330	H+1	-1.835E-04	-3.736	7.500	0.000
3301403	CO2 (g)	3.230E-06	-5.491	21.693	-0.530

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3021100	FECR2O4	2.732E-08	-7.563	0.419	24.860
2003002	DIASPORE	2.220E-06	-5.654	-7.352	24.630
3047000	HAUSMANNITE	1.211E-06	-5.917	-63.097	80.140

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

60	H3AsO3	3.176E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.238E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.796E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.847E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.441E-12	0.0	0.000E-01	0.0	5.464E-08	100.0
600	Pb+2	1.303E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	8.473E-09	0.2	0.000E-01	0.0	3.632E-06	99.8
30	Al+3	3.333E-09	0.1	0.000E-01	0.0	2.220E-06	99.9
1	E-1	-1.324E-10	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.809E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	8.680E-07	96.9	0.000E-01	0.0	2.732E-08	3.1
2	H2O	2.207E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.911E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 1.235E-03 Sum of ANIONS 1.697E-04
PERCENT DIFFERENCE = 7.583E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 1.196E-03
EQUILIBRIUM pH = 7.500
EQUILIBRIUM pe = 13.761 or Eh = 793.00 mv

PART 1 of OUTPUT FILE

Revuè river water-Site 9 - Run 3

Entered CO_3^{2-}, PCO2, PO2, fixed pH, solids allowed to precipitate
Fe redox pair, Mn redox pair

Temperature (Celsius): 17.30
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.162E-08	-7.500	0.000E-01
30	Al+3	2.239E-06	-5.650	6.000E-02
60	H3AsO3	3.162E-08	-7.500	4.000E-03
100	Ba+2	1.230E-06	-5.910	1.700E-01
150	Ca+2	1.778E-04	-3.750	7.200E+00
160	Cd+2	2.818E-09	-8.550	3.200E-04
211	Cr(OH)2+	5.495E-08	-7.260	4.700E-03
280	Fe+2	8.913E-07	-6.050	5.000E-02
410	K+1	1.950E-05	-4.710	7.644E-01
460	Mg+2	3.090E-04	-3.510	7.600E+00
470	Mn+2	3.631E-06	-5.440	2.000E-01
500	Na+1	2.239E-04	-3.650	5.200E+00
600	Pb+2	1.288E-07	-6.890	2.700E-02
800	Sr+2	4.571E-07	-6.340	4.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	1.259E-06	-5.900	1.105E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
471	Mn+3	1.820E-21	-20.740	0.000E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 1.250E-03 Sum of ANIONS = 3.683E-04
PERCENT DIFFERENCE = 5.448E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	3.286E-08	3.162E-08	-7.50000	0.96226	0.017
30	Al+3	1.005E-15	7.106E-16	-15.14839	0.70732	0.150
60	H3AsO3	3.131E-08	3.132E-08	-7.50424	1.00028	0.000
100	Ba+2	1.238E-06	1.061E-06	-5.97417	0.85736	0.067
150	Ca+2	1.794E-04	1.538E-04	-3.81303	0.85736	0.067
160	Cd+2	2.688E-09	2.305E-09	-8.63741	0.85736	0.067
211	Cr(OH)2+	8.663E-10	8.336E-10	-9.07905	0.96226	0.017
280	Fe+2	2.129E-25	1.825E-25	-24.73867	0.85736	0.067
410	K+1	1.955E-05	1.881E-05	-4.72557	0.96226	0.017
460	Mg+2	3.121E-04	2.675E-04	-3.57260	0.85736	0.067
470	Mn+2	9.549E-17	8.187E-17	-16.08688	0.85736	0.067
500	Na+1	2.262E-04	2.176E-04	-3.66226	0.96226	0.017
600	Pb+2	2.792E-08	2.394E-08	-7.62087	0.85736	0.067
800	Sr+2	4.565E-07	3.914E-07	-6.40737	0.85736	0.067
471	Mn+3	6.572E-28	4.649E-28	-27.33266	0.70732	0.150
140	CO3-2	2.364E-07	2.027E-07	-6.69321	0.85736	0.067
281	Fe+3	8.832E-25	6.247E-25	-24.20431	0.70732	0.150

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	1.954E-09	1.954E-09	-8.70906	1.00028	-7.130

2113303	Cr(OH)4-	6.133E-13	5.901E-13	-12.22907	0.96226	-18.133
2113304	CrO2-	1.556E-12	1.497E-12	-11.82465	0.96226	-17.729
3300020	OH-	1.817E-07	1.749E-07	-6.75732	0.96226	-14.241
4603300	MgOH +	7.263E-09	6.989E-09	-8.15559	0.96226	-12.066
4601400	MgCO3 AQ	4.597E-08	4.598E-08	-7.33744	1.00028	2.928
4601401	MgHCO3 +	5.033E-07	4.843E-07	-6.31485	0.96226	11.468
1503300	CaOH +	6.656E-10	6.405E-10	-9.19347	0.96226	-12.864
1501400	CaHCO3 +	2.128E-07	2.048E-07	-6.68868	0.96226	11.334
1501401	CaCO3 AQ	3.798E-08	3.799E-08	-7.42035	1.00028	3.086
5001400	NaCO3 -	5.703E-10	5.488E-10	-9.26062	0.96226	1.112
5001401	NaHCO3 AQ	1.677E-08	1.677E-08	-7.77547	1.00028	10.080
303300	AlOH +2	1.575E-13	1.350E-13	-12.86961	0.85736	-5.154
303301	Al(OH)2 +	5.865E-11	5.644E-11	-10.24841	0.96226	-10.083
303302	Al(OH)4 -	1.028E-09	9.895E-10	-9.00456	0.96226	-23.839
303303	Al(OH)3 AQ	2.246E-09	2.247E-09	-8.64842	1.00028	-16.000
2803300	FeOH +	1.051E-27	1.011E-27	-26.99515	0.96226	-9.740
2803301	FeOH3 -1	1.546E-34	1.488E-34	-33.82746	0.96226	-31.572
2803302	FeOH2 AQ	1.368E-31	1.369E-31	-30.86374	1.00028	-21.125
2813300	FeOH +2	9.342E-20	8.010E-20	-19.09638	0.85736	-2.325
2813301	FeOH2 +	1.388E-15	1.336E-15	-14.87433	0.96226	-5.653
2813302	FeOH3 AQ	4.961E-16	4.962E-16	-15.30433	1.00028	-13.600
2813303	FeOH4 -	1.631E-16	1.569E-16	-15.80434	0.96226	-21.583
2813304	Fe2(OH)2+4	4.430E-37	2.394E-37	-36.62096	0.54032	-2.945
2813305	Fe3(OH)4+5	1.686E-49	6.444E-50	-49.19083	0.38218	-6.160
8003300	SrOH +	4.464E-13	4.295E-13	-12.36703	0.96226	-13.443
1003300	BaOH +	7.784E-13	7.490E-13	-12.12549	0.96226	-13.635
4703300	MnOH +	3.631E-20	3.494E-20	-19.45668	0.96226	-10.853
4703301	Mn(OH)3 -1	4.264E-29	4.103E-29	-28.38690	0.96226	-34.783
4700020	MnO4 -	3.001E-19	2.887E-19	-18.53948	0.96226	-131.239
4700021	MnO4 -2	4.651E-23	3.988E-23	-22.39928	0.85736	-121.288
4701400	MnHCO3 +	2.171E-19	2.089E-19	-18.68009	0.96226	11.617
1601400	Cd(CO3)3-4	5.893E-23	3.184E-23	-22.49703	0.54032	6.487
1603300	CdOH +	3.505E-12	3.373E-12	-11.47197	0.96226	-10.318
1603301	Cd(OH)2 AQ	1.029E-14	1.029E-14	-13.98742	1.00028	-20.350
1603302	Cd(OH)3 -	3.796E-20	3.652E-20	-19.43743	0.96226	-33.283
1603303	Cd(OH)4 -2	1.201E-26	1.029E-26	-25.98744	0.85736	-47.283
1603304	Cd2OH +3	5.940E-20	4.201E-20	-19.37661	0.70732	-9.451
1601400	CdHCO3 +	3.856E-11	3.710E-11	-10.43062	0.96226	12.417
1601401	CdCO3 AQ	1.170E-10	1.171E-10	-9.93161	1.00028	5.399
6001400	Pb(CO3)2-2	5.007E-11	4.293E-11	-10.36728	0.85736	10.707
6003300	PbOH +	1.534E-08	1.476E-08	-7.83087	0.96226	-7.693
6003301	Pb(OH)2 AQ	1.816E-10	1.816E-10	-9.74088	1.00028	-17.120
6003302	Pb(OH)3 -	6.852E-14	6.593E-14	-13.18089	0.96226	-28.043
6003303	Pb2OH +3	1.119E-14	7.912E-15	-14.10174	0.70732	-6.210
6003304	Pb3(OH)4+2	6.446E-18	5.526E-18	-17.25755	0.85736	-24.328
6001401	PbCO3 AQ	8.430E-08	8.432E-08	-7.07407	1.00028	7.240
6003305	Pb(OH)4 -2	5.584E-18	4.787E-18	-17.31990	0.85736	-39.632
6001402	PbHCO3 +	2.527E-09	2.432E-09	-8.61407	0.96226	13.217
3300600	H2AsO3 -	4.539E-10	4.368E-10	-9.35970	0.96226	-9.339
3300601	HAsO3 -2	9.051E-15	7.760E-15	-14.11014	0.85736	-21.539
3300602	AsO3 -3	1.020E-20	7.216E-21	-20.14172	0.70732	-34.987
3300603	H4AsO3 +	5.099E-16	4.906E-16	-15.30924	0.96226	-0.288
3301400	HCO3 -	1.690E-04	1.626E-04	-3.78877	0.96226	10.421
3301401	H2CO3 AQ	1.075E-05	1.075E-05	-4.96854	1.00028	16.725
2113300	Cr+3	1.210E-14	8.557E-15	-14.06769	0.70732	10.162
2113301	Cr(OH)+2	1.282E-11	1.099E-11	-10.95904	0.85736	5.687

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-5.934E-06	-5.227	0.000	0.000
4704710	Mn+2/Mn+3	-3.641E-06	-5.439	25.006	25.760
330	H+1	-1.818E-04	-3.741	7.500	0.000
3301403	CO2 (g)	3.235E-06	-5.490	21.693	-0.530
3300021	O2 (g)	-2.044E-06	-5.689	-85.043	133.830
2802810	Fe+2/Fe+3	-8.953E-07	-6.048	13.226	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	4.477E-07	-6.349	3.409	30.845
2047000	PYROLUSITE	3.641E-06	-5.439	-16.428	29.180
2003002	DIASPORE	2.220E-06	-5.654	-7.352	24.630
3021102	CR2O3	2.591E-08	-7.587	3.158	12.125

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	3.176E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.238E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.796E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	2.847E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.303E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.835E-09	5.2	0.000E-01	0.0	5.181E-08	94.8
470	Mn+2	9.604E-17	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.333E-09	0.1	0.000E-01	0.0	2.220E-06	99.9
140	CO3-2	1.809E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
471	Mn+3	6.572E-28	0.0	0.000E-01	0.0	3.641E-06	100.0
280	Fe+2	2.139E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.047E-15	0.0	0.000E-01	0.0	8.953E-07	100.0
1	E-1	-1.501E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.911E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	2.183E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 1.233E-03 Sum of ANIONS 1.697E-04
PERCENT DIFFERENCE = 7.580E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 1.195E-03
EQUILIBRIUM pH = 7.500
EQUILIBRIUM pe = 13.761 or Eh = 793.00 mv

PART 1 of OUTPUT FILE

Revuè river water-Site 9 - Run 4

Entered CO_3^{2-}, P_{CO2}, P_{O2}, fixed pH, Fe redox pair, Mn redox pair, solids allowed to precipitate

Adsorption

Temperature (Celsius): 17.30
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.162E-08	-7.500	0.000E-01
30	Al+3	2.239E-06	-5.650	6.000E-02
60	H3AsO3	3.162E-08	-7.500	4.000E-03
100	Ba+2	1.230E-06	-5.910	1.700E-01
150	Ca+2	1.778E-04	-3.750	7.200E+00
160	Cd+2	2.818E-09	-8.550	3.200E-04
211	Cr(OH)2+	5.495E-08	-7.260	4.700E-03
280	Fe+2	8.913E-07	-6.050	5.000E-02
410	K+1	1.950E-05	-4.710	7.644E-01
460	Mg+2	3.090E-04	-3.510	7.600E+00
470	Mn+2	3.631E-06	-5.440	2.000E-01
500	Na+1	2.239E-04	-3.650	5.200E+00
600	Pb+2	1.288E-07	-6.890	2.700E-02
800	Sr+2	4.571E-07	-6.340	4.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	1.259E-06	-5.900	1.105E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
471	Mn+3	1.820E-21	-20.740	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E+00	0.890	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 1.250E-03 Sum of ANIONS = 3.683E-04
PERCENT DIFFERENCE = 5.448E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	3.280E-08	3.162E-08	-7.50000	0.96418	0.016
30	Al+3	9.867E-16	7.106E-16	-15.14839	0.72017	0.143
60	H3AsO3	2.057E-11	2.058E-11	-10.68666	1.00025	0.000
100	Ba+2	5.010E-07	4.330E-07	-6.36352	0.86425	0.063
150	Ca+2	1.173E-04	1.014E-04	-3.99402	0.86425	0.063
160	Cd+2	1.521E-12	1.315E-12	-11.88112	0.86425	0.063
211	Cr(OH)2+	8.645E-10	8.336E-10	-9.07905	0.96418	0.016
280	Fe+2	2.112E-25	1.825E-25	-24.73867	0.86425	0.063
410	K+1	1.955E-05	1.885E-05	-4.72470	0.96418	0.016
460	Mg+2	3.121E-04	2.697E-04	-3.56913	0.86425	0.063
470	Mn+2	9.473E-17	8.187E-17	-16.08688	0.86425	0.063
500	Na+1	2.262E-04	2.181E-04	-3.66139	0.96418	0.016
600	Pb+2	3.745E-15	3.237E-15	-14.48986	0.86425	0.063
800	Sr+2	4.565E-07	3.946E-07	-6.40388	0.86425	0.063
811	ADS1TYP1	1.040E-04	1.040E-04	-3.98289	1.00000	0.000
140	CO3-2	2.345E-07	2.027E-07	-6.69321	0.86425	0.063

281	Fe+3	8.675E-25	6.247E-25	-24.20431	0.72017	0.143
471	Mn+3	6.455E-28	4.649E-28	-27.33266	0.72017	0.143
812	ADS1TYP2	5.898E-03	5.898E-03	-2.22933	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8120600	=S2H2AsO3(o)	3.119E-08	3.119E-08	-7.50598	1.00000	5.410
2113302	Cr(OH)3 AQ	1.954E-09	1.954E-09	-8.70906	1.00025	-7.130
2113303	Cr(OH)4-	6.120E-13	5.901E-13	-12.22907	0.96418	-18.134
2113304	CrO2-	1.553E-12	1.497E-12	-11.82465	0.96418	-17.730
3300020	OH-	1.814E-07	1.749E-07	-6.75732	0.96418	-14.241
4603300	MgOH +	7.307E-09	7.045E-09	-8.15211	0.96418	-12.067
4601400	MgCO3 AQ	4.634E-08	4.635E-08	-7.33396	1.00025	2.928
4601401	MgHCO3 +	5.064E-07	4.882E-07	-6.31137	0.96418	11.467
1503300	CaOH +	4.379E-10	4.222E-10	-9.37446	0.96418	-12.865
1501400	CaHCO3 +	1.400E-07	1.350E-07	-6.86967	0.96418	11.333
1501401	CaCO3 AQ	2.504E-08	2.504E-08	-7.60134	1.00025	3.086
5001400	NaCO3 -	5.703E-10	5.499E-10	-9.25975	0.96418	1.111
5001401	NaHCO3 AQ	1.680E-08	1.680E-08	-7.77460	1.00025	10.080
303300	AlOH +2	1.562E-13	1.350E-13	-12.86961	0.86425	-5.158
303301	Al(OH)2 +	5.854E-11	5.644E-11	-10.24841	0.96418	-10.084
303302	Al(OH)4 -	1.026E-09	9.895E-10	-9.00456	0.96418	-23.840
303303	Al(OH)3 AQ	2.246E-09	2.247E-09	-8.64842	1.00025	-16.000
2803300	FeOH +	1.049E-27	1.011E-27	-26.99515	0.96418	-9.741
2803301	FeOH3 -1	1.543E-34	1.488E-34	-33.82746	0.96418	-31.573
2803302	FeOH2 AQ	1.368E-31	1.369E-31	-30.86374	1.00025	-21.125
2813300	FeOH +2	9.268E-20	8.010E-20	-19.09638	0.86425	-2.329
2813301	FeOH2 +	1.385E-15	1.336E-15	-14.87433	0.96418	-5.654
2813302	FeOH3 AQ	4.961E-16	4.962E-16	-15.30433	1.00025	-13.600
2813303	FeOH4 -	1.627E-16	1.569E-16	-15.80434	0.96418	-21.584
2813304	Fe2(OH)2+4	4.290E-37	2.394E-37	-36.62096	0.55790	-2.959
2813305	Fe3(OH)4+5	1.604E-49	6.444E-50	-49.19083	0.40178	-6.182
8003300	SrOH +	4.490E-13	4.330E-13	-12.36355	0.96418	-13.444
1003300	BaOH +	3.170E-13	3.056E-13	-12.51484	0.96418	-13.635
4703300	MnOH +	3.624E-20	3.494E-20	-19.45668	0.96418	-10.854
4703301	Mn(OH)3 -1	4.255E-29	4.103E-29	-28.38690	0.96418	-34.784
4700020	MnO4 -	2.995E-19	2.887E-19	-18.53948	0.96418	-131.240
4700021	MnO4 -2	4.614E-23	3.988E-23	-22.39928	0.86425	-121.292
4701400	MnHCO3 +	2.166E-19	2.089E-19	-18.68008	0.96418	11.616
1601400	Cd(CO3)3-4	3.256E-26	1.817E-26	-25.74074	0.55790	6.473
1603300	CdOH +	1.996E-15	1.925E-15	-14.71568	0.96418	-10.319
1603301	Cd(OH)2 AQ	5.872E-18	5.873E-18	-17.23114	1.00025	-20.350
1603302	Cd(OH)3 -	2.161E-23	2.084E-23	-22.68115	0.96418	-33.284
1603303	Cd(OH)4 -2	6.795E-30	5.873E-30	-29.23115	0.86425	-47.287
1603304	Cd2OH +3	1.899E-26	1.368E-26	-25.86404	0.72017	-9.459
1601400	CdHCO3 +	2.195E-14	2.117E-14	-13.67433	0.96418	12.416
1601401	CdCO3 AQ	6.677E-14	6.678E-14	-13.17533	1.00025	5.399
6001400	Pb(CO3)2-2	6.716E-18	5.804E-18	-17.23627	0.86425	10.703
6003300	PbOH +	2.070E-15	1.996E-15	-14.69987	0.96418	-7.694
6003301	Pb(OH)2 AQ	2.455E-17	2.455E-17	-16.60987	1.00025	-17.120
6003302	Pb(OH)3 -	9.246E-21	8.915E-21	-20.04988	0.96418	-28.044
6003303	Pb2OH +3	2.008E-28	1.446E-28	-27.83972	0.72017	-6.217
6003304	Pb3(OH)4+2	1.581E-38	1.366E-38	-37.86453	0.86425	-24.332
6001401	PbCO3 AQ	1.140E-14	1.140E-14	-13.94306	1.00025	7.240
6003305	Pb(OH)4 -2	7.490E-25	6.473E-25	-24.18889	0.86425	-39.636
6001402	PbHCO3 +	3.410E-16	3.288E-16	-15.48307	0.96418	13.216
3300600	H2AsO3 -	2.977E-13	2.870E-13	-12.54213	0.96418	-9.340
3300601	HAsO3 -2	5.899E-18	5.098E-18	-17.29256	0.86425	-21.543
3300602	AsO3 -3	6.583E-24	4.741E-24	-23.32414	0.72017	-34.995
3300603	H4AsO3 +	3.343E-19	3.224E-19	-18.49166	0.96418	-0.289
3301400	HCO3 -	1.687E-04	1.626E-04	-3.78877	0.96418	10.420
3301401	H2CO3 AQ	1.075E-05	1.075E-05	-4.96854	1.00025	16.725
2113300	Cr+3	1.188E-14	8.557E-15	-14.06769	0.72017	10.154
2113301	Cr(OH)+2	1.272E-11	1.099E-11	-10.95904	0.86425	5.683
8123301	=SO2-	9.202E-04	9.202E-04	-3.03614	1.00000	-8.930
8123302	=SO2H2+	8.659E-04	8.659E-04	-3.06252	1.00000	7.290
8113301	=SO1-	1.623E-05	1.623E-05	-4.78970	1.00000	-8.930
8113302	=SO1H2+	1.527E-05	1.527E-05	-4.81608	1.00000	7.290

8121600	=SO2Cd+	7.351E-11	7.351E-11	-10.13365	1.00000	-2.900
8111600	=SO1Cd+	2.772E-09	2.772E-09	-8.55721	1.00000	0.430
8116000	=SO1Pb+	1.300E-07	1.300E-07	-6.88595	1.00000	4.710
8126000	=SO2Pb+	2.868E-10	2.868E-10	-9.54239	1.00000	0.300
8121500	=SO2Ca+	6.360E-06	6.360E-06	-5.19654	1.00000	-5.850
8111500	=SO1HCa++	5.581E-05	5.581E-05	-4.25329	1.00000	4.970
8111000	=SO1HBa++	7.366E-07	7.366E-07	-6.13279	1.00000	5.460
8121000	=SO2Ba+	2.889E-10	2.889E-10	-9.53923	1.00000	-7.200
8110600	=S1H2AsO3(o)	5.501E-10	5.501E-10	-9.25954	1.00000	5.410

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-5.511E-06	-5.259	0.000	0.000
3300021	O2 (g)	-2.044E-06	-5.689	-85.043	133.830
2802810	Fe+2/Fe+3	-8.953E-07	-6.048	13.226	-10.000
4704710	Mn+2/Mn+3	-3.641E-06	-5.439	25.006	25.760
330	H+1	-1.207E-04	-3.918	7.500	0.000
3301403	CO2 (g)	3.744E-06	-5.427	21.693	-0.530

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	4.477E-07	-6.349	3.409	30.845
2047000	PYROLUSITE	3.641E-06	-5.439	-16.428	29.180
2003002	DIASPORE	2.220E-06	-5.654	-7.352	24.630
3021102	CR2O3	2.591E-08	-7.587	3.158	12.125

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
800	Sr+2	4.565E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
60	H3AsO3	2.087E-11	0.1	3.174E-08	99.9	0.000E-01	0.0
100	Ba+2	5.010E-07	40.5	7.368E-07	59.5	0.000E-01	0.0
150	Ca+2	1.175E-04	65.4	6.217E-05	34.6	0.000E-01	0.0
160	Cd+2	1.612E-12	0.1	2.845E-09	99.9	0.000E-01	0.0
600	Pb+2	1.759E-14	0.0	1.303E-07	100.0	0.000E-01	0.0
410	K+1	1.955E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.126E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.833E-09	5.2	0.000E-01	0.0	5.181E-08	94.8
1	E-1	-1.498E-18	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.122E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
470	Mn+2	9.528E-17	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.331E-09	0.1	0.000E-01	0.0	2.220E-06	99.9
140	CO3-2	1.804E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	2.044E-15	0.0	0.000E-01	0.0	8.953E-07	100.0
471	Mn+3	6.455E-28	0.0	0.000E-01	0.0	3.641E-06	100.0
330	H+1	1.907E-04	147.8	-6.168E-05	-47.8	0.000E-01	0.0
2	H2O	2.020E-07	66.6	1.014E-07	33.4	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 2.108E-03 Sum of ANIONS 1.106E-03
PERCENT DIFFERENCE = 3.118E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 1.069E-03
EQUILIBRIUM pH = 7.500
EQUILIBRIUM pe = 13.761 or Eh = 793.00 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
**** Parameters For Adsorbent Number 1 ****
Electrostatic Variables: psi0 = 0.035914 sig0 = 0.003009
psib = 0.000000 sigb = 0.000000
psid = 0.000000 sigd = 0.000000
Adsorbent Concentration (g/l): 3.442
Specific Surface Area (sq. meters/g): 600.00

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.554	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-2.418	[1.000] 150 [1.000] 140
5046000	ARTINITE	-8.990	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.773	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-5.863	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-2.254	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-4.111	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.595	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.369	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.861	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.277	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.486	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-12.007	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-21.867	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.795	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-2.353	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.865	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.399	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-4.754	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.985	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.860	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.195	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.465	[1.000] 100 [1.000] 140
2047000	PYROLUSITE	0.000	[-4.000] 330 [-1.000] 1 [1.000] 471 [2.000] 2
2047001	BIRNESSITE	-1.663	[-4.000] 330 [-1.000] 1 [1.000] 471 [2.000] 2
2047002	NSUTITE	-1.076	[-4.000] 330 [-1.000] 1 [1.000] 471 [2.000] 2
3047100	BIXBYITE	-9.351	[-6.000] 330 [2.000] 471 [3.000] 2
3047000	HAUSMANNITE	-23.837	[-8.000] 330 [-2.000] 1 [3.000] 470 [4.000] 2
2047003	PYROCROITE	-16.614	[-2.000] 330 [1.000] 470 [2.000] 2
2047100	MANGANITE	-4.595	[-3.000] 330 [1.000] 471 [2.000] 2
5047000	RHODOCHROSIT	-12.410	[1.000] 470 [1.000] 140
16000	CD METAL	-53.242	[1.000] 160 [2.000] 1
16001	GAMMA CD	-53.345	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.846	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-11.015	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-10.531	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-12.482	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-46.273	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-7.959	[1.000] 600 [1.000] 140
2060000	MASSICOT	-12.726	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-12.528	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-12.470	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-20.396	[-2.000] 330 [2.000] 600 [1.000] 2 [1.000] 140
5060002	PB3O2CO3	-31.696	[-4.000] 330 [3.000] 600 [1.000] 140 [2.000] 2
2060003	PLATTNERITE	-7.643	[-4.000] 330 [-2.000] 1 [1.000] 600 [2.000] 2
3060000	PB2O3	-17.498	[-6.000] 330 [-2.000] 1 [2.000] 600 [3.000] 2
3060001	MINIUM	-31.635	[-8.000] 330 [-2.000] 1 [3.000] 600 [4.000] 2
2060004	PB(OH)2 (C)	-7.912	[-2.000] 330 [1.000] 600 [2.000] 2
5060003	HYDCERRUSITE	-24.396	[-2.000] 330 [3.000] 600 [2.000] 140 [2.000] 2

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2060005 PB2O(OH)2      -25.180    [ -4.000] 330  [  2.000] 600  [  3.000]   2
 3006000 ARSENOLITE     -39.667    [  4.000]  60  [ -6.000]   2
3006001 CLAUDETITE     -39.423    [  4.000]  60  [ -6.000]   2
2015000 LIME           -22.690    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE    -12.265    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE        -20.597    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE      -10.781    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE      -23.720    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                  [  4.000]   2
3046000 SPINEL         -11.930    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                  [  4.000]   2
3046001 MAG-FERRITE    -10.038    [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                  [  4.000]   2
3028102 LEPIDOCROCIT    -3.075    [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021100 FECR2O4        -12.478    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4         -4.581    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3            0.000    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)     -0.829    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)     -3.418    [  1.000] 211  [  1.000]   2  [ -1.000] 330
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3 - Modelling of water quality of Site 14

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - Initial run

Entered Alkalinity, PCO_2, PO_2, fixed pH, solids not allowed to precipitate

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
140	CO3-2	6.761E-21	-20.170	1.930E+01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 6.433E-04
PERCENT DIFFERENCE = 1.349E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.593E-08	2.512E-08	-7.60000	0.96880	0.014
140	CO3-2	3.669E-07	3.232E-07	-6.49048	0.88091	0.055
30	Al+3	5.117E-13	3.847E-13	-12.41485	0.75180	0.124
100	Ba+2	1.383E-06	1.219E-06	-5.91409	0.88091	0.055
150	Ca+2	1.295E-04	1.141E-04	-3.94281	0.88091	0.055
160	Cd+2	4.319E-09	3.804E-09	-8.41970	0.88091	0.055
211	Cr(OH)2+	7.203E-09	6.978E-09	-8.15626	0.96880	0.014
231	Cu+2	9.796E-09	8.629E-09	-8.06402	0.88091	0.055
280	Fe+2	5.332E-07	4.697E-07	-6.32814	0.88091	0.055
410	K+1	6.647E-05	6.440E-05	-4.19114	0.96880	0.014
460	Mg+2	1.436E-04	1.265E-04	-3.89780	0.88091	0.055
500	Na+1	2.088E-04	2.023E-04	-3.69409	0.96880	0.014
540	Ni+2	5.973E-09	5.261E-09	-8.27889	0.88091	0.055
600	Pb+2	2.632E-08	2.319E-08	-7.63479	0.88091	0.055
800	Sr+2	5.707E-07	5.027E-07	-6.29868	0.88091	0.055
950	Zn+2	2.734E-07	2.409E-07	-6.61821	0.88091	0.055

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	2.059E-08	2.059E-08	-7.68627	1.00018	-7.130
2113303	Cr(OH)4-	8.082E-12	7.829E-12	-11.10627	0.96880	-18.136

2113304	CrO2-	2.051E-11	1.987E-11	-10.70186	0.96880	-17.732
3300020	OH-	2.661E-07	2.578E-07	-6.58865	0.96880	-14.175
4603300	MgOH +	5.151E-09	4.991E-09	-8.30184	0.96880	-11.990
4601400	MgCO3 AQ	3.576E-08	3.576E-08	-7.44657	1.00018	2.942
4601401	MgHCO3 +	2.887E-07	2.796E-07	-6.55339	0.96880	11.449
1503300	CaOH +	7.333E-10	7.105E-10	-9.14846	0.96880	-12.792
1501400	CaHCO3 +	2.013E-07	1.950E-07	-6.70989	0.96880	11.337
1501401	CaCO3 AQ	4.656E-08	4.657E-08	-7.33193	1.00018	3.101
5001400	NaCO3 -	9.330E-10	9.039E-10	-9.04387	0.96880	1.154
5001401	NaHCO3 AQ	1.974E-08	1.974E-08	-7.70457	1.00018	10.080
303300	AlOH +2	1.203E-10	1.060E-10	-9.97485	0.88091	-5.105
303301	Al(OH)2 +	4.999E-08	4.843E-08	-7.31487	0.96880	-10.086
303302	Al(OH)4 -	2.341E-06	2.268E-06	-5.64431	0.96880	-23.616
303303	Al(OH)3 AQ	2.427E-06	2.427E-06	-5.61487	1.00018	-16.000
2803300	FeOH +	3.954E-09	3.831E-09	-8.41670	0.96880	-9.675
2803301	FeOH3 -1	1.129E-15	1.094E-15	-14.96102	0.96880	-31.419
2803302	FeOH2 AQ	7.829E-13	7.830E-13	-12.10622	1.00018	-20.978
8003300	SrOH +	8.511E-13	8.246E-13	-12.08376	0.96880	-13.371
1003300	BaOH +	1.337E-12	1.295E-12	-11.88775	0.96880	-13.560
2311400	CuCO3 AQ	1.498E-08	1.498E-08	-7.82449	1.00018	6.730
2311401	Cu(CO3)2-2	6.920E-12	6.096E-12	-11.21497	0.88091	9.885
2313300	CuOH +	3.546E-09	3.435E-09	-8.46402	0.96880	-7.986
2313301	Cu(OH)2 AQ	2.857E-07	2.857E-07	-6.54403	1.00018	-13.680
2313302	Cu(OH)3 -	7.091E-13	6.870E-13	-12.16304	0.96880	-26.885
2313303	Cu(OH)4 -2	6.181E-18	5.444E-18	-17.26404	0.88091	-39.545
2313304	Cu2(OH)2+2	3.296E-12	2.903E-12	-11.53711	0.88091	-10.554
2311402	CuHCO3 +	7.232E-10	7.007E-10	-9.15449	0.96880	13.014
9503300	ZnOH +	6.984E-09	6.767E-09	-8.16963	0.96880	-9.138
9503301	Zn(OH)2 AQ	4.816E-09	4.817E-09	-8.31722	1.00018	-16.899
9503302	Zn(OH)3 -	6.259E-13	6.064E-13	-12.21723	0.96880	-28.385
9503303	Zn(OH)4 -2	4.343E-18	3.826E-18	-17.41724	0.88091	-41.144
9501400	ZnHCO3 +	5.071E-09	4.913E-09	-8.30869	0.96880	12.414
9501401	ZnCO3 AQ	1.553E-08	1.554E-08	-7.80869	1.00018	5.300
9501402	Zn(CO3)2-2	1.219E-10	1.074E-10	-9.96917	0.88091	9.685
1601400	Cd(CO3)3-4	3.541E-22	2.132E-22	-21.67114	0.60219	6.440
1603300	CdOH +	8.451E-12	8.187E-12	-11.08685	0.96880	-10.253
1603301	Cd(OH)2 AQ	2.693E-14	2.693E-14	-13.56972	1.00018	-20.350
1603302	Cd(OH)3 -	1.242E-19	1.203E-19	-18.91972	0.96880	-33.286
1603303	Cd(OH)4 -2	4.845E-26	4.268E-26	-25.36973	0.88091	-47.295
1603304	Cd2OH +3	2.182E-19	1.640E-19	-18.78512	0.75180	-9.422
1601400	CdHCO3 +	8.009E-11	7.759E-11	-10.11018	0.96880	12.414
1601401	CdCO3 AQ	3.081E-10	3.082E-10	-9.51118	1.00018	5.399
6001400	Pb(CO3)2-2	1.200E-10	1.057E-10	-9.97575	0.88091	10.695
6003300	PbOH +	1.858E-08	1.800E-08	-7.74480	0.96880	-7.696
6003301	Pb(OH)2 AQ	2.787E-10	2.787E-10	-9.55480	1.00018	-17.120
6003302	Pb(OH)3 -	1.315E-13	1.274E-13	-12.89481	0.96880	-28.046
6003303	Pb2OH +3	1.243E-14	9.341E-15	-14.02959	0.75180	-6.236
6003304	Pb3(OH)4+2	1.959E-17	1.726E-17	-16.76297	0.88091	-24.204
6001401	PbCO3 AQ	1.302E-07	1.302E-07	-6.88527	1.00018	7.240
6003305	Pb(OH)4 -2	1.322E-17	1.165E-17	-16.93382	0.88091	-39.644
6001402	PbHCO3 +	3.080E-09	2.984E-09	-8.52527	0.96880	13.214
5403300	NiOH +	1.984E-11	1.922E-11	-10.71633	0.96880	-10.024
5403301	Ni(OH)2 AQ	8.337E-13	8.339E-13	-12.07890	1.00018	-19.000
5403302	Ni(OH)3 -	3.427E-16	3.320E-16	-15.47891	0.96880	-29.986
5401400	NiHCO3 +	1.301E-10	1.261E-10	-9.89937	0.96880	12.484
5401401	NiCO3 AQ	1.261E-08	1.261E-08	-7.89937	1.00018	6.870
5401402	Ni(CO3)2-2	8.039E-12	7.082E-12	-11.14985	0.88091	10.165
3301400	HCO3 -	2.028E-04	1.964E-04	-3.70680	0.96880	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00018	16.713
2113300	Cr+3	4.736E-14	3.560E-14	-13.44853	0.75180	10.032
2113301	Cr(OH)+2	8.295E-11	7.307E-11	-10.13625	0.88091	5.675

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	8.954E-05	-4.048	0.000	0.000
3300021	O2 (g)	1.656E-04	-3.781	-84.354	133.830
330	H+1	-4.211E-04	-3.376	7.600	0.000
3301403	CO2 (g)	4.385E-04	-3.358	21.690	-0.530

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
1	E-1	3.247E-14	-13.489	0.000	0.000
3301404	CH4 (g)	0.000E-01	-149.427	40.971	-61.000

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Sr+2	100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
Zn+2	89.4	PERCENT BOUND IN SPECIES #	950	Zn+2
	2.3	PERCENT BOUND IN SPECIES #	9503300	ZnOH +
	1.6	PERCENT BOUND IN SPECIES #	9503301	Zn(OH)2 AQ
	1.7	PERCENT BOUND IN SPECIES #	9501400	ZnHCO3 +
	5.1	PERCENT BOUND IN SPECIES #	9501401	ZnCO3 AQ
Al+3	1.0	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
	48.6	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
	50.4	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
Ba+2	100.0	PERCENT BOUND IN SPECIES #	100	Ba+2
Ca+2	99.8	PERCENT BOUND IN SPECIES #	150	Ca+2
Cd+2	91.6	PERCENT BOUND IN SPECIES #	160	Cd+2
	1.7	PERCENT BOUND IN SPECIES #	1601400	CdHCO3 +
	6.5	PERCENT BOUND IN SPECIES #	1601401	CdCO3 AQ
Cr(OH)2+	25.8	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
	73.8	PERCENT BOUND IN SPECIES #	2113302	Cr(OH)3 AQ
Cu+2	3.1	PERCENT BOUND IN SPECIES #	231	Cu+2
	4.8	PERCENT BOUND IN SPECIES #	2311400	CuCO3 AQ
	1.1	PERCENT BOUND IN SPECIES #	2313300	CuOH +
	90.8	PERCENT BOUND IN SPECIES #	2313301	Cu(OH)2 AQ
Fe+2	99.3	PERCENT BOUND IN SPECIES #	280	Fe+2
K+1	100.0	PERCENT BOUND IN SPECIES #	410	K+1
Mg+2	99.8	PERCENT BOUND IN SPECIES #	460	Mg+2
Na+1	100.0	PERCENT BOUND IN SPECIES #	500	Na+1
Ni+2	31.9	PERCENT BOUND IN SPECIES #	540	Ni+2
	67.3	PERCENT BOUND IN SPECIES #	5401401	NiCO3 AQ
Pb+2	14.7	PERCENT BOUND IN SPECIES #	600	Pb+2
	10.4	PERCENT BOUND IN SPECIES #	6003300	PbOH +
	72.9	PERCENT BOUND IN SPECIES #	6001401	PbCO3 AQ
	1.7	PERCENT BOUND IN SPECIES #	6001402	PbHCO3 +
E-1				
CO3-2	94.6	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
	4.9	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ
H+1	98.1	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
	10.2	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ
H2O	1.5	PERCENT BOUND IN SPECIES #	3300020	OH-
	53.1	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
	41.2	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
	3.2	PERCENT BOUND IN SPECIES #	2313301	Cu(OH)2 AQ

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	3.060E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	4.818E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.383E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.297E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	4.715E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.790E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
231	Cu+2	3.147E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	5.372E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.874E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.786E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	2.144E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	2.067E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	1.765E-05	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 8.277E-04 Sum of ANIONS 2.061E-04
PERCENT DIFFERENCE = 6.013E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
NON-CARBONATE ALKALINITY = 2.409E-07
EQUILIBRIUM IONIC STRENGTH (m) = 7.932E-04
EQUILIBRIUM pH = 7.600
EQUILIBRIUM pe = 13.489 or Eh = 782.67 mv

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-0.381	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-2.148	[1.000] 150 [1.000] 140
5046000	ARTINITE	-9.097	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	1.405	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-5.859	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-1.991	[1.000] 150 [1.000] 140
2003002	DIASPORE	3.160	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-3.940	[1.000] 150 [1.000] 460 [2.000] 140
2003003	GIBBSITE (C)	1.289	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-2.210	[2.000] 30 [3.000] 2 [-6.000] 330
5015003	HUNTITE	-11.998	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-22.231	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
5046002	MAGNESITE	-2.447	[1.000] 460 [1.000] 140
3050000	NATRON	-12.343	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-4.850	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-2.345	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.549	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.044	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-3.814	[1.000] 100 [1.000] 140
5023100	CUCO3	-4.924	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-1.722	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-0.702	[-2.000] 330 [1.000] 231 [1.000] 2
95000	ZN METAL	-59.878	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-3.171	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-2.849	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-3.868	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-3.618	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-3.168	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-3.128	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-2.918	[-2.000] 330 [1.000] 950 [2.000] 2

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2095005 ZNO(ACTIVE)     -2.728    [ -2.000] 330  [  1.000] 950  [  1.000]   2
2095006 ZINCITE         -2.871    [ -2.000] 330  [  1.000] 950  [  1.000]   2
  16000 CD METAL       -49.144    [  1.000] 160  [  2.000]   1
  16001 GAMMA CD       -49.246    [  1.000] 160  [  2.000]   1
5016000 OTAVITE         -1.178    [  1.000] 160  [  1.000] 140
2016000 CD(OH)2 (A)     -7.246    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)     -6.870    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE     -8.693    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL       -38.876    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE       -0.926    [  1.000] 600  [  1.000] 140
2060000 MASSICOT        -5.585    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE        -5.389    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O      -5.415    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3         -6.224    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                  [  1.000] 140
5060002 PB3O2CO3       -10.392    [ -4.000] 330  [  3.000] 600  [  1.000] 140
                                  [  2.000]   2
2060003 PLATTNERITE     -0.568    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                  [  2.000]   2
3060000 PB2O3           -3.733    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                  [  3.000]   2
3060001 MINIUM         -10.285    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                  [  4.000]   2
2060004 PB(OH)2 (C)     -0.785    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE    -3.225    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                  [  2.000]   2
2060005 PB2O(OH)2      -11.070    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3           -8.071    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2         -3.444    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE       -5.871    [ -2.000] 330  [  1.000] 540  [  1.000]   2
5023101 MALACHITE       -2.462    [  2.000] 231  [  2.000]   2  [  1.000] 140
                                  [ -2.000] 330
5023102 AZURITE         -5.393    [  3.000] 231  [  2.000]   2  [  2.000] 140
                                  [ -2.000] 330
2015000 LIME           -22.201    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE    -11.856    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE         -2.835    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE      -10.724    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE        1.361    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                  [  4.000]   2
3046000 SPINEL          -5.533    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                  [  4.000]   2
3021100 FECR2O4          8.306    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4         -2.459    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3            2.108    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)      0.194    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)     -2.358    [  1.000] 211  [  1.000]   2  [ -1.000] 330
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PART 1 of OUTPUT FILE

Revuè river water-Site 14 - Run 2

Entered CO_3^{2-}, P_{CO2}, P_{O2}, fixed pH, Solids allowed to precipitate

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	1.905E-06	-5.720	1.310E+01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.593E-08	2.512E-08	-7.60000	0.96882	0.014
30	Al+3	3.537E-16	2.660E-16	-15.57513	0.75196	0.124
100	Ba+2	1.383E-06	1.219E-06	-5.91406	0.88100	0.055
150	Ca+2	1.295E-04	1.141E-04	-3.94277	0.88100	0.055
160	Cd+2	4.319E-09	3.805E-09	-8.41967	0.88100	0.055
211	Cr(OH)2+	5.132E-13	4.972E-13	-12.30346	0.96882	0.014
231	Cu+2	9.795E-09	8.629E-09	-8.06402	0.88100	0.055
280	Fe+2	5.194E-07	4.576E-07	-6.33953	0.88100	0.055
410	K+1	6.647E-05	6.440E-05	-4.19114	0.96882	0.014
460	Mg+2	1.436E-04	1.265E-04	-3.89776	0.88100	0.055
500	Na+1	2.088E-04	2.023E-04	-3.69408	0.96882	0.014
540	Ni+2	5.972E-09	5.262E-09	-8.27888	0.88100	0.055
600	Pb+2	2.632E-08	2.319E-08	-7.63479	0.88100	0.055
800	Sr+2	5.707E-07	5.028E-07	-6.29865	0.88100	0.055
950	Zn+2	2.734E-07	2.409E-07	-6.61818	0.88100	0.055
140	CO3-2	3.669E-07	3.232E-07	-6.49048	0.88100	0.055

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	1.467E-12	1.467E-12	-11.83347	1.00018	-7.130
2113303	Cr(OH)4-	5.758E-16	5.579E-16	-15.25347	0.96882	-18.136
2113304	CrO2-	1.461E-15	1.416E-15	-14.84906	0.96882	-17.732
3300020	OH-	2.661E-07	2.578E-07	-6.58865	0.96882	-14.175

4603300	MgOH +	5.152E-09	4.991E-09	-8.30180	0.96882	-11.990
4601400	MgCO3 AQ	3.576E-08	3.577E-08	-7.44653	1.00018	2.942
4601401	MgHCO3 +	2.887E-07	2.797E-07	-6.55335	0.96882	11.449
1503300	CaOH +	7.334E-10	7.105E-10	-9.14842	0.96882	-12.792
1501400	CaHCO3 +	2.013E-07	1.951E-07	-6.70985	0.96882	11.337
1501401	CaCO3 AQ	4.656E-08	4.657E-08	-7.33189	1.00018	3.101
5001400	NaCO3 -	9.330E-10	9.039E-10	-9.04386	0.96882	1.154
5001401	NaHCO3 AQ	1.974E-08	1.974E-08	-7.70456	1.00018	10.080
303300	AlOH +2	8.316E-14	7.326E-14	-13.13512	0.88100	-5.105
303301	Al(OH)2 +	3.456E-11	3.349E-11	-10.47514	0.96882	-10.086
303302	Al(OH)4 -	1.619E-09	1.568E-09	-8.80458	0.96882	-23.616
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00018	-16.000
2803300	FeOH +	3.852E-09	3.732E-09	-8.42809	0.96882	-9.675
2803301	FeOH3 -1	1.100E-15	1.066E-15	-14.97240	0.96882	-31.419
2803302	FeOH2 AQ	7.626E-13	7.628E-13	-12.11761	1.00018	-20.978
8003300	SrOH +	8.512E-13	8.247E-13	-12.08372	0.96882	-13.371
1003300	BaOH +	1.337E-12	1.295E-12	-11.88771	0.96882	-13.560
2311400	CuCO3 AQ	1.498E-08	1.498E-08	-7.82450	1.00018	6.730
2311401	Cu(CO3)2-2	6.919E-12	6.096E-12	-11.21497	0.88100	9.885
2313300	CuOH +	3.546E-09	3.435E-09	-8.46403	0.96882	-7.986
2313301	Cu(OH)2 AQ	2.857E-07	2.857E-07	-6.54403	1.00018	-13.680
2313302	Cu(OH)3 -	7.091E-13	6.870E-13	-12.16304	0.96882	-26.885
2313303	Cu(OH)4 -2	6.180E-18	5.444E-18	-17.26404	0.88100	-39.545
2313304	Cu2(OH)2+2	3.295E-12	2.903E-12	-11.53712	0.88100	-10.554
2311402	CuHCO3 +	7.232E-10	7.007E-10	-9.15450	0.96882	13.014
9503300	ZnOH +	6.985E-09	6.767E-09	-8.16960	0.96882	-9.138
9503301	Zn(OH)2 AQ	4.817E-09	4.817E-09	-8.31719	1.00018	-16.899
9503302	Zn(OH)3 -	6.260E-13	6.065E-13	-12.21719	0.96882	-28.385
9503303	Zn(OH)4 -2	4.343E-18	3.826E-18	-17.41720	0.88100	-41.144
9501400	ZnHCO3 +	5.071E-09	4.913E-09	-8.30865	0.96882	12.414
9501401	ZnCO3 AQ	1.553E-08	1.554E-08	-7.80865	1.00018	5.300
9501402	Zn(CO3)2-2	1.219E-10	1.074E-10	-9.96913	0.88100	9.685
1601400	Cd(CO3)3-4	3.540E-22	2.133E-22	-21.67110	0.60242	6.440
1603300	CdOH +	8.452E-12	8.188E-12	-11.08682	0.96882	-10.253
1603301	Cd(OH)2 AQ	2.693E-14	2.694E-14	-13.56968	1.00018	-20.350
1603302	Cd(OH)3 -	1.242E-19	1.203E-19	-18.91969	0.96882	-33.286
1603303	Cd(OH)4 -2	4.845E-26	4.269E-26	-25.36969	0.88100	-47.295
1603304	Cd2OH +3	2.182E-19	1.640E-19	-18.78504	0.75196	-9.422
1601400	CdHCO3 +	8.010E-11	7.760E-11	-10.11015	0.96882	12.414
1601401	CdCO3 AQ	3.082E-10	3.082E-10	-9.51115	1.00018	5.399
6001400	Pb(CO3)2-2	1.200E-10	1.057E-10	-9.97574	0.88100	10.695
6003300	PbOH +	1.858E-08	1.800E-08	-7.74479	0.96882	-7.696
6003301	Pb(OH)2 AQ	2.787E-10	2.787E-10	-9.55480	1.00018	-17.120
6003302	Pb(OH)3 -	1.315E-13	1.274E-13	-12.89480	0.96882	-28.046
6003303	Pb2OH +3	1.242E-14	9.342E-15	-14.02958	0.75196	-6.236
6003304	Pb3(OH)4+2	1.959E-17	1.726E-17	-16.76296	0.88100	-24.204
6001401	PbCO3 AQ	1.302E-07	1.302E-07	-6.88526	1.00018	7.240
6003305	Pb(OH)4 -2	1.322E-17	1.165E-17	-16.93381	0.88100	-39.644
6001402	PbHCO3 +	3.080E-09	2.984E-09	-8.52526	0.96882	13.214
5403300	NiOH +	1.984E-11	1.922E-11	-10.71632	0.96882	-10.024
5403301	Ni(OH)2 AQ	8.337E-13	8.339E-13	-12.07889	1.00018	-19.000
5403302	Ni(OH)3 -	3.427E-16	3.320E-16	-15.47890	0.96882	-29.986
5401400	NiHCO3 +	1.301E-10	1.261E-10	-9.89936	0.96882	12.484
5401401	NiCO3 AQ	1.261E-08	1.261E-08	-7.89936	1.00018	6.870
5401402	Ni(CO3)2-2	8.039E-12	7.082E-12	-11.14984	0.88100	10.165
3301400	HCO3 -	2.027E-04	1.964E-04	-3.70680	0.96882	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00018	16.713
2113300	Cr+3	3.373E-18	2.537E-18	-17.59574	0.75196	10.032
2113301	Cr(OH)+2	5.910E-15	5.206E-15	-14.28346	0.88100	5.675

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-6.648E-06	-5.177	0.000	0.000
3300021	O2 (g)	0.000E-01	0.000	-84.354	133.830
330	H+1	-2.167E-04	-3.664	7.600	0.000
3301403	CO2 (g)	3.880E-06	-5.411	21.690	-0.530

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3021100	FECR2O4	1.395E-08	-7.855	0.546	24.860
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
950	Zn+2	3.060E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.786E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.383E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.297E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	4.715E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	1.988E-12	0.0	0.000E-01	0.0	2.790E-08	100.0
231	Cu+2	3.147E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.874E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.331E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	2.144E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	5.232E-07	97.4	0.000E-01	0.0	1.395E-08	2.6
2	H2O	8.982E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	2.235E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 8.277E-04 Sum of ANIONS 2.038E-04
PERCENT DIFFERENCE = 6.049E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 7.920E-04
EQUILIBRIUM pH = 7.600
EQUILIBRIUM pe = 13.489 or Eh = 782.67 mv

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - Run 3

Enter CO_3^{2-}, P_{CO2}, P_{O2}, fixed pH, solids allowed to precipitate
Fe redox pair, Mn redox pair

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	1.905E-06	-5.720	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.593E-08	2.512E-08	-7.60000	0.96884	0.014
30	Al+3	3.537E-16	2.660E-16	-15.57513	0.75209	0.124
100	Ba+2	1.383E-06	1.219E-06	-5.91402	0.88107	0.055
150	Ca+2	1.295E-04	1.141E-04	-3.94273	0.88107	0.055
160	Cd+2	4.319E-09	3.805E-09	-8.41964	0.88107	0.055
211	Cr(OH)2+	6.361E-10	6.162E-10	-9.21025	0.96884	0.014
231	Cu+2	9.794E-09	8.629E-09	-8.06402	0.88107	0.055
280	Fe+2	1.438E-25	1.267E-25	-24.89733	0.88107	0.055
410	K+1	6.647E-05	6.440E-05	-4.19113	0.96884	0.014
460	Mg+2	1.436E-04	1.266E-04	-3.89773	0.88107	0.055
500	Na+1	2.088E-04	2.023E-04	-3.69407	0.96884	0.014
540	Ni+2	5.972E-09	5.262E-09	-8.27887	0.88107	0.055
600	Pb+2	2.632E-08	2.319E-08	-7.63478	0.88107	0.055
800	Sr+2	5.707E-07	5.028E-07	-6.29861	0.88107	0.055
950	Zn+2	2.734E-07	2.409E-07	-6.61814	0.88107	0.055
281	Fe+3	3.468E-25	2.608E-25	-24.58367	0.75209	0.124
140	CO3-2	3.669E-07	3.232E-07	-6.49048	0.88107	0.055

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00018	-7.130
2113303	Cr(OH)4-	7.137E-13	6.914E-13	-12.16026	0.96884	-18.136
2113304	CrO2-	1.811E-12	1.755E-12	-11.75585	0.96884	-17.732
3300020	OH-	2.661E-07	2.578E-07	-6.58865	0.96884	-14.175
4603300	MgOH +	5.152E-09	4.992E-09	-8.30177	0.96884	-11.990
4601400	MgCO3 AQ	3.576E-08	3.577E-08	-7.44649	1.00018	2.942
4601401	MgHCO3 +	2.887E-07	2.797E-07	-6.55331	0.96884	11.449
1503300	CaOH +	7.334E-10	7.106E-10	-9.14838	0.96884	-12.792
1501400	CaHCO3 +	2.013E-07	1.951E-07	-6.70981	0.96884	11.337
1501401	CaCO3 AQ	4.657E-08	4.657E-08	-7.33185	1.00018	3.101
5001400	NaCO3 -	9.330E-10	9.040E-10	-9.04385	0.96884	1.154
5001401	NaHCO3 AQ	1.974E-08	1.974E-08	-7.70455	1.00018	10.080
303300	AlOH +2	8.315E-14	7.326E-14	-13.13512	0.88107	-5.105
303301	Al(OH)2 +	3.456E-11	3.349E-11	-10.47514	0.96884	-10.086
303302	Al(OH)4 -	1.619E-09	1.568E-09	-8.80458	0.96884	-23.616
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00018	-16.000
2803300	FeOH +	1.066E-27	1.033E-27	-26.98589	0.96884	-9.675
2803301	FeOH3 -1	3.045E-34	2.950E-34	-33.53021	0.96884	-31.419
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67541	1.00018	-20.978
2813300	FeOH +2	5.405E-20	4.762E-20	-19.32223	0.88107	-2.284
2813301	FeOH2 +	9.122E-16	8.837E-16	-15.05368	0.96884	-5.656
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00018	-13.600
2813303	FeOH4 -	1.698E-16	1.646E-16	-15.78370	0.96884	-21.586
2813304	Fe2(OH)2+4	1.288E-37	7.759E-38	-37.11020	0.60261	-2.923
2813305	Fe3(OH)4+5	3.079E-50	1.395E-50	-49.85531	0.45322	-6.161
8003300	SrOH +	8.513E-13	8.247E-13	-12.08369	0.96884	-13.371
1003300	BaOH +	1.337E-12	1.295E-12	-11.88767	0.96884	-13.560
2311400	CuCO3 AQ	1.498E-08	1.498E-08	-7.82449	1.00018	6.730
2311401	Cu(CO3)2-2	6.919E-12	6.096E-12	-11.21497	0.88107	9.885
2313300	CuOH +	3.546E-09	3.435E-09	-8.46402	0.96884	-7.986
2313301	Cu(OH)2 AQ	2.857E-07	2.857E-07	-6.54403	1.00018	-13.680
2313302	Cu(OH)3 -	7.091E-13	6.870E-13	-12.16304	0.96884	-26.885
2313303	Cu(OH)4 -2	6.179E-18	5.444E-18	-17.26404	0.88107	-39.545
2313304	Cu2(OH)2+2	3.295E-12	2.903E-12	-11.53711	0.88107	-10.554
2311402	CuHCO3 +	7.232E-10	7.007E-10	-9.15450	0.96884	13.014
9503300	ZnOH +	6.985E-09	6.768E-09	-8.16957	0.96884	-9.138
9503301	Zn(OH)2 AQ	4.817E-09	4.818E-09	-8.31716	1.00018	-16.899
9503302	Zn(OH)3 -	6.260E-13	6.065E-13	-12.21717	0.96884	-28.385
9503303	Zn(OH)4 -2	4.343E-18	3.827E-18	-17.41717	0.88107	-41.144
9501400	ZnHCO3 +	5.071E-09	4.913E-09	-8.30862	0.96884	12.414
9501401	ZnCO3 AQ	1.553E-08	1.554E-08	-7.80862	1.00018	5.300
9501402	Zn(CO3)2-2	1.219E-10	1.074E-10	-9.96910	0.88107	9.685
1601400	Cd(CO3)3-4	3.539E-22	2.133E-22	-21.67107	0.60261	6.440
1603300	CdOH +	8.452E-12	8.189E-12	-11.08679	0.96884	-10.253
1603301	Cd(OH)2 AQ	2.693E-14	2.694E-14	-13.56965	1.00018	-20.350
1603302	Cd(OH)3 -	1.242E-19	1.203E-19	-18.91966	0.96884	-33.286
1603303	Cd(OH)4 -2	4.845E-26	4.269E-26	-25.36966	0.88107	-47.295
1603304	Cd2OH +3	2.181E-19	1.641E-19	-18.78498	0.75209	-9.422
1601400	CdHCO3 +	8.010E-11	7.760E-11	-10.11012	0.96884	12.414
1601401	CdCO3 AQ	3.082E-10	3.082E-10	-9.51111	1.00018	5.399
6001400	Pb(CO3)2-2	1.200E-10	1.057E-10	-9.97574	0.88107	10.695
6003300	PbOH +	1.858E-08	1.800E-08	-7.74479	0.96884	-7.696
6003301	Pb(OH)2 AQ	2.787E-10	2.787E-10	-9.55479	1.00018	-17.120
6003302	Pb(OH)3 -	1.315E-13	1.274E-13	-12.89480	0.96884	-28.046
6003303	Pb2OH +3	1.242E-14	9.342E-15	-14.02957	0.75209	-6.236
6003304	Pb3(OH)4+2	1.959E-17	1.726E-17	-16.76294	0.88107	-24.204
6001401	PbCO3 AQ	1.302E-07	1.302E-07	-6.88526	1.00018	7.240
6003305	Pb(OH)4 -2	1.322E-17	1.165E-17	-16.93381	0.88107	-39.644
6001402	PbHCO3 +	3.080E-09	2.984E-09	-8.52526	0.96884	13.214
5403300	NiOH +	1.984E-11	1.922E-11	-10.71631	0.96884	-10.024
5403301	Ni(OH)2 AQ	8.338E-13	8.339E-13	-12.07888	1.00018	-19.000
5403302	Ni(OH)3 -	3.427E-16	3.320E-16	-15.47889	0.96884	-29.986
5401400	NiHCO3 +	1.301E-10	1.261E-10	-9.89935	0.96884	12.484
5401401	NiCO3 AQ	1.261E-08	1.261E-08	-7.89935	1.00018	6.870
5401402	Ni(CO3)2-2	8.038E-12	7.082E-12	-11.14983	0.88107	10.165

3301400	HCO3 -	2.027E-04	1.964E-04	-3.70680	0.96884	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00018	16.713
2113300	Cr+3	4.180E-15	3.144E-15	-14.50252	0.75209	10.031
2113301	Cr(OH)+2	7.324E-12	6.453E-12	-11.19024	0.88107	5.675

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-7.166E-06	-5.145	0.000	0.000
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000
330	H+1	-2.157E-04	-3.666	7.600	0.000
3301403	CO2 (g)	3.885E-06	-5.411	21.690	-0.530
3300021	O2 (g)	-1.343E-07	-6.872	-84.354	133.830

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.272E-08	-7.896	3.220	12.125

PART 5 of OUTPUT FILE

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
600	Pb+2	1.786E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	1.383E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.297E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
160	Cd+2	4.715E-09	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.874E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
231	Cu+2	3.147E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	3.060E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.464E-09	8.8	0.000E-01	0.0	2.544E-08	91.2
280	Fe+2	1.448E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
30	Al+3	3.331E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.144E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.495E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.235E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	8.961E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 8.266E-04 Sum of ANIONS 2.037E-04
PERCENT DIFFERENCE = 6.045E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
EQUILIBRIUM IONIC STRENGTH (m) = 7.910E-04
EQUILIBRIUM pH = 7.600
EQUILIBRIUM pe = 13.489 or Eh = 782.67 mv

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - Run 4

Entered CO_3^{2-}, P_{CO2}, P_{O2}, fixed pH, Fe redox pair, Mn redox pair, solids allowed to precipitate
Adsorption

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	1.905E-06	-5.720	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.586E-08	2.512E-08	-7.60000	0.97123	0.013
30	Al+3	3.459E-16	2.660E-16	-15.57513	0.76898	0.114
100	Ba+2	4.101E-07	3.649E-07	-6.43787	0.88980	0.051
150	Ca+2	6.986E-05	6.216E-05	-4.20649	0.88980	0.051
160	Cd+2	1.546E-12	1.376E-12	-11.86154	0.88980	0.051
211	Cr(OH)2+	6.345E-10	6.162E-10	-9.21025	0.97123	0.013
231	Cu+2	3.061E-13	2.724E-13	-12.56487	0.88980	0.051
280	Fe+2	1.424E-25	1.267E-25	-24.89733	0.88980	0.051
410	K+1	6.647E-05	6.456E-05	-4.19006	0.97123	0.013
460	Mg+2	1.436E-04	1.278E-04	-3.89344	0.88980	0.051
500	Na+1	2.088E-04	2.028E-04	-3.69300	0.97123	0.013
540	Ni+2	1.065E-11	9.481E-12	-11.02315	0.88980	0.051
600	Pb+2	3.147E-15	2.801E-15	-14.55275	0.88980	0.051
800	Sr+2	5.707E-07	5.078E-07	-6.29432	0.88980	0.051
950	Zn+2	2.797E-11	2.489E-11	-10.60397	0.88980	0.051
811	ADS1TYP1	1.050E-04	1.050E-04	-3.97864	1.00000	0.000

140	CO3-2	3.633E-07	3.232E-07	-6.49048	0.88980	0.051
281	Fe+3	3.392E-25	2.608E-25	-24.58367	0.76898	0.114
812	ADS1TYP2	5.897E-03	5.897E-03	-2.22936	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	4.757E-10	4.757E-10	-9.32262	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00015	-7.130
2113303	Cr(OH)4-	7.119E-13	6.914E-13	-12.16026	0.97123	-18.137
2113304	CrO2-	1.806E-12	1.755E-12	-11.75585	0.97123	-17.733
3300020	OH-	2.655E-07	2.578E-07	-6.58865	0.97123	-14.176
4603300	MgOH +	5.190E-09	5.041E-09	-8.29749	0.97123	-11.991
4601400	MgCO3 AQ	3.612E-08	3.612E-08	-7.44221	1.00015	2.942
4601401	MgHCO3 +	2.908E-07	2.825E-07	-6.54903	0.97123	11.448
1503300	CaOH +	3.986E-10	3.871E-10	-9.41214	0.97123	-12.793
1501400	CaHCO3 +	1.094E-07	1.063E-07	-6.97357	0.97123	11.336
1501401	CaCO3 AQ	2.537E-08	2.537E-08	-7.59561	1.00015	3.101
5001400	NaCO3 -	9.330E-10	9.062E-10	-9.04278	0.97123	1.153
5001401	NaHCO3 AQ	1.979E-08	1.979E-08	-7.70348	1.00015	10.080
303300	AlOH +2	8.233E-14	7.326E-14	-13.13512	0.88980	-5.109
303301	Al(OH)2 +	3.448E-11	3.349E-11	-10.47514	0.97123	-10.087
303302	Al(OH)4 -	1.615E-09	1.568E-09	-8.80458	0.97123	-23.617
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00015	-16.000
2803300	FeOH +	1.064E-27	1.033E-27	-26.98589	0.97123	-9.676
2803301	FeOH3 -1	3.037E-34	2.950E-34	-33.53021	0.97123	-31.420
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00015	-20.978
2813300	FeOH +2	5.351E-20	4.762E-20	-19.32223	0.88980	-2.288
2813301	FeOH2 +	9.099E-16	8.837E-16	-15.05368	0.97123	-5.657
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00015	-13.600
2813303	FeOH4 -	1.694E-16	1.646E-16	-15.78369	0.97123	-21.587
2813304	Fe2(OH)2+4	1.238E-37	7.759E-38	-37.11021	0.62687	-2.940
2813305	Fe3(OH)4+5	2.895E-50	1.395E-50	-49.85531	0.48205	-6.187
8003300	SrOH +	8.576E-13	8.329E-13	-12.07940	0.97123	-13.372
1003300	BaOH +	3.992E-13	3.877E-13	-12.41152	0.97123	-13.561
2311400	CuCO3 AQ	4.727E-13	4.728E-13	-12.32534	1.00015	6.730
2311401	Cu(CO3)2-2	2.162E-16	1.924E-16	-15.71582	0.88980	9.881
2313300	CuOH +	1.116E-13	1.084E-13	-12.96487	0.97123	-7.987
2313301	Cu(OH)2 AQ	9.017E-12	9.018E-12	-11.04488	1.00015	-13.680
2313302	Cu(OH)3 -	2.232E-17	2.168E-17	-16.66389	0.97123	-26.886
2313303	Cu(OH)4 -2	1.931E-22	1.718E-22	-21.76489	0.88980	-39.549
2313304	Cu2(OH)2+2	3.250E-21	2.892E-21	-20.53881	0.88980	-10.558
2311402	CuHCO3 +	2.277E-14	2.211E-14	-13.65535	0.97123	13.013
9503300	ZnOH +	7.199E-13	6.992E-13	-12.15539	0.97123	-9.139
9503301	Zn(OH)2 AQ	4.977E-13	4.978E-13	-12.30298	1.00015	-16.899
9503302	Zn(OH)3 -	6.452E-17	6.266E-17	-16.20299	0.97123	-28.386
9503303	Zn(OH)4 -2	4.443E-22	3.954E-22	-21.40300	0.88980	-41.148
9501400	ZnHCO3 +	5.227E-13	5.076E-13	-12.29445	0.97123	12.413
9501401	ZnCO3 AQ	1.605E-12	1.605E-12	-11.79445	1.00015	5.300
9501402	Zn(CO3)2-2	1.247E-14	1.109E-14	-13.95493	0.88980	9.681
1601400	Cd(CO3)3-4	1.230E-25	7.710E-26	-25.11297	0.62687	6.423
1603300	CdOH +	3.048E-15	2.960E-15	-14.52869	0.97123	-10.254
1603301	Cd(OH)2 AQ	9.736E-18	9.738E-18	-17.01155	1.00015	-20.350
1603302	Cd(OH)3 -	4.478E-23	4.350E-23	-22.36156	0.97123	-33.287
1603303	Cd(OH)4 -2	1.734E-29	1.543E-29	-28.81156	0.88980	-47.299
1603304	Cd2OH +3	2.788E-26	2.144E-26	-25.66878	0.76898	-9.432
1601400	CdHCO3 +	2.888E-14	2.805E-14	-13.55202	0.97123	12.413
1601401	CdCO3 AQ	1.114E-13	1.114E-13	-12.95301	1.00015	5.399
6001400	Pb(CO3)2-2	1.435E-17	1.277E-17	-16.89370	0.88980	10.691
6003300	PbOH +	2.238E-15	2.174E-15	-14.66276	0.97123	-7.697
6003301	Pb(OH)2 AQ	3.366E-17	3.367E-17	-16.47276	1.00015	-17.120
6003302	Pb(OH)3 -	1.585E-20	1.539E-20	-19.81277	0.97123	-28.047
6003303	Pb2OH +3	1.772E-28	1.363E-28	-27.86551	0.76898	-6.246
6003304	Pb3(OH)4+2	3.419E-38	3.042E-38	-37.51685	0.88980	-24.208
6001401	PbCO3 AQ	1.573E-14	1.573E-14	-13.80323	1.00015	7.240
6003305	Pb(OH)4 -2	1.581E-24	1.407E-24	-23.85178	0.88980	-39.648
6001402	PbHCO3 +	3.711E-16	3.604E-16	-15.44323	0.97123	13.213
5403300	NiOH +	3.565E-14	3.463E-14	-13.46059	0.97123	-10.025
5403301	Ni(OH)2 AQ	1.502E-15	1.503E-15	-14.82317	1.00015	-19.000

5403302	Ni(OH)3 -	6.159E-19	5.982E-19	-18.22317	0.97123	-29.987
5401400	NiHCO3 +	2.339E-13	2.272E-13	-12.64363	0.97123	12.483
5401401	NiCO3 AQ	2.271E-11	2.272E-11	-10.64363	1.00015	6.870
5401402	Ni(CO3)2-2	1.434E-14	1.276E-14	-13.89411	0.88980	10.161
3301400	HCO3 -	2.022E-04	1.964E-04	-3.70680	0.97123	10.396
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00015	16.713
2113300	Cr+3	4.089E-15	3.144E-15	-14.50252	0.76898	10.022
2113301	Cr(OH)+2	7.252E-12	6.453E-12	-11.19024	0.88980	5.671
8123301	=SO2-	9.297E-04	9.297E-04	-3.03166	1.00000	-8.930
8123302	=SO2H2+	8.569E-04	8.569E-04	-3.06706	1.00000	7.290
8113301	=SO1-	1.656E-05	1.656E-05	-4.78094	1.00000	-8.930
8113302	=SO1H2+	1.526E-05	1.526E-05	-4.81634	1.00000	7.290
8129500	=SO2Zn+	1.774E-08	1.774E-08	-7.75104	1.00000	-1.990
8119500	=SO1Zn+	2.882E-07	2.882E-07	-6.54032	1.00000	0.970
8121600	=SO2Cd+	1.206E-10	1.206E-10	-9.91860	1.00000	-2.900
8111600	=SO1Cd+	4.593E-09	4.593E-09	-8.33789	1.00000	0.430
8112310	=SO1Cu+	2.392E-07	2.392E-07	-6.62122	1.00000	2.850
8122310	=SO2Cu+	7.552E-08	7.552E-08	-7.12193	1.00000	0.600
8115400	=SO1Ni+	1.661E-08	1.661E-08	-7.77950	1.00000	0.150
8125400	=SO2Ni+	2.088E-09	2.088E-09	-8.68022	1.00000	-2.500
8116000	=SO1Pb+	1.782E-07	1.782E-07	-6.74910	1.00000	4.710
8126000	=SO2Pb+	3.892E-10	3.892E-10	-9.40981	1.00000	0.300
8121500	=SO2Ca+	6.116E-06	6.116E-06	-5.21355	1.00000	-5.850
8111500	=SO1HCa++	5.364E-05	5.364E-05	-4.27054	1.00000	4.970
8111000	=SO1HBa++	9.729E-07	9.729E-07	-6.01191	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-6.580E-06	-5.182	0.000	0.000
330	H+1	-1.363E-04	-3.866	7.600	0.000
3301403	CO2 (g)	4.681E-06	-5.330	21.690	-0.530
3300021	O2 (g)	-1.343E-07	-6.872	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.272E-08	-7.895	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP2

76.7	PERCENT BOUND IN SPECIES # 812	ADS1TYP2
12.1	PERCENT BOUND IN SPECIES #8123301	=SO2-
11.1	PERCENT BOUND IN SPECIES #8123302	=SO2H2+

Ba+2

29.6	PERCENT BOUND IN SPECIES # 100	Ba+2
70.3	PERCENT BOUND IN SPECIES #8111000	=SO1HBa++

Ca+2

53.8	PERCENT BOUND IN SPECIES # 150	Ca+2
4.7	PERCENT BOUND IN SPECIES #8121500	=SO2Ca+
41.3	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++

Cd+2

2.6	PERCENT BOUND IN SPECIES #8121600	=SO2Cd+
97.4	PERCENT BOUND IN SPECIES #8111600	=SO1Cd+

Zn+2

5.8	PERCENT BOUND IN SPECIES #8129500	=SO2Zn+
94.2	PERCENT BOUND IN SPECIES #8119500	=SO1Zn+

Cu+2

76.0	PERCENT BOUND IN SPECIES #8112310	=SO1Cu+
24.0	PERCENT BOUND IN SPECIES #8122310	=SO2Cu+

ADS1TYP1

54.7	PERCENT BOUND IN SPECIES # 811	ADS1TYP1

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                 8.6     PERCENT BOUND IN SPECIES #8113301   =SO1-
                 7.9     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
                27.9     PERCENT BOUND IN SPECIES #8111500   =SO1HCa++
K+1
               100.0     PERCENT BOUND IN SPECIES #    410   K+1

Mg+2
                99.8     PERCENT BOUND IN SPECIES #    460   Mg+2
Na+1
               100.0     PERCENT BOUND IN SPECIES #    500   Na+1
Ni+2
                88.7     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                11.1     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
                99.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
               100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Cr(OH)2+
                25.8     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
                73.8     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
Al+3
                 1.0     PERCENT BOUND IN SPECIES # 303301   Al(OH)2 +
                48.5     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                50.4     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
                94.7     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 4.9     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
                99.3     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
                61.0     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                27.7     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                11.4     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
               142.0     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                14.8     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
               601.5     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                10.7     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                24.0     PERCENT BOUND IN SPECIES #3300020   OH-
                 1.6     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                26.0     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                21.6     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                 6.8     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                 1.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                16.1     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	4.101E-07	29.6	9.734E-07	70.4	0.000E-01	0.0
150	Ca+2	6.999E-05	53.9	5.975E-05	46.1	0.000E-01	0.0
160	Cd+2	1.689E-12	0.0	4.714E-09	100.0	0.000E-01	0.0
950	Zn+2	3.133E-11	0.0	3.059E-07	100.0	0.000E-01	0.0
231	Cu+2	9.930E-12	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.365E-11	0.2	1.870E-08	99.8	0.000E-01	0.0
600	Pb+2	2.153E-14	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.463E-09	8.8	0.000E-01	0.0	2.544E-08	91.2
30	Al+3	3.327E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.136E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	1.434E-25	100.0	0.000E-01	0.0	0.000E-01	0.0

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  1  E-1            0.000E-01     0.0   0.000E-01      0.0   0.000E-01      0.0
281  Fe+3           1.493E-15     0.0   0.000E-01      0.0   5.372E-07    100.0
330  H+1            2.235E-04   156.9  -8.101E-05    -56.9   0.000E-01      0.0
  2  H2O            2.845E-07    25.7   8.227E-07     74.3   0.000E-01      0.0

     Charge Balance: SPECIATED
       Sum of CATIONS =  1.693E-03 Sum of ANIONS   1.150E-03
       PERCENT DIFFERENCE =   1.912E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
     EQUILIBRIUM IONIC STRENGTH (m) =   6.688E-04
     EQUILIBRIUM pH                 =   7.600
     EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv
******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.030620      sig0 = 0.001966
                            psib = 0.000000      sigb = 0.000000
                            psid = 0.000000      sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-2.411	[1.000] 150 [1.000] 140
5046000	ARTINITE	-9.088	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-5.855	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-2.255	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-4.199	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-12.249	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-22.209	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-2.443	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.341	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-4.846	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.545	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.042	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.338	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.425	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.223	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.203	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.365	[-8.000] 330 [1.000] 231 [2.000] 281 [4.000] 2
95000	ZN METAL	-63.863	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.157	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-6.834	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-7.854	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.604	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.154	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.114	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-6.904	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.714	[-2.000] 330 [1.000] 950 [1.000] 2
2095006	ZINCITE	-6.856	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.586	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.688	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.620	[1.000] 160 [1.000] 140

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2016000 CD(OH)2 (A)    -10.688    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)    -10.312    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE    -12.135    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL       -45.794    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE       -7.844    [  1.000] 600  [  1.000] 140
2060000 MASSICOT       -12.502    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE       -12.307    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O     -12.333    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3        -20.060    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                  [  1.000] 140
5060002 PB3O2CO3       -31.146    [ -4.000] 330  [  3.000] 600  [  1.000] 140
                                  [  2.000]   2
2060003 PLATTNERITE     -7.486    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                  [  2.000]   2
3060000 PB2O3          -17.568    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                  [  3.000]   2
3060001 MINIUM         -31.039    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                  [  4.000]   2
2060004 PB(OH)2 (C)     -7.703    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE   -23.979    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                  [  2.000]   2
2060005 PB2O(OH)2      -24.906    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3          -10.816    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2         -6.188    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE       -8.615    [ -2.000] 330  [  1.000] 540  [  1.000]   2
5023101 MALACHITE      -11.463    [  2.000] 231  [  2.000]   2  [  1.000] 140
                                  [ -2.000] 330
5023102 AZURITE        -18.895    [  3.000] 231  [  2.000]   2  [  2.000] 140
                                  [ -2.000] 330
2015000 LIME           -22.464    [ -2.000] 330  [  1.000] 150  [  1.000]
2015001 PORTLANDITE    -12.120    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE        -20.420    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE      -10.720    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE      -23.529    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                  [  4.000]   2
3046000 SPINEL         -11.849    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                  [  4.000]   2
3046001 MAG-FERRITE     -9.978    [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                  [  4.000]   2
3028102 LEPIDOCROCIT    -3.155    [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021100 FECR2O4        -12.371    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4         -4.563    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3            0.000    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)     -0.860    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)     -3.412    [  1.000] 211  [  1.000]   2  [ -1.000] 330
```

APPENDIX II

EFFECT OF pH CHANGES IN METALS ADSORPTION AND PRECIPITATION IN THE WATER OF THE CHICAMBA DAM (SITE 14):
Output files of modelling with the Minteqa2 Program

Extended output files of the site 14 water quality modelling with different pH values. The modelling was undertaken with the geochemical speciation program MINTEQA2 only for site 14 in order to see what would be the influence of pH changes in the water quality supplied to Chimoio City from the Chicamba Dam. pH values of 6.0, 6.5, 7.0, 7.6 (actual water pH), 8.0 and 8.5 were introduced in the model after the four runs were undertaken. The output file has been reduced.

1 – Modelling with pH = 6.0

```
                              PART 1 of OUTPUT FILE
Revuè river water-Site 14 - pH = 6.0
Entered PCO2, PO2, fixed pH, solids allowed to precipitate, Fe redox pair and
adsorption
--------------------------------------------------------------------------------
 Temperature (Celsius):  19.30
 Units of concentration: MG/L
 Ionic strength to be computed.
 Carbonate concentration represents carbonate alkalinity.
 Do not automatically terminate if charge imbalance exceeds 30%
 Precipitation is allowed for all solids in the thermodynamic database and
   the print option for solids is set to: 1
 The maximum number of iterations is: 200
 The method used to compute activity coefficients is: Davies equation
 Intermediate output file
 Adsorption model: Diffuse Layer
 Number of adsorbing surfaces: 1
--------------------------------------------------------------------------------
INPUT DATA BEFORE TYPE MODIFICATIONS
   ID        NAME        ACTIVITY GUESS     LOG GUESS    ANAL TOTAL
    330  H+1                  1.000E-06         -6.000    0.000E-01
     30  Al+3                 4.786E-06         -5.320    1.300E-01
    100  Ba+2                 1.380E-06         -5.860    1.900E-01
    150  Ca+2                 1.288E-04         -3.890    5.200E+00
    160  Cd+2                 4.677E-09         -8.330    5.300E-04
    211  Cr(OH)2+             2.818E-08         -7.550    2.400E-03
    231  Cu+2                 3.162E-07         -6.500    2.000E-02
    280  Fe+2                 5.370E-07         -6.270    3.000E-02
    410  K+1                  6.607E-05         -4.180    2.599E+00
    460  Mg+2                 1.445E-04         -3.840    3.500E+00
    500  Na+1                 2.089E-04         -3.680    4.800E+00
    540  Ni+2                 1.862E-08         -7.730    1.100E-03
    600  Pb+2                 1.778E-07         -6.750    3.700E-02
    800  Sr+2                 5.754E-07         -6.240    5.000E-02
    950  Zn+2                 3.090E-07         -6.510    2.000E-02
      1  E-1                  1.000E-16        -16.000    0.000E-01
    140  CO3-2                2.188E-04         -3.660    1.310E+01
    281  Fe+3                 1.778E-21        -20.750    0.000E-01
    813  ADS1PSIo             1.000E+00          0.000    0.000E-01
    811  ADS1TYP1             1.905E-04         -3.720    1.922E-04
    812  ADS1TYP2             7.762E-03         -2.110    7.690E-03
      2  H2O                  1.000E+00          0.000    0.000E-01
```

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	1.030E-06	1.000E-06	-6.00000	0.97077	0.013
30	Al+3	2.192E-11	1.678E-11	-10.77513	0.76565	0.116
100	Ba+2	1.379E-06	1.225E-06	-5.91199	0.88809	0.052
150	Ca+2	1.296E-04	1.151E-04	-3.93896	0.88809	0.052
160	Cd+2	1.090E-09	9.678E-10	-9.01420	0.88809	0.052
211	Cr(OH)2+	1.814E-08	1.761E-08	-7.75414	0.97077	0.013
231	Cu+2	2.986E-10	2.652E-10	-9.57639	0.88809	0.052
280	Fe+2	2.261E-22	2.008E-22	-21.69733	0.88809	0.052
410	K+1	6.647E-05	6.453E-05	-4.19026	0.97077	0.013
460	Mg+2	1.440E-04	1.278E-04	-3.89330	0.88809	0.052
500	Na+1	2.088E-04	2.027E-04	-3.69317	0.97077	0.013
540	Ni+2	6.529E-09	5.799E-09	-8.23668	0.88809	0.052
600	Pb+2	2.866E-12	2.545E-12	-11.59427	0.88809	0.052
800	Sr+2	5.707E-07	5.068E-07	-6.29516	0.88809	0.052
950	Zn+2	2.386E-08	2.119E-08	-7.67380	0.88809	0.052
811	ADS1TYP1	1.463E-04	1.463E-04	-3.83477	1.00000	0.000
140	CO3-2	2.296E-10	2.039E-10	-9.69048	0.88809	0.052
281	Fe+3	2.149E-20	1.646E-20	-19.78367	0.76565	0.116
812	ADS1TYP2	5.880E-03	5.880E-03	-2.23065	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	3.961E-14	3.961E-14	-13.40223	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.306E-09	1.306E-09	-8.88414	1.00016	-7.130
2113303	Cr(OH)4-	1.285E-14	1.247E-14	-13.90415	0.97077	-18.137
2113304	CrO2-	3.259E-14	3.164E-14	-13.49974	0.97077	-17.733
3300020	OH-	6.672E-09	6.477E-09	-8.18865	0.97077	-14.176
4603300	MgOH +	1.305E-10	1.267E-10	-9.89734	0.97077	-11.991
4601400	MgCO3 AQ	2.280E-11	2.280E-11	-10.64207	1.00016	2.942
4601401	MgHCO3 +	7.311E-09	7.098E-09	-8.14889	0.97077	11.448
1503300	CaOH +	1.855E-11	1.801E-11	-10.74461	0.97077	-12.793
1501400	CaHCO3 +	5.092E-09	4.943E-09	-8.30603	0.97077	11.336
1501401	CaCO3 AQ	2.964E-11	2.964E-11	-10.52807	1.00016	3.101
5001400	NaCO3 -	5.888E-13	5.716E-13	-12.24294	0.97077	1.154
5001401	NaHCO3 AQ	4.969E-10	4.970E-10	-9.30364	1.00016	10.080
303300	AlOH +2	1.307E-10	1.161E-10	-9.93512	0.88809	-5.108
303301	Al(OH)2 +	1.373E-09	1.333E-09	-8.87514	0.97077	-10.087
303302	Al(OH)4 -	4.058E-11	3.939E-11	-10.40458	0.97077	-23.617
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00016	-16.000
2803300	FeOH +	4.236E-26	4.112E-26	-25.38589	0.97077	-9.676
2803301	FeOH3 -1	7.633E-36	7.410E-36	-35.13021	0.97077	-31.420
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00016	-20.978
2813300	FeOH +2	8.498E-17	7.547E-17	-16.12223	0.88809	-2.287
2813301	FeOH2 +	3.624E-14	3.518E-14	-13.45368	0.97077	-5.657
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00016	-13.600
2813303	FeOH4 -	4.258E-18	4.133E-18	-17.38369	0.97077	-21.587
2813304	Fe2(OH)2+4	3.133E-31	1.949E-31	-30.71021	0.62205	-2.937
2813305	Fe3(OH)4+5	2.930E-42	1.395E-42	-41.85532	0.47627	-6.182
8003300	SrOH +	2.151E-14	2.088E-14	-13.68024	0.97077	-13.372
1003300	BaOH +	3.367E-14	3.269E-14	-13.48563	0.97077	-13.561
2311400	CuCO3 AQ	2.904E-13	2.905E-13	-12.53687	1.00016	6.730
2311401	Cu(CO3)2-2	8.398E-20	7.459E-20	-19.12734	0.88809	9.882
2313300	CuOH +	2.732E-12	2.652E-12	-11.57640	0.97077	-7.987
2313301	Cu(OH)2 AQ	5.540E-12	5.541E-12	-11.25640	1.00016	-13.680
2313302	Cu(OH)3 -	3.447E-19	3.347E-19	-18.47541	0.97077	-26.886
2313303	Cu(OH)4 -2	7.501E-26	6.662E-26	-25.17641	0.88809	-39.548
2313304	Cu2(OH)2+2	1.948E-18	1.730E-18	-17.76186	0.88809	-10.558

2311402	CuHCO3 +	5.572E-13	5.409E-13	-12.26687	0.97077	13.013
9503300	ZnOH +	1.541E-11	1.495E-11	-10.82522	0.97077	-9.139
9503301	Zn(OH)2 AQ	2.674E-13	2.674E-13	-12.57281	1.00016	-16.899
9503302	Zn(OH)3 -	8.711E-19	8.456E-19	-18.07282	0.97077	-28.386
9503303	Zn(OH)4 -2	1.509E-25	1.340E-25	-24.87282	0.88809	-41.147
9501400	ZnHCO3 +	1.118E-11	1.086E-11	-10.96428	0.97077	12.413
9501401	ZnCO3 AQ	8.623E-13	8.624E-13	-12.06428	1.00016	5.300
9501402	Zn(CO3)2-2	4.234E-18	3.760E-18	-17.42476	0.88809	9.682
1601400	Cd(CO3)3-4	2.190E-32	1.363E-32	-31.86563	0.62205	6.426
1603300	CdOH +	5.389E-14	5.232E-14	-13.28135	0.97077	-10.254
1603301	Cd(OH)2 AQ	4.322E-18	4.323E-18	-17.36421	1.00016	-20.350
1603302	Cd(OH)3 -	4.997E-25	4.850E-25	-24.31422	0.97077	-33.287
1603303	Cd(OH)4 -2	4.868E-33	4.323E-33	-32.36422	0.88809	-47.298
1603304	Cd2OH +3	3.482E-22	2.666E-22	-21.57410	0.76565	-9.430
1601400	CdHCO3 +	5.108E-13	4.958E-13	-12.30468	0.97077	12.413
1601401	CdCO3 AQ	4.946E-14	4.947E-14	-13.30568	1.00016	5.399
6001400	Pb(CO3)2-2	5.204E-21	4.621E-21	-20.33522	0.88809	10.692
6003300	PbOH +	5.112E-14	4.963E-14	-13.30427	0.97077	-7.697
6003301	Pb(OH)2 AQ	1.930E-17	1.931E-17	-16.71428	1.00016	-17.120
6003302	Pb(OH)3 -	2.283E-22	2.217E-22	-21.65428	0.97077	-28.047
6003303	Pb2OH +3	3.693E-24	2.828E-24	-23.54854	0.76565	-6.244
6003304	Pb3(OH)4+2	1.024E-35	9.091E-36	-35.04140	0.88809	-24.207
6001401	PbCO3 AQ	9.020E-15	9.021E-15	-14.04474	1.00016	7.240
6003305	Pb(OH)4 -2	5.731E-28	5.090E-28	-27.29329	0.88809	-39.647
6001402	PbHCO3 +	8.475E-15	8.227E-15	-14.08474	0.97077	13.213
5403300	NiOH +	5.480E-13	5.320E-13	-12.27411	0.97077	-10.025
5403301	Ni(OH)2 AQ	5.798E-16	5.798E-16	-15.23669	1.00016	-19.000
5403302	Ni(OH)3 -	5.973E-21	5.798E-21	-20.23669	0.97077	-29.987
5401400	NiHCO3 +	3.595E-12	3.490E-12	-11.45715	0.97077	12.483
5401401	NiCO3 AQ	8.766E-12	8.767E-12	-11.05715	1.00016	6.870
5401402	Ni(CO3)2-2	3.499E-18	3.107E-18	-17.50763	0.88809	10.162
3301400	HCO3 -	5.083E-06	4.934E-06	-5.30680	0.97077	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00016	16.713
2113300	Cr+3	1.860E-10	1.424E-10	-9.84641	0.76565	10.024
2113301	Cr(OH)+2	8.268E-09	7.343E-09	-8.13413	0.88809	5.672
8123301	=SO2-	7.399E-04	7.399E-04	-3.13085	1.00000	-8.930
8123302	=SO2H2+	1.070E-03	1.070E-03	-2.97045	1.00000	7.290
8113301	=SO1-	1.841E-05	1.841E-05	-4.73497	1.00000	-8.930
8113302	=SO1H2+	2.663E-05	2.663E-05	-4.57457	1.00000	7.290
8129500	=SO2Zn+	1.191E-08	1.191E-08	-7.92425	1.00000	-1.990
8119500	=SO1Zn+	2.702E-07	2.702E-07	-6.56837	1.00000	0.970
8121600	=SO2Cd+	6.689E-11	6.689E-11	-10.17465	1.00000	-2.900
8111600	=SO1Cd+	3.558E-09	3.558E-09	-8.44877	1.00000	0.430
8112310	=SO1Cu+	2.565E-07	2.565E-07	-6.59096	1.00000	2.850
8122310	=SO2Cu+	5.796E-08	5.796E-08	-7.23684	1.00000	0.600
8115400	=SO1Ni+	1.119E-08	1.119E-08	-7.95125	1.00000	0.150
8125400	=SO2Ni+	1.007E-09	1.007E-09	-8.99713	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74884	1.00000	4.710
8126000	=SO2Pb+	2.788E-10	2.788E-10	-9.55472	1.00000	0.300
8121500	=SO2Ca+	8.925E-09	8.925E-09	-8.04940	1.00000	-5.850
8111500	=SO1HCa++	1.370E-07	1.370E-07	-6.86332	1.00000	4.970
8111000	=SO1HBa++	4.505E-09	4.505E-09	-8.34635	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	1.917E-04	-3.717	0.000	0.000
330	H+1	-7.550E-04	-3.122	6.000	0.000
3301403	CO2 (g)	4.325E-04	-3.364	21.690	-0.530
3300021	O2 (g)	1.148E-04	-3.940	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1PSIo				
	315.0	PERCENT BOUND IN SPECIES	#8123302	=SO2H2+
	7.8	PERCENT BOUND IN SPECIES	#8113302	=SO1H2+
ADS1TYP2				
	76.5	PERCENT BOUND IN SPECIES	# 812	ADS1TYP2
	9.6	PERCENT BOUND IN SPECIES	#8123301	=SO2-
	13.9	PERCENT BOUND IN SPECIES	#8123302	=SO2H2+
Ba+2				
	99.7	PERCENT BOUND IN SPECIES	# 100	Ba+2
Ca+2				
	99.9	PERCENT BOUND IN SPECIES	# 150	Ca+2
Cd+2				
	23.1	PERCENT BOUND IN SPECIES	# 160	Cd+2
	1.4	PERCENT BOUND IN SPECIES	#8121600	=SO2Cd+
	75.5	PERCENT BOUND IN SPECIES	#8111600	=SO1Cd+
Cr(OH)2+				
	65.0	PERCENT BOUND IN SPECIES	# 211	Cr(OH)2+
	4.7	PERCENT BOUND IN SPECIES	#2113302	Cr(OH)3 AQ
	29.6	PERCENT BOUND IN SPECIES	#2113301	Cr(OH)+2
Cu+2				
	81.5	PERCENT BOUND IN SPECIES	#8112310	=SO1Cu+
	18.4	PERCENT BOUND IN SPECIES	#8122310	=SO2Cu+
ADS1TYP1				
	76.1	PERCENT BOUND IN SPECIES	# 811	ADS1TYP1
	9.6	PERCENT BOUND IN SPECIES	#8113301	=SO1-
	13.9	PERCENT BOUND IN SPECIES	#8113302	=SO1H2+
K+1				
	100.0	PERCENT BOUND IN SPECIES	# 410	K+1
Mg+2				
	100.0	PERCENT BOUND IN SPECIES	# 460	Mg+2
Na+1				
	100.0	PERCENT BOUND IN SPECIES	# 500	Na+1
Ni+2				
	34.8	PERCENT BOUND IN SPECIES	# 540	Ni+2
	59.7	PERCENT BOUND IN SPECIES	#8115400	=SO1Ni+
	5.4	PERCENT BOUND IN SPECIES	#8125400	=SO2Ni+
Pb+2				
	99.8	PERCENT BOUND IN SPECIES	#8116000	=SO1Pb+
Sr+2				
	100.0	PERCENT BOUND IN SPECIES	# 800	Sr+2
Zn+2				
	7.8	PERCENT BOUND IN SPECIES	# 950	Zn+2
	3.9	PERCENT BOUND IN SPECIES	#8129500	=SO2Zn+
	88.3	PERCENT BOUND IN SPECIES	#8119500	=SO1Zn+
Al+3				
	4.0	PERCENT BOUND IN SPECIES	# 303300	AlOH +2
	42.3	PERCENT BOUND IN SPECIES	# 303301	Al(OH)2 +
	1.3	PERCENT BOUND IN SPECIES	# 303302	Al(OH)4 -
	51.7	PERCENT BOUND IN SPECIES	# 303303	Al(OH)3 AQ
Fe+2				
	100.0	PERCENT BOUND IN SPECIES	# 280	Fe+2
CO3-2				
	32.5	PERCENT BOUND IN SPECIES	#3301400	HCO3 -
	67.4	PERCENT BOUND IN SPECIES	#3301401	H2CO3 AQ
H+1				
	1.4	PERCENT BOUND IN SPECIES	#3301400	HCO3 -

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                5.8     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
              293.1     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                7.3     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
E-1
Fe+3
               98.6     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                1.1     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ

H2O
                1.5     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
               33.8     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
               32.1     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                7.3     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                1.4     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
               22.3     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.379E-06	99.7	4.505E-09	0.3	0.000E-01	0.0
150	Ca+2	1.296E-04	99.9	1.459E-07	0.1	0.000E-01	0.0
160	Cd+2	1.090E-09	23.1	3.625E-09	76.9	0.000E-01	0.0
211	Cr(OH)2+	2.790E-08	100.0	0.000E-01	0.0	0.000E-01	0.0
231	Cu+2	3.078E-10	0.1	3.144E-07	99.9	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	6.542E-09	34.9	1.219E-08	65.1	0.000E-01	0.0
600	Pb+2	2.935E-12	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	2.389E-08	7.8	2.821E-07	92.2	0.000E-01	0.0
30	Al+3	3.244E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
280	Fe+2	2.261E-22	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.563E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	2.718E-05	7.4	3.380E-04	92.6	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	3.674E-14	0.0	0.000E-01	0.0	5.372E-07	100.0
2	H2O	7.590E-09	1.0	7.909E-07	99.0	0.000E-01	0.0

```
     Charge Balance: SPECIATED
       Sum of CATIONS =  1.926E-03 Sum of ANIONS   7.634E-04
       PERCENT DIFFERENCE =   4.322E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =  -1.023E-06
     EQUILIBRIUM IONIC STRENGTH (m) =   6.918E-04
     EQUILIBRIUM pH                 =   6.000
     EQUILIBRIUM pe                 =  15.089   or Eh  =   875.51 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.117781     sig0 = 0.015880
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

```
Saturation indices and stoichiometry of all minerals
    ID #      NAME       Sat. Index        Stoichiometry in [brackets]
  2003000 ALOH3(A)         -3.542    [  1.000]  30  [  3.000]   2  [ -3.000] 330
  5015000 ARAGONITE        -5.344    [  1.000] 150  [  1.000] 140
  5046000 ARTINITE        -15.488    [ -2.000] 330  [  2.000] 460  [  1.000] 140
                                     [  5.000]   2
```

2003001	BOEHMITE	-1.755	[-3.000]	330	[1.000]	30	[2.000]	2			
2046000	BRUCITE	-9.054	[1.000]	460	[2.000]	2	[-2.000]	330			
5015001	CALCITE	-5.187	[1.000]	150	[1.000]	140					
2003002	DIASPORE	0.000	[-3.000]	330	[1.000]	30	[2.000]	2			
5015002	DOLOMITE	-10.332	[1.000]	150	[1.000]	460	[2.000]	140			
2028100	FERRIHYDRITE	-6.675	[-3.000]	330	[1.000]	281	[3.000]	2			
2028101	FE3(OH)8	-33.487	[-8.000]	330	[2.000]	281	[1.000]	280			
			[8.000]	2							
2003003	GIBBSITE (C)	-1.871	[-3.000]	330	[1.000]	30	[3.000]	2			
3003000	Al2O3	-8.530	[2.000]	30	[3.000]	2	[-6.000]	330			
2028102	GOETHITE	-2.491	[-3.000]	330	[1.000]	281	[2.000]	2			
3028100	HEMATITE	0.000	[-6.000]	330	[2.000]	281	[3.000]	2			
5015003	HUNTITE	-24.781	[3.000]	460	[1.000]	150	[4.000]	140			
5046001	HYDRMAGNESIT	-38.208	[5.000]	460	[4.000]	140	[-2.000]	330			
			[6.000]	2							
3028101	MAGHEMITE	-9.953	[-6.000]	330	[2.000]	281	[3.000]	2			
5046002	MAGNESITE	-5.643	[1.000]	460	[1.000]	140					
3028000	MAGNETITE	-17.723	[-8.000]	330	[2.000]	281	[1.000]	280			
			[4.000]	2							
3050000	NATRON	-15.541	[2.000]	500	[1.000]	140	[10.000]	2			
5046003	NESQUEHONITE	-8.045	[1.000]	460	[1.000]	140	[3.000]	2			
5028000	SIDERITE	-20.914	[1.000]	280	[1.000]	140					
5080000	STRONTIANITE	-6.745	[1.000]	800	[1.000]	140					
5050001	THERMONATR	-17.242	[2.000]	500	[1.000]	140	[1.000]	2			
5010000	WITHERITE	-7.012	[1.000]	100	[1.000]	140					
5023100	CUCO3	-9.637	[1.000]	231	[1.000]	140					
2023100	CU(OH)2	-6.434	[-2.000]	330	[1.000]	231	[2.000]	2			
2023101	TENORITE	-5.414	[-2.000]	330	[1.000]	231	[1.000]	2			
3023100	CUPRICFERIT	-7.576	[-8.000]	330	[1.000]	231	[2.000]	281			
			[4.000]	2							
95000	ZN METAL	-64.133	[1.000]	950	[2.000]	1					
5095000	SMITHSONITE	-7.427	[1.000]	950	[1.000]	140					
5095001	ZNCO3, 1H2O	-7.104	[1.000]	950	[1.000]	140	[1.000]	2			
2095000	ZN(OH)2 (A)	-8.124	[-2.000]	330	[1.000]	950	[2.000]	2			
2095001	ZN(OH)2 (C)	-7.874	[-2.000]	330	[1.000]	950	[2.000]	2			
2095002	ZN(OH)2 (B)	-7.424	[-2.000]	330	[1.000]	950	[2.000]	2			
2095003	ZN(OH)2 (G)	-7.384	[-2.000]	330	[1.000]	950	[2.000]	2			
2095004	ZN(OH)2 (E)	-7.174	[-2.000]	330	[1.000]	950	[2.000]	2			
2095005	ZNO(ACTIVE)	-6.984	[-2.000]	330	[1.000]	950	[1.000]	2			

ID #	NAME	Sat. Index	Stoichiometry in [brackets]								
2095006	ZINCITE	-7.126	[-2.000]	330	[1.000]	950	[1.000]	2			
16000	CD METAL	-52.938	[1.000]	160	[2.000]	1					
16001	GAMMA CD	-53.040	[1.000]	160	[2.000]	1					
5016000	OTAVITE	-4.973	[1.000]	160	[1.000]	140					
2016000	CD(OH)2 (A)	-11.041	[-2.000]	330	[1.000]	160	[2.000]	2			
2016001	CD(OH)2 (C)	-10.664	[-2.000]	330	[1.000]	160	[2.000]	2			
2016002	MONTEPONITE	-12.488	[-2.000]	330	[1.000]	160	[1.000]	2			
60000	PB METAL	-46.036	[1.000]	600	[2.000]	1					
5060000	CERRUSITE	-8.085	[1.000]	600	[1.000]	140					
2060000	MASSICOT	-12.744	[-2.000]	330	[1.000]	600	[1.000]	2			
2060001	LITHARGE	-12.548	[-2.000]	330	[1.000]	600	[1.000]	2			
2060002	PBO, .3H2O	-12.574	[-2.000]	330	[1.000]	600	[1.330]	2			
5060001	PB2OCO3	-20.543	[-2.000]	330	[2.000]	600	[1.000]	2			
			[1.000]	140							
5060002	PB3O2CO3	-31.871	[-4.000]	330	[3.000]	600	[1.000]	140			
			[2.000]	2							
2060003	PLATTNERITE	-7.728	[-4.000]	330	[-2.000]	1	[1.000]	600			
			[2.000]	2							
3060000	PB2O3	-18.052	[-6.000]	330	[-2.000]	1	[2.000]	600			
			[3.000]	2							
3060001	MINIUM	-31.764	[-8.000]	330	[-2.000]	1	[3.000]	600			
			[4.000]	2							
2060004	PB(OH)2 (C)	-7.944	[-2.000]	330	[1.000]	600	[2.000]	2			
5060003	HYDCERRUSITE	-24.704	[-2.000]	330	[3.000]	600	[2.000]	140			

			[2.000]	2					
2060005	PB2O(OH)2	-25.389	[-4.000]	330	[2.000]	600	[3.000]	2	
5054000	NICO3	-11.229	[1.000]	540	[1.000]	140			
2054000	NI(OH)2	-6.602	[-2.000]	330	[1.000]	540	[2.000]	2	
2054001	BUNSENITE	-9.028	[-2.000]	330	[1.000]	540	[1.000]	2	
5023101	MALACHITE	-11.886	[2.000]	231	[2.000]	2	[1.000]	140	
			[-2.000]	330					
5023102	AZURITE	-19.530	[3.000]	231	[2.000]	2	[2.000]	140	
			[-2.000]	330					
2015000	LIME	-25.397	[-2.000]	330	[1.000]	150	[1.000]	2	
2015001	PORTLANDITE	-15.052	[-2.000]	330	[1.000]	150	[2.000]	2	
2028000	WUSTITE	-20.589	[-2.000]	330	[0.947]	280	[1.000]	2	
2046001	PERICLASE	-13.920	[-2.000]	330	[1.000]	460	[1.000]	2	
3028001	HERCYNITE	-23.529	[-8.000]	330	[1.000]	280	[2.000]	30	
			[4.000]	2					
3046000	SPINEL	-15.049	[-8.000]	330	[1.000]	460	[2.000]	30	
			[4.000]	2					
3046001	MAG-FERRITE	-13.178	[-8.000]	330	[1.000]	460	[2.000]	281	
			[4.000]	2					
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2	
3021100	FECR2O4	-12.659	[2.000]	211	[1.000]	280	[-4.000]	330	
3021101	MGCR2O4	-8.051	[2.000]	211	[1.000]	460	[-4.000]	330	
3021102	CR2O3	-0.288	[2.000]	211	[-2.000]	330	[-1.000]	2	
2021102	CR(OH)3 (A)	-1.004	[1.000]	211	[1.000]	2	[-1.000]	330	
2021101	CR(OH)3 (C)	-3.556	[1.000]	211	[1.000]	2	[-1.000]	330	

2 – Modelling with pH = 6.5

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - pH = 6.5

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair and adsorption

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.162E-07	-6.500	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	3.258E-07	3.162E-07	-6.50000	0.97071	0.013
30	Al+3	6.935E-13	5.307E-13	-12.27513	0.76525	0.116
100	Ba+2	1.346E-06	1.195E-06	-5.92255	0.88788	0.052
150	Ca+2	1.285E-04	1.141E-04	-3.94275	0.88788	0.052
160	Cd+2	1.491E-10	1.324E-10	-9.87813	0.88788	0.052
211	Cr(OH)2+	7.992E-09	7.758E-09	-8.11025	0.97071	0.013
231	Cu+2	3.244E-11	2.880E-11	-10.54058	0.88788	0.052
280	Fe+2	2.261E-23	2.008E-23	-22.69733	0.88788	0.052
410	K+1	6.647E-05	6.452E-05	-4.19029	0.97071	0.013
460	Mg+2	1.439E-04	1.278E-04	-3.89343	0.88788	0.052
500	Na+1	2.088E-04	2.027E-04	-3.69319	0.97071	0.013
540	Ni+2	1.029E-09	9.133E-10	-9.03937	0.88788	0.052

600	Pb+2	3.114E-13	2.765E-13	-12.55837	0.88788	0.052
800	Sr+2	5.707E-07	5.067E-07	-6.29524	0.88788	0.052
950	Zn+2	2.786E-09	2.473E-09	-8.60669	0.88788	0.052
811	ADS1TYP1	1.459E-04	1.459E-04	-3.83605	1.00000	0.000
140	CO3-2	2.297E-09	2.039E-09	-8.69048	0.88788	0.052
281	Fe+3	6.800E-22	5.204E-22	-21.28367	0.76525	0.116
812	ADS1TYP2	5.895E-03	5.895E-03	-2.22949	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	1.045E-12	1.045E-12	-11.98085	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00016	-7.130
2113303	Cr(OH)4-	5.658E-14	5.492E-14	-13.26026	0.97071	-18.137
2113304	CrO2-	1.436E-13	1.394E-13	-12.85585	0.97071	-17.733
3300020	OH-	2.110E-08	2.048E-08	-7.68865	0.97071	-14.176
4603300	MgOH +	4.125E-10	4.004E-10	-9.39748	0.97071	-11.991
4601400	MgCO3 AQ	2.279E-10	2.279E-10	-9.64220	1.00016	2.942
4601401	MgHCO3 +	2.311E-08	2.244E-08	-7.64902	0.97071	11.448
1503300	CaOH +	5.814E-11	5.644E-11	-10.24840	0.97071	-12.793
1501400	CaHCO3 +	1.596E-08	1.549E-08	-7.80983	0.97071	11.336
1501401	CaCO3 AQ	2.938E-10	2.939E-10	-9.53187	1.00016	3.101
5001400	NaCO3 -	5.888E-12	5.715E-12	-11.24297	0.97071	1.154
5001401	NaHCO3 AQ	1.571E-09	1.572E-09	-8.80367	1.00016	10.080
303300	AlOH +2	1.308E-11	1.161E-11	-10.93512	0.88788	-5.108
303301	Al(OH)2 +	4.343E-10	4.216E-10	-9.37514	0.97071	-10.087
303302	Al(OH)4 -	1.283E-10	1.246E-10	-9.90458	0.97071	-23.617
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00016	-16.000
2803300	FeOH +	1.340E-26	1.300E-26	-25.88589	0.97071	-9.676
2803301	FeOH3 -1	2.414E-35	2.343E-35	-34.63021	0.97071	-31.420
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00016	-20.978
2813300	FeOH +2	8.500E-18	7.547E-18	-17.12223	0.88788	-2.287
2813301	FeOH2 +	1.146E-14	1.113E-14	-13.95368	0.97071	-5.657
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00016	-13.600
2813303	FeOH4 -	1.347E-17	1.307E-17	-16.88369	0.97071	-21.587
2813304	Fe2(OH)2+4	3.136E-33	1.949E-33	-32.71021	0.62148	-2.936
2813305	Fe3(OH)4+5	9.278E-45	4.413E-45	-44.35532	0.47558	-6.182
8003300	SrOH +	6.801E-14	6.602E-14	-13.18032	0.97071	-13.372
1003300	BaOH +	1.039E-13	1.009E-13	-12.99620	0.97071	-13.561
2311400	CuCO3 AQ	3.154E-13	3.155E-13	-12.50106	1.00016	6.730
2311401	Cu(CO3)2-2	9.122E-19	8.100E-19	-18.09153	0.88788	9.882
2313300	CuOH +	9.383E-13	9.108E-13	-12.04059	0.97071	-7.987
2313301	Cu(OH)2 AQ	6.016E-12	6.017E-12	-11.22059	1.00016	-13.680
2313302	Cu(OH)3 -	1.184E-18	1.149E-18	-17.93960	0.97071	-26.886
2313303	Cu(OH)4 -2	8.148E-25	7.234E-25	-24.14060	0.88788	-39.548
2313304	Cu2(OH)2+2	2.298E-19	2.041E-19	-18.69024	0.88788	-10.557
2311402	CuHCO3 +	1.914E-13	1.858E-13	-12.73106	0.97071	13.013
9503300	ZnOH +	5.686E-12	5.519E-12	-11.25811	0.97071	-9.139
9503301	Zn(OH)2 AQ	3.121E-13	3.121E-13	-12.50570	1.00016	-16.899
9503302	Zn(OH)3 -	3.215E-18	3.121E-18	-17.50571	0.97071	-28.386
9503303	Zn(OH)4 -2	1.762E-24	1.564E-24	-23.80572	0.88788	-41.147
9501400	ZnHCO3 +	4.128E-12	4.007E-12	-11.39717	0.97071	12.413
9501401	ZnCO3 AQ	1.006E-12	1.007E-12	-11.99717	1.00016	5.300
9501402	Zn(CO3)2-2	4.943E-17	4.389E-17	-16.35764	0.88788	9.682
1601400	Cd(CO3)3-4	2.999E-30	1.864E-30	-29.72956	0.62148	6.427
1603300	CdOH +	2.331E-14	2.263E-14	-13.64528	0.97071	-10.254
1603301	Cd(OH)2 AQ	5.913E-18	5.914E-18	-17.22814	1.00016	-20.350
1603302	Cd(OH)3 -	2.162E-24	2.098E-24	-23.67815	0.97071	-33.287
1603303	Cd(OH)4 -2	6.660E-32	5.914E-32	-31.22815	0.88788	-47.298
1603304	Cd2OH +3	2.062E-23	1.578E-23	-22.80196	0.76525	-9.430
1601400	CdHCO3 +	2.210E-13	2.145E-13	-12.66861	0.97071	12.413
1601401	CdCO3 AQ	6.766E-14	6.767E-14	-13.16961	1.00016	5.399
6001400	Pb(CO3)2-2	5.654E-20	5.020E-20	-19.29933	0.88788	10.692
6003300	PbOH +	1.756E-14	1.705E-14	-13.76838	0.97071	-7.697
6003301	Pb(OH)2 AQ	2.097E-17	2.097E-17	-16.67838	1.00016	-17.120

6003302	Pb(OH)3 -	7.844E-22	7.614E-22	-21.11839	0.97071	-28.047
6003303	Pb2OH +3	1.379E-25	1.055E-25	-24.97675	0.76525	-6.244
6003304	Pb3(OH)4+2	1.312E-36	1.165E-36	-35.93371	0.88788	-24.207
6001401	PbCO3 AQ	9.797E-15	9.798E-15	-14.00885	1.00016	7.240
6003305	Pb(OH)4 -2	6.227E-27	5.528E-27	-26.25740	0.88788	-39.647
6001402	PbHCO3 +	2.911E-15	2.826E-15	-14.54885	0.97071	13.213
5403300	NiOH +	2.730E-13	2.650E-13	-12.57681	0.97071	-10.025
5403301	Ni(OH)2 AQ	9.132E-16	9.133E-16	-15.03939	1.00016	-19.000
5403302	Ni(OH)3 -	2.975E-20	2.888E-20	-19.53939	0.97071	-29.987
5401400	NiHCO3 +	1.791E-12	1.738E-12	-11.75985	0.97071	12.483
5401401	NiCO3 AQ	1.381E-11	1.381E-11	-10.85985	1.00016	6.870
5401402	Ni(CO3)2-2	5.512E-17	4.894E-17	-16.31033	0.88788	10.162
3301400	HCO3 -	1.607E-05	1.560E-05	-4.80680	0.97071	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00016	16.713
2113300	Cr+3	8.197E-12	6.273E-12	-11.20252	0.76525	10.024
2113301	Cr(OH)+2	1.152E-09	1.023E-09	-8.99024	0.88788	5.672
8123301	=SO2-	8.034E-04	8.034E-04	-3.09508	1.00000	-8.930
8123302	=SO2H2+	9.911E-04	9.911E-04	-3.00389	1.00000	7.290
8113301	=SO1-	1.988E-05	1.988E-05	-4.70164	1.00000	-8.930
8113302	=SO1H2+	2.452E-05	2.452E-05	-4.61046	1.00000	7.290
8129500	=SO2Zn+	1.286E-08	1.286E-08	-7.89059	1.00000	-1.990
8119500	=SO1Zn+	2.903E-07	2.903E-07	-6.53716	1.00000	0.970
8121600	=SO2Cd+	8.472E-11	8.472E-11	-10.07203	1.00000	-2.900
8111600	=SO1Cd+	4.481E-09	4.481E-09	-8.34859	1.00000	0.430
8112310	=SO1Cu+	2.564E-07	2.564E-07	-6.59104	1.00000	2.850
8122310	=SO2Cu+	5.828E-08	5.828E-08	-7.23448	1.00000	0.600
8115400	=SO1Ni+	1.622E-08	1.622E-08	-7.78984	1.00000	0.150
8125400	=SO2Ni+	1.468E-09	1.468E-09	-8.83327	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74884	1.00000	4.710
8126000	=SO2Pb+	2.804E-10	2.804E-10	-9.55227	1.00000	0.300
8121500	=SO2Ca+	8.191E-08	8.191E-08	-7.08664	1.00000	-5.850
8111500	=SO1HCa++	1.154E-06	1.154E-06	-5.93762	1.00000	4.970
8111000	=SO1HBa++	3.738E-08	3.738E-08	-7.42742	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	1.806E-04	-3.743	0.000	0.000
330	H+1	-5.967E-04	-3.224	6.500	0.000
3301403	CO2 (g)	4.208E-04	-3.376	21.690	-0.530
3300021	O2 (g)	1.144E-04	-3.941	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.816E-06	-5.317	-7.225	24.630
3021102	CR2O3	8.467E-09	-8.072	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1PSIo

506.6	PERCENT BOUND IN SPECIES #8123302	=SO2H2+
12.5	PERCENT BOUND IN SPECIES #8113302	=SO1H2+
1.2	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++

ADS1TYP2

76.7	PERCENT BOUND IN SPECIES # 812	ADS1TYP2
10.4	PERCENT BOUND IN SPECIES #8123301	=SO2-
12.9	PERCENT BOUND IN SPECIES #8123302	=SO2H2+

Ba+2

97.3	PERCENT BOUND IN SPECIES # 100	Ba+2
2.7	PERCENT BOUND IN SPECIES #8111000	=SO1HBa++

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Ca+2
              99.0     PERCENT BOUND IN SPECIES #    150   Ca+2
Cd+2
               3.2     PERCENT BOUND IN SPECIES #    160   Cd+2
               1.8     PERCENT BOUND IN SPECIES #8121600   =SO2Cd+
              95.0     PERCENT BOUND IN SPECIES #8111600   =SO1Cd+
Zn+2
               4.2     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
              94.9     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
Cu+2
              81.5     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
              18.5     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
ADS1TYP1
              75.9     PERCENT BOUND IN SPECIES #    811   ADS1TYP1
              10.3     PERCENT BOUND IN SPECIES #8113301   =SO1-
              12.8     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
K+1
             100.0     PERCENT BOUND IN SPECIES #    410   K+1

Mg+2
             100.0     PERCENT BOUND IN SPECIES #    460   Mg+2
Na+1
             100.0     PERCENT BOUND IN SPECIES #    500   Na+1
Ni+2
               5.5     PERCENT BOUND IN SPECIES #    540   Ni+2
              86.6     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
               7.8     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
              99.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
             100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Cr(OH)2+
              72.8     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
              16.6     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
              10.5     PERCENT BOUND IN SPECIES #2113301   Cr(OH)+2
Al+3
              19.3     PERCENT BOUND IN SPECIES # 303301   Al(OH)2 +
               5.7     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
              74.4     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
              60.3     PERCENT BOUND IN SPECIES #3301400   HCO3 -
              39.5     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
              99.9     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
              96.3     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
               3.5     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
H+1
               7.0     PERCENT BOUND IN SPECIES #3301400   HCO3 -
               9.2     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
             432.9     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
              10.7     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
               2.5     PERCENT BOUND IN SPECIES #3300020   OH-
               1.5     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
              34.3     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
              30.3     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
               6.9     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
               1.9     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
              21.0     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.346E-06	97.3	3.738E-08	2.7	0.000E-01	0.0
150	Ca+2	1.285E-04	99.0	1.236E-06	1.0	0.000E-01	0.0
160	Cd+2	1.494E-10	3.2	4.566E-09	96.8	0.000E-01	0.0
950	Zn+2	2.797E-09	0.9	3.032E-07	99.1	0.000E-01	0.0
231	Cu+2	3.990E-11	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.045E-09	5.6	1.769E-08	94.4	0.000E-01	0.0
600	Pb+2	3.417E-13	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	1.097E-08	39.3	0.000E-01	0.0	1.693E-08	60.7
30	Al+3	2.254E-09	0.0	0.000E-01	0.0	4.816E-06	100.0
140	CO3-2	2.665E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.262E-23	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.190E-14	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	3.748E-05	16.4	1.914E-04	83.6	0.000E-01	0.0
2	H2O	2.867E-08	3.4	8.187E-07	96.6	0.000E-01	0.0

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 Charge Balance: SPECIATED
       Sum of CATIONS =  1.843E-03 Sum of ANIONS   8.394E-04
       PERCENT DIFFERENCE =   3.742E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =  -3.046E-07
     EQUILIBRIUM IONIC STRENGTH (m) =   6.946E-04
     EQUILIBRIUM pH                 =   6.500
     EQUILIBRIUM pe                 =  14.589   or Eh  =   846.50 mv
******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.090776     sig0 = 0.009143
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
```

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-4.348	[1.000] 150 [1.000] 140
5046000	ARTINITE	-13.488	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-8.055	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-4.191	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-8.336	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-20.785	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-33.209	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2

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5046002 MAGNESITE       -4.643    [  1.000] 460  [  1.000] 140
3028000 MAGNETITE      -17.723    [ -8.000] 330  [  2.000] 281  [  1.000] 280
                                  [  4.000]   2
3050000 NATRON         -14.541    [  2.000] 500  [  1.000] 140  [ 10.000]   2
5046003 NESQUEHONITE    -7.046    [  1.000] 460  [  1.000] 140  [  3.000]   2
5028000 SIDERITE       -20.914    [  1.000] 280  [  1.000] 140
5080000 STRONTIANITE    -5.746    [  1.000] 800  [  1.000] 140
5050001 THERMONATR     -16.242    [  2.000] 500  [  1.000] 140  [  1.000]   2
5010000 WITHERITE       -6.023    [  1.000] 100  [  1.000] 140
5023100 CUCO3           -9.601    [  1.000] 231  [  1.000] 140
2023100 CU(OH)2         -6.398    [ -2.000] 330  [  1.000] 231  [  2.000]   2
2023101 TENORITE        -5.378    [ -2.000] 330  [  1.000] 231  [  1.000]   2
3023100 CUPRICFERIT     -7.541    [ -8.000] 330  [  1.000] 231  [  2.000] 281
                                  [  4.000]   2
  95000 ZN METAL       -64.066    [  1.000] 950  [  2.000]   1
5095000 SMITHSONITE     -7.359    [  1.000] 950  [  1.000] 140
5095001 ZNCO3, 1H2O     -7.037    [  1.000] 950  [  1.000] 140  [  1.000]   2
2095000 ZN(OH)2 (A)     -8.057    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095001 ZN(OH)2 (C)     -7.807    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095002 ZN(OH)2 (B)     -7.357    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095003 ZN(OH)2 (G)     -7.317    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095004 ZN(OH)2 (E)     -7.107    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095005 ZNO(ACTIVE)     -6.917    [ -2.000] 330  [  1.000] 950  [  1.000]   2

ID #      NAME       Sat. Index       Stoichiometry in [brackets]
2095006 ZINCITE         -7.059    [ -2.000] 330  [  1.000] 950  [  1.000]   2
  16000 CD METAL       -52.802    [  1.000] 160  [  2.000]   1
  16001 GAMMA CD       -52.904    [  1.000] 160  [  2.000]   1
5016000 OTAVITE         -4.837    [  1.000] 160  [  1.000] 140
2016000 CD(OH)2 (A)    -10.905    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)    -10.528    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE    -12.352    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL       -46.000    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE       -8.049    [  1.000] 600  [  1.000] 140
2060000 MASSICOT       -12.708    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE       -12.512    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O     -12.538    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3        -20.471    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                  [  1.000] 140
5060002 PB3O2CO3       -31.763    [ -4.000] 330  [  3.000] 600  [  1.000] 140
                                  [  2.000]   2
2060003 PLATTNERITE     -7.692    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                  [  2.000]   2
3060000 PB2O3          -17.980    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                  [  3.000]   2
3060001 MINIUM         -31.656    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                  [  4.000]   2
2060004 PB(OH)2 (C)     -7.908    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE   -24.596    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                  [  2.000]   2
2060005 PB2O(OH)2      -25.317    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3          -11.032    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2         -6.404    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE       -8.831    [ -2.000] 330  [  1.000] 540  [  1.000]   2
5023101 MALACHITE      -11.815    [  2.000] 231  [  2.000]   2  [  1.000] 140
                                  [ -2.000] 330
5023102 AZURITE        -19.422    [  3.000] 231  [  2.000]   2  [  2.000] 140
                                  [ -2.000] 330
2015000 LIME           -24.401    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE    -14.056    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE        -20.536    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE      -12.920    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE      -23.529    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                  [  4.000]   2
3046000 SPINEL         -14.049    [ -8.000] 330  [  1.000] 460  [  2.000]  30
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			[4.000]	2					
3046001	MAG-FERRITE	-12.178	[-8.000]	330	[1.000]	460	[2.000]	281	
			[4.000]	2					
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2	
3021100	FECR2O4	-12.371	[2.000]	211	[1.000]	280	[-4.000]	330	
3021101	MGCR2O4	-6.763	[2.000]	211	[1.000]	460	[-4.000]	330	
3021102	CR2O3	0.000	[2.000]	211	[-2.000]	330	[-1.000]	2	
2021102	CR(OH)3 (A)	-0.860	[1.000]	211	[1.000]	2	[-1.000]	330	
2021101	CR(OH)3 (C)	-3.412	[1.000]	211	[1.000]	2	[-1.000]	330	

3 – Modelling with pH = 7.0

PART 1 of OUTPUT FILE

Revuè river water-Site 14 – pH = 7.0

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair and adsorption

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	2.449E-11	2.449E-11	-10.61101	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00016	-7.130
2113303	Cr(OH)4-	1.789E-13	1.737E-13	-12.76026	0.97072	-18.137
2113304	CrO2-	4.540E-13	4.407E-13	-12.35585	0.97072	-17.733
3300020	OH-	6.672E-08	6.477E-08	-7.18865	0.97072	-14.176
4603300	MgOH +	1.304E-09	1.266E-09	-8.89763	0.97072	-11.991
4601400	MgCO3 AQ	2.278E-09	2.278E-09	-8.64236	1.00016	2.942
4601401	MgHCO3 +	7.307E-08	7.093E-08	-7.14918	0.97072	11.448
1503300	CaOH +	1.714E-10	1.664E-10	-9.77885	0.97072	-12.793
1501400	CaHCO3 +	4.706E-08	4.568E-08	-7.34028	0.97072	11.336
1501401	CaCO3 AQ	2.739E-09	2.740E-09	-8.56232	1.00016	3.101
5001400	NaCO3 -	5.887E-11	5.715E-11	-10.24297	0.97072	1.154

5001401	NaHCO3 AQ	4.969E-09	4.970E-09	-8.30368	1.00016	10.080
303300	AlOH +2	1.308E-12	1.161E-12	-11.93512	0.88793	-5.108
303301	Al(OH)2 +	1.373E-10	1.333E-10	-9.87514	0.97072	-10.087
303302	Al(OH)4 -	4.058E-10	3.939E-10	-9.40458	0.97072	-23.617
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00016	-16.000
2803300	FeOH +	4.237E-27	4.113E-27	-26.38589	0.97072	-9.676
2803301	FeOH3 -1	7.633E-35	7.410E-35	-34.13021	0.97072	-31.420
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00016	-20.978
2813300	FeOH +2	8.499E-19	7.547E-19	-18.12223	0.88793	-2.287
2813301	FeOH2 +	3.624E-15	3.518E-15	-14.45368	0.97072	-5.657
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00016	-13.600
2813303	FeOH4 -	4.258E-17	4.133E-17	-16.38369	0.97072	-21.587
2813304	Fe2(OH)2+4	3.135E-35	1.949E-35	-34.71021	0.62160	-2.936
2813305	Fe3(OH)4+5	2.933E-47	1.395E-47	-46.85532	0.47573	-6.182
8003300	SrOH +	2.151E-13	2.088E-13	-12.68032	0.97072	-13.372
1003300	BaOH +	2.731E-13	2.651E-13	-12.57664	0.97072	-13.561
2311400	CuCO3 AQ	3.461E-13	3.461E-13	-12.46076	1.00016	6.730
2311401	Cu(CO3)2-2	1.001E-17	8.887E-18	-17.05124	0.88793	9.882
2313300	CuOH +	3.256E-13	3.160E-13	-12.50029	0.97072	-7.987
2313301	Cu(OH)2 AQ	6.601E-12	6.602E-12	-11.18029	1.00016	-13.680
2313302	Cu(OH)3 -	4.108E-18	3.987E-18	-17.39930	0.97072	-26.886
2313303	Cu(OH)4 -2	8.940E-24	7.938E-24	-23.10031	0.88793	-39.548
2313304	Cu2(OH)2+2	2.767E-20	2.457E-20	-19.60964	0.88793	-10.557
2311402	CuHCO3 +	6.640E-14	6.445E-14	-13.19076	0.97072	13.013
9503300	ZnOH +	2.002E-12	1.943E-12	-11.71152	0.97072	-9.139
9503301	Zn(OH)2 AQ	3.474E-13	3.474E-13	-12.45911	1.00016	-16.899
9503302	Zn(OH)3 -	1.132E-17	1.099E-17	-16.95912	0.97072	-28.386
9503303	Zn(OH)4 -2	1.961E-23	1.741E-23	-22.75912	0.88793	-41.147
9501400	ZnHCO3 +	1.453E-12	1.411E-12	-11.85058	0.97072	12.413
9501401	ZnCO3 AQ	1.120E-12	1.121E-12	-11.95057	1.00016	5.300
9501402	Zn(CO3)2-2	5.503E-16	4.886E-16	-15.31105	0.88793	9.682
1601400	Cd(CO3)3-4	3.411E-28	2.120E-28	-27.67364	0.62160	6.426
1603300	CdOH +	8.386E-15	8.140E-15	-14.08935	0.97072	-10.254
1603301	Cd(OH)2 AQ	6.725E-18	6.726E-18	-17.17222	1.00016	-20.350
1603302	Cd(OH)3 -	7.775E-24	7.547E-24	-23.12222	0.97072	-33.287
1603303	Cd(OH)4 -2	7.575E-31	6.726E-31	-30.17223	0.88793	-47.298
1603304	Cd2OH +3	8.434E-25	6.455E-25	-24.19011	0.76533	-9.430
1601400	CdHCO3 +	7.947E-14	7.715E-14	-13.11268	0.97072	12.413
1601401	CdCO3 AQ	7.696E-14	7.697E-14	-13.11368	1.00016	5.399
6001400	Pb(CO3)2-2	6.254E-19	5.553E-19	-18.25547	0.88793	10.692
6003300	PbOH +	6.143E-15	5.963E-15	-14.22452	0.97072	-7.697
6003301	Pb(OH)2 AQ	2.320E-17	2.320E-17	-16.63453	1.00016	-17.120
6003302	Pb(OH)3 -	2.744E-21	2.664E-21	-20.57454	0.97072	-28.047
6003303	Pb2OH +3	5.335E-27	4.083E-27	-26.38904	0.76533	-6.244
6003304	Pb3(OH)4+2	1.776E-37	1.577E-37	-36.80215	0.88793	-24.207
6001401	PbCO3 AQ	1.084E-14	1.084E-14	-13.96499	1.00016	7.240
6003305	Pb(OH)4 -2	6.888E-26	6.116E-26	-25.21354	0.88793	-39.647
6001402	PbHCO3 +	1.018E-15	9.886E-16	-15.00500	0.97072	13.213
5403300	NiOH +	1.000E-13	9.710E-14	-13.01280	0.97072	-10.025
5403301	Ni(OH)2 AQ	1.058E-15	1.058E-15	-14.97538	1.00016	-19.000
5403302	Ni(OH)3 -	1.090E-19	1.058E-19	-18.97539	0.97072	-29.987
5401400	NiHCO3 +	6.562E-13	6.370E-13	-12.19584	0.97072	12.483
5401401	NiCO3 AQ	1.600E-11	1.600E-11	-10.79584	1.00016	6.870
5401402	Ni(CO3)2-2	6.387E-16	5.671E-16	-15.24632	0.88793	10.162
3301400	HCO3 -	5.083E-05	4.934E-05	-4.30680	0.97072	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00016	16.713
2113300	Cr+3	2.592E-13	1.984E-13	-12.70252	0.76533	10.024
2113301	Cr(OH)+2	1.152E-10	1.023E-10	-9.99024	0.88793	5.672
8123301	=SO2-	8.519E-04	8.519E-04	-3.06961	1.00000	-8.930
8123302	=SO2H2+	9.364E-04	9.364E-04	-3.02855	1.00000	7.290
8113301	=SO1-	2.016E-05	2.016E-05	-4.69541	1.00000	-8.930
8113302	=SO1H2+	2.216E-05	2.216E-05	-4.65434	1.00000	7.290
8129500	=SO2Zn+	1.353E-08	1.353E-08	-7.86865	1.00000	-1.990
8119500	=SO1Zn+	2.921E-07	2.921E-07	-6.53445	1.00000	0.970
8121600	=SO2Cd+	9.104E-11	9.104E-11	-10.04076	1.00000	-2.900

8111600	=SO1Cd+	4.607E-09	4.607E-09	-8.33655	1.00000	0.430
8112310	=SO1Cu+	2.543E-07	2.543E-07	-6.59463	1.00000	2.850
8122310	=SO2Cu+	6.042E-08	6.042E-08	-7.21883	1.00000	0.600
8115400	=SO1Ni+	1.699E-08	1.699E-08	-7.76972	1.00000	0.150
8125400	=SO2Ni+	1.607E-09	1.607E-09	-8.79392	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74887	1.00000	4.710
8126000	=SO2Pb+	2.930E-10	2.930E-10	-9.53307	1.00000	0.300
8121500	=SO2Ca+	7.215E-07	7.215E-07	-6.14175	1.00000	-5.850
8111500	=SO1HCa++	9.183E-06	9.183E-06	-5.03701	1.00000	4.970
8111000	=SO1HBa++	2.650E-07	2.650E-07	-6.57681	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	1.457E-04	-3.836	0.000	0.000
330	H+1	-4.550E-04	-3.342	7.000	0.000
3301403	CO2 (g)	3.856E-04	-3.414	21.690	-0.530
3300021	O2 (g)	1.143E-04	-3.942	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.816E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.172E-08	-7.931	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1PSIo

875.8	PERCENT BOUND IN SPECIES	#8123302	=SO2H2+
20.7	PERCENT BOUND IN SPECIES	#8113302	=SO1H2+
17.2	PERCENT BOUND IN SPECIES	#8111500	=SO1HCa++

ADS1TYP2

76.7	PERCENT BOUND IN SPECIES	# 812	ADS1TYP2
11.1	PERCENT BOUND IN SPECIES	#8123301	=SO2-
12.2	PERCENT BOUND IN SPECIES	#8123302	=SO2H2+

Ba+2

80.8	PERCENT BOUND IN SPECIES	# 100	Ba+2
19.2	PERCENT BOUND IN SPECIES	#8111000	=SO1HBa++

Ca+2

92.3	PERCENT BOUND IN SPECIES	# 150	Ca+2
7.1	PERCENT BOUND IN SPECIES	#8111500	=SO1HCa++

Cd+2

1.9	PERCENT BOUND IN SPECIES	#8121600	=SO2Cd+
97.7	PERCENT BOUND IN SPECIES	#8111600	=SO1Cd+

Zn+2

4.4	PERCENT BOUND IN SPECIES	#8129500	=SO2Zn+
95.5	PERCENT BOUND IN SPECIES	#8119500	=SO1Zn+

Cu+2

80.8	PERCENT BOUND IN SPECIES	#8112310	=SO1Cu+
19.2	PERCENT BOUND IN SPECIES	#8122310	=SO2Cu+

ADS1TYP1

72.7	PERCENT BOUND IN SPECIES	# 811	ADS1TYP1
10.5	PERCENT BOUND IN SPECIES	#8113301	=SO1-
11.5	PERCENT BOUND IN SPECIES	#8113302	=SO1H2+
4.8	PERCENT BOUND IN SPECIES	#8111500	=SO1HCa++

K+1

100.0	PERCENT BOUND IN SPECIES	# 410	K+1

Mg+2

99.9	PERCENT BOUND IN SPECIES	# 460	Mg+2

Na+1

100.0	PERCENT BOUND IN SPECIES	# 500	Na+1

Ni+2

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                 90.7     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                  8.6     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
                 99.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
                100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Cr(OH)2+
                 56.6     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
                 40.8     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
                  2.6     PERCENT BOUND IN SPECIES #2113301   Cr(OH)+2
Al+3
                  6.2     PERCENT BOUND IN SPECIES # 303301   Al(OH)2 +
                 18.3     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                 75.5     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
                 82.6     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 17.1     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
                 99.8     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
                 88.8     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                 10.1     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                  1.0     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
                 32.4     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 13.4     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
                596.5     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                 14.1     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                  7.4     PERCENT BOUND IN SPECIES #3300020   OH-
                  1.5     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                 32.5     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                 28.3     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                  6.7     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                  1.9     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                 19.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
100	Ba+2	1.118E-06	80.8	2.650E-07	19.2	0.000E-01	0.0
150	Ca+2	1.198E-04	92.4	9.905E-06	7.6	0.000E-01	0.0
160	Cd+2	1.712E-11	0.4	4.698E-09	99.6	0.000E-01	0.0
950	Zn+2	3.150E-10	0.1	3.056E-07	99.9	0.000E-01	0.0
231	Cu+2	1.090E-11	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.360E-10	0.7	1.860E-08	99.3	0.000E-01	0.0
600	Pb+2	5.247E-14	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	4.462E-09	16.0	0.000E-01	0.0	2.344E-08	84.0
30	Al+3	2.222E-09	0.0	0.000E-01	0.0	4.816E-06	100.0
140	CO3-2	6.151E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.265E-24	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	4.081E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	7.205E-05	45.9	8.494E-05	54.1	0.000E-01	0.0
2	H2O	7.685E-08	8.5	8.223E-07	91.5	0.000E-01	0.0

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     Charge Balance: SPECIATED
       Sum of CATIONS =  1.785E-03 Sum of ANIONS   9.230E-04
       PERCENT DIFFERENCE =   3.184E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =  -3.613E-08
     EQUILIBRIUM IONIC STRENGTH (m) =   6.940E-04
     EQUILIBRIUM pH                 =   7.000
     EQUILIBRIUM pe                 =  14.089   or Eh  =   817.49 mv
******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.063218     sig0 = 0.004996
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-3.378	[1.000] 150 [1.000] 140
5046000	ARTINITE	-11.488	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-7.055	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-3.221	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-6.366	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-16.816	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-28.210	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-3.643	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-13.541	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-6.046	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-4.746	[1.000] 800 [1.000] 140
5050001	THERMONATR	-15.242	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-5.103	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.561	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.358	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.338	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.500	[-8.000] 330 [1.000] 231 [2.000] 281 [4.000] 2
95000	ZN METAL	-64.020	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.313	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-6.991	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-8.010	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.760	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.310	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.270	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-7.060	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.870	[-2.000] 330 [1.000] 950 [1.000] 2
ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2095006	ZINCITE	-7.012	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.746	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.848	[1.000] 160 [2.000] 1

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5016000 OTAVITE          -4.781    [  1.000] 160  [  1.000] 140
2016000 CD(OH)2 (A)     -10.849    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)     -10.472    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE     -12.296    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL        -45.956    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE        -8.006    [  1.000] 600  [  1.000] 140
2060000 MASSICOT        -12.664    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE        -12.469    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O      -12.495    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3         -20.383    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                   [  1.000] 140
5060002 PB3O2CO3        -31.632    [ -4.000] 330  [  3.000] 600  [  1.000] 140
                                   [  2.000]   2
2060003 PLATTNERITE      -7.648    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                   [  2.000]   2
3060000 PB2O3           -17.892    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                   [  3.000]   2
3060001 MINIUM          -31.525    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                   [  4.000]   2
2060004 PB(OH)2 (C)      -7.864    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE    -24.465    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                   [  2.000]   2
2060005 PB2O(OH)2       -25.229    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3           -10.968    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2          -6.340    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE        -8.767    [ -2.000] 330  [  1.000] 540  [  1.000]   2
5023101 MALACHITE       -11.734    [  2.000] 231  [  2.000]   2  [  1.000] 140
                                   [ -2.000] 330
5023102 AZURITE         -19.301    [  3.000] 231  [  2.000]   2  [  2.000] 140
                                   [ -2.000] 330
2015000 LIME            -23.431    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE     -13.087    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE         -20.483    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE       -11.920    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE       -23.529    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                   [  4.000]   2
3046000 SPINEL          -13.050    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                   [  4.000]   2
3046001 MAG-FERRITE     -11.178    [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                   [  4.000]   2
3028102 LEPIDOCROCIT     -3.155    [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021100 FECR2O4         -12.371    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4          -5.763    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3             0.000    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)      -0.860    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)      -3.412    [  1.000] 211  [  1.000]   2  [ -1.000] 330
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4 – Modelling with pH = 7.6

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - pH = 7.6

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair and adsorption

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Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.586E-08	2.512E-08	-7.60000	0.97123	0.013
30	Al+3	3.459E-16	2.660E-16	-15.57513	0.76898	0.114
100	Ba+2	4.101E-07	3.649E-07	-6.43787	0.88980	0.051
150	Ca+2	6.986E-05	6.216E-05	-4.20649	0.88980	0.051
160	Cd+2	1.546E-12	1.376E-12	-11.86154	0.88980	0.051
211	Cr(OH)2+	6.345E-10	6.162E-10	-9.21025	0.97123	0.013
231	Cu+2	3.061E-13	2.724E-13	-12.56487	0.88980	0.051
280	Fe+2	1.424E-25	1.267E-25	-24.89733	0.88980	0.051
410	K+1	6.647E-05	6.456E-05	-4.19006	0.97123	0.013
460	Mg+2	1.436E-04	1.278E-04	-3.89344	0.88980	0.051
500	Na+1	2.088E-04	2.028E-04	-3.69300	0.97123	0.013
540	Ni+2	1.065E-11	9.481E-12	-11.02315	0.88980	0.051

600	Pb+2	3.147E-15	2.801E-15	-14.55275	0.88980	0.051
800	Sr+2	5.707E-07	5.078E-07	-6.29432	0.88980	0.051
950	Zn+2	2.797E-11	2.489E-11	-10.60397	0.88980	0.051
811	ADS1TYP1	1.050E-04	1.050E-04	-3.97864	1.00000	0.000
140	CO3-2	3.633E-07	3.232E-07	-6.49048	0.88980	0.051
281	Fe+3	3.392E-25	2.608E-25	-24.58367	0.76898	0.114
812	ADS1TYP2	5.897E-03	5.897E-03	-2.22936	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	4.757E-10	4.757E-10	-9.32262	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00015	-7.130
2113303	Cr(OH)4-	7.119E-13	6.914E-13	-12.16026	0.97123	-18.137
2113304	CrO2-	1.806E-12	1.755E-12	-11.75585	0.97123	-17.733
3300020	OH-	2.655E-07	2.578E-07	-6.58865	0.97123	-14.176
4603300	MgOH +	5.190E-09	5.041E-09	-8.29749	0.97123	-11.991
4601400	MgCO3 AQ	3.612E-08	3.612E-08	-7.44221	1.00015	2.942
4601401	MgHCO3 +	2.908E-07	2.825E-07	-6.54903	0.97123	11.448
1503300	CaOH +	3.986E-10	3.871E-10	-9.41214	0.97123	-12.793
1501400	CaHCO3 +	1.094E-07	1.063E-07	-6.97357	0.97123	11.336
1501401	CaCO3 AQ	2.537E-08	2.537E-08	-7.59561	1.00015	3.101
5001400	NaCO3 -	9.330E-10	9.062E-10	-9.04278	0.97123	1.153
5001401	NaHCO3 AQ	1.979E-08	1.979E-08	-7.70348	1.00015	10.080
303300	AlOH +2	8.233E-14	7.326E-14	-13.13512	0.88980	-5.109
303301	Al(OH)2 +	3.448E-11	3.349E-11	-10.47514	0.97123	-10.087
303302	Al(OH)4 -	1.615E-09	1.568E-09	-8.80458	0.97123	-23.617
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00015	-16.000
2803300	FeOH +	1.064E-27	1.033E-27	-26.98589	0.97123	-9.676
2803301	FeOH3 -1	3.037E-34	2.950E-34	-33.53021	0.97123	-31.420
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00015	-20.978
2813300	FeOH +2	5.351E-20	4.762E-20	-19.32223	0.88980	-2.288
2813301	FeOH2 +	9.099E-16	8.837E-16	-15.05368	0.97123	-5.657
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00015	-13.600
2813303	FeOH4 -	1.694E-16	1.646E-16	-15.78369	0.97123	-21.587
2813304	Fe2(OH)2+4	1.238E-37	7.759E-38	-37.11021	0.62687	-2.940
2813305	Fe3(OH)4+5	2.895E-50	1.395E-50	-49.85531	0.48205	-6.187
8003300	SrOH +	8.576E-13	8.329E-13	-12.07940	0.97123	-13.372
1003300	BaOH +	3.992E-13	3.877E-13	-12.41152	0.97123	-13.561
2311400	CuCO3 AQ	4.727E-13	4.728E-13	-12.32534	1.00015	6.730
2311401	Cu(CO3)2-2	2.162E-16	1.924E-16	-15.71582	0.88980	9.881
2313300	CuOH +	1.116E-13	1.084E-13	-12.96487	0.97123	-7.987
2313301	Cu(OH)2 AQ	9.017E-12	9.018E-12	-11.04488	1.00015	-13.680
2313302	Cu(OH)3 -	2.232E-17	2.168E-17	-16.66389	0.97123	-26.886
2313303	Cu(OH)4 -2	1.931E-22	1.718E-22	-21.76489	0.88980	-39.549
2313304	Cu2(OH)2+2	3.250E-21	2.892E-21	-20.53881	0.88980	-10.558
2311402	CuHCO3 +	2.277E-14	2.211E-14	-13.65535	0.97123	13.013
9503300	ZnOH +	7.199E-13	6.992E-13	-12.15539	0.97123	-9.139
9503301	Zn(OH)2 AQ	4.977E-13	4.978E-13	-12.30298	1.00015	-16.899
9503302	Zn(OH)3 -	6.452E-17	6.266E-17	-16.20299	0.97123	-28.386
9503303	Zn(OH)4 -2	4.443E-22	3.954E-22	-21.40300	0.88980	-41.148
9501400	ZnHCO3 +	5.227E-13	5.076E-13	-12.29445	0.97123	12.413
9501401	ZnCO3 AQ	1.605E-12	1.605E-12	-11.79445	1.00015	5.300
9501402	Zn(CO3)2-2	1.247E-14	1.109E-14	-13.95493	0.88980	9.681
1601400	Cd(CO3)3-4	1.230E-25	7.710E-26	-25.11297	0.62687	6.423
1603300	CdOH +	3.048E-15	2.960E-15	-14.52869	0.97123	-10.254
1603301	Cd(OH)2 AQ	9.736E-18	9.738E-18	-17.01155	1.00015	-20.350
1603302	Cd(OH)3 -	4.478E-23	4.350E-23	-22.36156	0.97123	-33.287
1603303	Cd(OH)4 -2	1.734E-29	1.543E-29	-28.81156	0.88980	-47.299
1603304	Cd2OH +3	2.788E-26	2.144E-26	-25.66878	0.76898	-9.432
1601400	CdHCO3 +	2.888E-14	2.805E-14	-13.55202	0.97123	12.413
1601401	CdCO3 AQ	1.114E-13	1.114E-13	-12.95301	1.00015	5.399
6001400	Pb(CO3)2-2	1.435E-17	1.277E-17	-16.89370	0.88980	10.691
6003300	PbOH +	2.238E-15	2.174E-15	-14.66276	0.97123	-7.697
6003301	Pb(OH)2 AQ	3.366E-17	3.367E-17	-16.47276	1.00015	-17.120

6003302	Pb(OH)3 -	1.585E-20	1.539E-20	-19.81277	0.97123	-28.047
6003303	Pb2OH +3	1.772E-28	1.363E-28	-27.86551	0.76898	-6.246
6003304	Pb3(OH)4+2	3.419E-38	3.042E-38	-37.51685	0.88980	-24.208
6001401	PbCO3 AQ	1.573E-14	1.573E-14	-13.80323	1.00015	7.240
6003305	Pb(OH)4 -2	1.581E-24	1.407E-24	-23.85178	0.88980	-39.648
6001402	PbHCO3 +	3.711E-16	3.604E-16	-15.44323	0.97123	13.213
5403300	NiOH +	3.565E-14	3.463E-14	-13.46059	0.97123	-10.025
5403301	Ni(OH)2 AQ	1.502E-15	1.503E-15	-14.82317	1.00015	-19.000
5403302	Ni(OH)3 -	6.159E-19	5.982E-19	-18.22317	0.97123	-29.987
5401400	NiHCO3 +	2.339E-13	2.272E-13	-12.64363	0.97123	12.483
5401401	NiCO3 AQ	2.271E-11	2.272E-11	-10.64363	1.00015	6.870
5401402	Ni(CO3)2-2	1.434E-14	1.276E-14	-13.89411	0.88980	10.161
3301400	HCO3 -	2.022E-04	1.964E-04	-3.70680	0.97123	10.396
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00015	16.713
2113300	Cr+3	4.089E-15	3.144E-15	-14.50252	0.76898	10.022
2113301	Cr(OH)+2	7.252E-12	6.453E-12	-11.19024	0.88980	5.671
8123301	=SO2-	9.297E-04	9.297E-04	-3.03166	1.00000	-8.930
8123302	=SO2H2+	8.569E-04	8.569E-04	-3.06706	1.00000	7.290
8113301	=SO1-	1.656E-05	1.656E-05	-4.78094	1.00000	-8.930
8113302	=SO1H2+	1.526E-05	1.526E-05	-4.81634	1.00000	7.290
8129500	=SO2Zn+	1.774E-08	1.774E-08	-7.75104	1.00000	-1.990
8119500	=SO1Zn+	2.882E-07	2.882E-07	-6.54032	1.00000	0.970
8121600	=SO2Cd+	1.206E-10	1.206E-10	-9.91860	1.00000	-2.900
8111600	=SO1Cd+	4.593E-09	4.593E-09	-8.33789	1.00000	0.430
8112310	=SO1Cu+	2.392E-07	2.392E-07	-6.62122	1.00000	2.850
8122310	=SO2Cu+	7.552E-08	7.552E-08	-7.12193	1.00000	0.600
8115400	=SO1Ni+	1.661E-08	1.661E-08	-7.77950	1.00000	0.150
8125400	=SO2Ni+	2.088E-09	2.088E-09	-8.68022	1.00000	-2.500
8116000	=SO1Pb+	1.782E-07	1.782E-07	-6.74910	1.00000	4.710
8126000	=SO2Pb+	3.892E-10	3.892E-10	-9.40981	1.00000	0.300
8121500	=SO2Ca+	6.116E-06	6.116E-06	-5.21355	1.00000	-5.850
8111500	=SO1HCa++	5.364E-05	5.364E-05	-4.27054	1.00000	4.970
8111000	=SO1HBa++	9.729E-07	9.729E-07	-6.01191	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-6.580E-06	-5.182	0.000	0.000
330	H+1	-1.363E-04	-3.866	7.600	0.000
3301403	CO2 (g)	2.329E-04	-3.633	21.690	-0.530
3300021	O2 (g)	1.140E-04	-3.943	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.272E-08	-7.895	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP2

76.7	PERCENT BOUND IN SPECIES # 812	ADS1TYP2
12.1	PERCENT BOUND IN SPECIES #8123301	=SO2-
11.1	PERCENT BOUND IN SPECIES #8123302	=SO2H2+

Ba+2

29.6	PERCENT BOUND IN SPECIES # 100	Ba+2
70.3	PERCENT BOUND IN SPECIES #8111000	=SO1HBa++

Ca+2

53.8	PERCENT BOUND IN SPECIES # 150	Ca+2
4.7	PERCENT BOUND IN SPECIES #8121500	=SO2Ca+
41.3	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++

Cd+2

2.6	PERCENT BOUND IN SPECIES #8121600	=SO2Cd+

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                97.4     PERCENT BOUND IN SPECIES #8111600   =SO1Cd+
Zn+2
                 5.8     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                94.2     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
Cu+2
                76.0     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                24.0     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
ADS1TYP1
                54.7     PERCENT BOUND IN SPECIES #    811   ADS1TYP1
                 8.6     PERCENT BOUND IN SPECIES #8113301   =SO1-
                 7.9     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
                27.9     PERCENT BOUND IN SPECIES #8111500   =SO1HCa++
K+1
               100.0     PERCENT BOUND IN SPECIES #    410   K+1
Mg+2
                99.8     PERCENT BOUND IN SPECIES #    460   Mg+2
Na+1
               100.0     PERCENT BOUND IN SPECIES #    500   Na+1
Ni+2
                88.7     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                11.1     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
                99.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
               100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Cr(OH)2+
                25.8     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
                73.8     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
Al+3
                 1.0     PERCENT BOUND IN SPECIES # 303301   Al(OH)2 +
                48.5     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                50.4     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
                94.7     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 4.9     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
                99.3     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
                61.0     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                27.7     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                11.4     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
               142.0     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                14.8     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
               601.5     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                10.7     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                24.0     PERCENT BOUND IN SPECIES #3300020   OH-
                 1.6     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                26.0     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                21.6     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                 6.8     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                 1.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                16.1     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
100	Ba+2	4.101E-07	29.6	9.734E-07	70.4	0.000E-01	0.0
150	Ca+2	6.999E-05	53.9	5.975E-05	46.1	0.000E-01	0.0
160	Cd+2	1.689E-12	0.0	4.714E-09	100.0	0.000E-01	0.0

950	Zn+2	3.133E-11	0.0	3.059E-07	100.0	0.000E-01	0.0
231	Cu+2	9.930E-12	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.365E-11	0.2	1.870E-08	99.8	0.000E-01	0.0
600	Pb+2	2.153E-14	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.463E-09	8.8	0.000E-01	0.0	2.544E-08	91.2
30	Al+3	3.327E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.136E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	1.434E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.493E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.235E-04	156.9	-8.101E-05	-56.9	0.000E-01	0.0
2	H2O	2.845E-07	25.7	8.227E-07	74.3	0.000E-01	0.0

```
     Charge Balance: SPECIATED
       Sum of CATIONS =  1.693E-03 Sum of ANIONS   1.150E-03
       PERCENT DIFFERENCE =   1.912E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =   2.400E-07
     EQUILIBRIUM IONIC STRENGTH (m) =   6.688E-04
     EQUILIBRIUM pH                 =   7.600
     EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.030620     sig0 = 0.001966
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
```

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-2.411	[1.000] 150 [1.000] 140
5046000	ARTINITE	-9.088	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-5.855	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-2.255	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-4.199	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-12.249	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-22.209	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-2.443	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.341	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-4.846	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.545	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.042	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.338	[1.000] 100 [1.000] 140

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5023100 CUCO3          -9.425    [  1.000] 231  [  1.000] 140
2023100 CU(OH)2        -6.223    [ -2.000] 330  [  1.000] 231  [  2.000]   2
2023101 TENORITE       -5.203    [ -2.000] 330  [  1.000] 231  [  1.000]   2
3023100 CUPRICFERIT    -7.365    [ -8.000] 330  [  1.000] 231  [  2.000] 281
                                 [  4.000]   2
  95000 ZN METAL      -63.863    [  1.000] 950  [  2.000]   1
5095000 SMITHSONITE    -7.157    [  1.000] 950  [  1.000] 140
5095001 ZNCO3, 1H2O    -6.834    [  1.000] 950  [  1.000] 140  [  1.000]   2
2095000 ZN(OH)2 (A)    -7.854    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095001 ZN(OH)2 (C)    -7.604    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095002 ZN(OH)2 (B)    -7.154    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095003 ZN(OH)2 (G)    -7.114    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095004 ZN(OH)2 (E)    -6.904    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095005 ZNO(ACTIVE)    -6.714    [ -2.000] 330  [  1.000] 950  [  1.000]   2

 ID #      NAME       Sat. Index        Stoichiometry in [brackets]
2095006 ZINCITE        -6.856    [ -2.000] 330  [  1.000] 950  [  1.000]   2
  16000 CD METAL      -52.586    [  1.000] 160  [  2.000]   1
  16001 GAMMA CD      -52.688    [  1.000] 160  [  2.000]   1
5016000 OTAVITE        -4.620    [  1.000] 160  [  1.000] 140
2016000 CD(OH)2 (A)   -10.688    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)   -10.312    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE   -12.135    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL      -45.794    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE      -7.844    [  1.000] 600  [  1.000] 140
2060000 MASSICOT      -12.502    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE      -12.307    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O    -12.333    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3       -20.060    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                 [  1.000] 140
5060002 PB3O2CO3      -31.146    [ -4.000] 330  [  3.000] 600  [  1.000] 140
                                 [  2.000]   2
2060003 PLATTNERITE    -7.486    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                 [  2.000]   2
3060000 PB2O3         -17.568    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                 [  3.000]   2
3060001 MINIUM        -31.039    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                 [  4.000]   2
2060004 PB(OH)2 (C)    -7.703    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE  -23.979    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                 [  2.000]   2
2060005 PB2O(OH)2     -24.906    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3         -10.816    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2        -6.188    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE      -8.615    [ -2.000] 330  [  1.000] 540  [  1.000]   2
5023101 MALACHITE     -11.463    [  2.000] 231  [  2.000]   2  [  1.000] 140
                                 [ -2.000] 330
5023102 AZURITE       -18.895    [  3.000] 231  [  2.000]   2  [  2.000] 140
                                 [ -2.000] 330
2015000 LIME          -22.464    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE   -12.120    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE       -20.420    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE     -10.720    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE     -23.529    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                 [  4.000]   2
3046000 SPINEL        -11.849    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                 [  4.000]   2
3046001 MAG-FERRITE    -9.978    [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                 [  4.000]   2
3028102 LEPIDOCROCIT   -3.155    [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021100 FECR2O4       -12.371    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4        -4.563    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3           0.000    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)    -0.860    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)    -3.412    [  1.000] 211  [  1.000]   2  [ -1.000] 330
```

5 – Modelling with pH = 8.0

PART 1 of OUTPUT FILE

Revuè river water-Site 14 – pH = 8.0

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair and adsorption

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	1.000E-08	-8.000	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	1.031E-08	1.000E-08	-8.00000	0.96982	0.013
30	Al+3	2.211E-17	1.678E-17	-16.77513	0.75894	0.120
100	Ba+2	1.270E-07	1.124E-07	-6.94938	0.88462	0.053
150	Ca+2	2.750E-05	2.432E-05	-4.61395	0.88462	0.053
160	Cd+2	3.471E-13	3.070E-13	-12.51280	0.88462	0.053
211	Cr(OH)2+	2.530E-10	2.453E-10	-9.61025	0.96982	0.013
231	Cu+2	6.413E-14	5.673E-14	-13.24616	0.88462	0.053
280	Fe+2	2.269E-26	2.008E-26	-25.69733	0.88462	0.053
410	K+1	6.647E-05	6.446E-05	-4.19069	0.96982	0.013
460	Mg+2	1.430E-04	1.265E-04	-3.89789	0.88462	0.053
500	Na+1	2.087E-04	2.024E-04	-3.69371	0.96982	0.013
540	Ni+2	2.325E-12	2.057E-12	-11.68678	0.88462	0.053

600	Pb+2	7.121E-16	6.299E-16	-15.20072	0.88462	0.053
800	Sr+2	5.707E-07	5.048E-07	-6.29686	0.88462	0.053
950	Zn+2	6.213E-12	5.496E-12	-11.25997	0.88462	0.053
811	ADS1TYP1	7.849E-05	7.849E-05	-4.10519	1.00000	0.000
140	CO3-2	2.305E-06	2.039E-06	-5.69048	0.88462	0.053
281	Fe+3	2.168E-26	1.646E-26	-25.78367	0.75894	0.120
812	ADS1TYP2	5.885E-03	5.885E-03	-2.23024	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	2.058E-09	2.058E-09	-8.68661	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00017	-7.130
2113303	Cr(OH)4-	1.791E-12	1.737E-12	-11.76026	0.96982	-18.137
2113304	CrO2-	4.544E-12	4.407E-12	-11.35585	0.96982	-17.732
3300020	OH-	6.678E-07	6.477E-07	-6.18865	0.96982	-14.175
4603300	MgOH +	1.292E-08	1.253E-08	-7.90193	0.96982	-11.991
4601400	MgCO3 AQ	2.256E-07	2.256E-07	-6.64666	1.00017	2.942
4601401	MgHCO3 +	7.242E-07	7.023E-07	-6.15348	0.96982	11.448
1503300	CaOH +	3.924E-10	3.805E-10	-9.41960	0.96982	-12.792
1501400	CaHCO3 +	1.077E-07	1.045E-07	-6.98103	0.96982	11.337
1501401	CaCO3 AQ	6.264E-08	6.265E-08	-7.20307	1.00017	3.101
5001400	NaCO3 -	5.886E-09	5.708E-09	-8.24348	0.96982	1.154
5001401	NaHCO3 AQ	4.963E-08	4.964E-08	-7.30418	1.00017	10.080
303300	AlOH +2	1.313E-14	1.161E-14	-13.93512	0.88462	-5.107
303301	Al(OH)2 +	1.375E-11	1.333E-11	-10.87514	0.96982	-10.087
303302	Al(OH)4 -	4.062E-09	3.939E-09	-8.40458	0.96982	-23.616
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00017	-16.000
2803300	FeOH +	4.241E-28	4.113E-28	-27.38589	0.96982	-9.675
2803301	FeOH3 -1	7.640E-34	7.410E-34	-33.13021	0.96982	-31.420
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00017	-20.978
2813300	FeOH +2	8.531E-21	7.547E-21	-20.12223	0.88462	-2.285
2813301	FeOH2 +	3.628E-16	3.518E-16	-15.45368	0.96982	-5.657
2813302	FeOH3 AQ	4.133E-16	4.133E-16	-15.38369	1.00017	-13.600
2813303	FeOH4 -	4.262E-16	4.133E-16	-15.38369	0.96982	-21.587
2813304	Fe2(OH)2+4	3.182E-39	1.949E-39	-38.71021	0.61240	-2.930
2813305	Fe3(OH)4+5	3.002E-52	1.395E-52	-51.85531	0.46477	-6.172
8003300	SrOH +	2.145E-12	2.080E-12	-11.68194	0.96982	-13.372
1003300	BaOH +	3.092E-13	2.999E-13	-12.52303	0.96982	-13.560
2311400	CuCO3 AQ	6.213E-13	6.214E-13	-12.20664	1.00017	6.730
2311401	Cu(CO3)2-2	1.804E-15	1.595E-15	-14.79712	0.88462	9.883
2313300	CuOH +	5.850E-14	5.673E-14	-13.24617	0.96982	-7.987
2313301	Cu(OH)2 AQ	1.185E-11	1.185E-11	-10.92617	1.00017	-13.680
2313302	Cu(OH)3 -	7.381E-17	7.158E-17	-16.14518	0.96982	-26.886
2313303	Cu(OH)4 -2	1.611E-21	1.425E-21	-20.84619	0.88462	-39.547
2313304	Cu2(OH)2+2	8.950E-22	7.918E-22	-21.10140	0.88462	-10.556
2311402	CuHCO3 +	1.193E-14	1.157E-14	-13.93664	0.96982	13.013
9503300	ZnOH +	3.999E-13	3.878E-13	-12.41139	0.96982	-9.138
9503301	Zn(OH)2 AQ	6.933E-13	6.935E-13	-12.15898	1.00017	-16.899
9503302	Zn(OH)3 -	2.261E-16	2.193E-16	-15.65899	0.96982	-28.386
9503303	Zn(OH)4 -2	3.929E-21	3.475E-21	-20.45899	0.88462	-41.146
9501400	ZnHCO3 +	2.903E-13	2.815E-13	-12.55045	0.96982	12.413
9501401	ZnCO3 AQ	2.236E-12	2.236E-12	-11.65044	1.00017	5.300
9501402	Zn(CO3)2-2	1.102E-13	9.752E-14	-13.01092	0.88462	9.683
1601400	Cd(CO3)3-4	7.059E-24	4.323E-24	-23.36423	0.61240	6.433
1603300	CdOH +	1.711E-15	1.660E-15	-14.77995	0.96982	-10.254
1603301	Cd(OH)2 AQ	1.371E-17	1.371E-17	-16.86281	1.00017	-20.350
1603302	Cd(OH)3 -	1.587E-22	1.539E-22	-21.81282	0.96982	-33.287
1603303	Cd(OH)4 -2	1.550E-28	1.371E-28	-27.86282	0.88462	-47.297
1603304	Cd2OH +3	3.536E-27	2.683E-27	-26.57130	0.75894	-9.426
1601400	CdHCO3 +	1.622E-14	1.573E-14	-13.80328	0.96982	12.413
1601401	CdCO3 AQ	1.569E-13	1.569E-13	-12.80428	1.00017	5.399
6001400	Pb(CO3)2-2	1.293E-16	1.144E-16	-15.94168	0.88462	10.693
6003300	PbOH +	1.266E-15	1.228E-15	-14.91073	0.96982	-7.697
6003301	Pb(OH)2 AQ	4.777E-17	4.778E-17	-16.32074	1.00017	-17.120

6003302	Pb(OH)3 -	5.657E-20	5.486E-20	-19.26074	0.96982	-28.047
6003303	Pb2OH +3	2.282E-29	1.732E-29	-28.76145	0.75894	-6.240
6003304	Pb3(OH)4+2	1.558E-38	1.378E-38	-37.86077	0.88462	-24.205
6001401	PbCO3 AQ	2.232E-14	2.233E-14	-13.65120	1.00017	7.240
6003305	Pb(OH)4 -2	1.424E-23	1.260E-23	-22.89975	0.88462	-39.646
6001402	PbHCO3 +	2.099E-16	2.036E-16	-15.69120	0.96982	13.213
5403300	NiOH +	1.946E-14	1.887E-14	-13.72422	0.96982	-10.024
5403301	Ni(OH)2 AQ	2.056E-15	2.057E-15	-14.68680	1.00017	-19.000
5403302	Ni(OH)3 -	2.121E-18	2.057E-18	-17.68681	0.96982	-29.987
5401400	NiHCO3 +	1.277E-13	1.238E-13	-12.90726	0.96982	12.483
5401401	NiCO3 AQ	3.109E-11	3.110E-11	-10.50726	1.00017	6.870
5401402	Ni(CO3)2-2	1.246E-13	1.102E-13	-12.95774	0.88462	10.163
3301400	HCO3 -	5.088E-04	4.934E-04	-3.30680	0.96982	10.397
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00017	16.713
2113300	Cr+3	2.614E-16	1.984E-16	-15.70252	0.75894	10.028
2113301	Cr(OH)+2	1.156E-12	1.023E-12	-11.99024	0.88462	5.673
8123301	=SO2-	9.846E-04	9.846E-04	-3.00674	1.00000	-8.930
8123302	=SO2H2+	8.059E-04	8.059E-04	-3.09373	1.00000	7.290
8113301	=SO1-	1.313E-05	1.313E-05	-4.88170	1.00000	-8.930
8113302	=SO1H2+	1.075E-05	1.075E-05	-4.96869	1.00000	7.290
8129500	=SO2Zn+	2.324E-08	2.324E-08	-7.63371	1.00000	-1.990
8119500	=SO1Zn+	2.827E-07	2.827E-07	-6.54866	1.00000	0.970
8121600	=SO2Cd+	1.598E-10	1.598E-10	-9.79654	1.00000	-2.900
8111600	=SO1Cd+	4.555E-09	4.555E-09	-8.34149	1.00000	0.430
8112310	=SO1Cu+	2.214E-07	2.214E-07	-6.65486	1.00000	2.850
8122310	=SO2Cu+	9.335E-08	9.335E-08	-7.02990	1.00000	0.600
8115400	=SO1Ni+	1.601E-08	1.601E-08	-7.79548	1.00000	0.150
8125400	=SO2Ni+	2.688E-09	2.688E-09	-8.57053	1.00000	-2.500
8116000	=SO1Pb+	1.781E-07	1.781E-07	-6.74942	1.00000	4.710
8126000	=SO2Pb+	5.194E-10	5.194E-10	-9.28446	1.00000	0.300
8121500	=SO2Ca+	1.420E-05	1.420E-05	-4.84768	1.00000	-5.850
8111500	=SO1HCa++	8.788E-05	8.788E-05	-4.05613	1.00000	4.970
8111000	=SO1HBa++	1.254E-06	1.254E-06	-5.90157	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-3.161E-04	-3.500	0.000	0.000
330	H+1	2.906E-04	-3.537	8.000	0.000
3301403	CO2 (g)	-7.889E-05	-4.103	21.690	-0.530
3300021	O2 (g)	1.127E-04	-3.948	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.813E-06	-5.318	-7.225	24.630
3021102	CR2O3	1.291E-08	-7.889	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1PSIo

>1000.	PERCENT BOUND IN SPECIES	#8123302	=SO2H2+
88.2	PERCENT BOUND IN SPECIES	#8113302	=SO1H2+
2.3	PERCENT BOUND IN SPECIES	#8119500	=SO1Zn+
1.8	PERCENT BOUND IN SPECIES	#8112310	=SO1Cu+
1.5	PERCENT BOUND IN SPECIES	#8116000	=SO1Pb+
116.6	PERCENT BOUND IN SPECIES	#8121500	=SO2Ca+
>1000.	PERCENT BOUND IN SPECIES	#8111500	=SO1HCa++
20.6	PERCENT BOUND IN SPECIES	#8111000	=SO1HBa++

ADS1TYP2

76.5	PERCENT BOUND IN SPECIES	# 812	ADS1TYP2
12.8	PERCENT BOUND IN SPECIES	#8123301	=SO2-

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                10.5     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
Ba+2
                 9.2     PERCENT BOUND IN SPECIES #    100   Ba+2
                90.7     PERCENT BOUND IN SPECIES #8111000   =SO1HBa++
Ca+2
                21.2     PERCENT BOUND IN SPECIES #    150   Ca+2
                10.9     PERCENT BOUND IN SPECIES #8121500   =SO2Ca+
                67.7     PERCENT BOUND IN SPECIES #8111500   =SO1HCa++
Cd+2
                 3.4     PERCENT BOUND IN SPECIES #8121600   =SO2Cd+
                96.6     PERCENT BOUND IN SPECIES #8111600   =SO1Cd+
Zn+2
                 7.6     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                92.4     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
Cu+2
                70.3     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                29.7     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
ADS1TYP1
                40.8     PERCENT BOUND IN SPECIES #    811   ADS1TYP1
                 6.8     PERCENT BOUND IN SPECIES #8113301   =SO1-
                 5.6     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
                45.7     PERCENT BOUND IN SPECIES #8111500   =SO1HCa++
K+1
               100.0     PERCENT BOUND IN SPECIES #    410   K+1
Mg+2
                99.3     PERCENT BOUND IN SPECIES #    460   Mg+2
Na+1
               100.0     PERCENT BOUND IN SPECIES #    500   Na+1
Ni+2
                85.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                14.3     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
                99.7     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
               100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Cr(OH)2+
                12.2     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
                87.5     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
Al+3
                70.6     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                29.2     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
                97.3     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 2.0     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
                98.2     PERCENT BOUND IN SPECIES #    280   Fe+2
                 1.8     PERCENT BOUND IN SPECIES #2803300   FeOH +
E-1
Fe+3
                30.2     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                34.4     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                35.5     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
               152.4     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 6.3     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
               241.4     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                 3.2     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                43.7     PERCENT BOUND IN SPECIES #3300020   OH-
                 1.1     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                 1.5     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                18.5     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                14.5     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                 6.1     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                 1.0     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
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11.7 PERCENT BOUND IN SPECIES #8116000 =SO1Pb+

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.270E-07	9.2	1.256E-06	90.8	0.000E-01	0.0
150	Ca+2	2.767E-05	21.3	1.021E-04	78.7	0.000E-01	0.0
160	Cd+2	5.219E-13	0.0	4.715E-09	100.0	0.000E-01	0.0
950	Zn+2	9.943E-12	0.0	3.060E-07	100.0	0.000E-01	0.0
231	Cu+2	1.261E-11	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.369E-11	0.2	1.870E-08	99.8	0.000E-01	0.0
600	Pb+2	2.469E-14	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	2.079E-09	7.4	0.000E-01	0.0	2.583E-08	92.6
30	Al+3	5.754E-09	0.1	0.000E-01	0.0	4.813E-06	99.9
140	CO3-2	5.228E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.312E-26	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.202E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	5.300E-04	158.7	-1.961E-04	-58.7	0.000E-01	0.0
2	H2O	7.043E-07	46.1	8.227E-07	53.9	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 1.628E-03 Sum of ANIONS 1.512E-03
PERCENT DIFFERENCE = 3.713E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)
NON-CARBONATE ALKALINITY = 6.579E-07
EQUILIBRIUM IONIC STRENGTH (m) = 7.398E-04
EQUILIBRIUM pH = 8.000
EQUILIBRIUM pe = 13.089 or Eh = 759.46 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
**** Parameters For Adsorbent Number 1 ****
Electrostatic Variables: psi0 = 0.008907 sig0 = 0.000569
psib = 0.000000 sigb = 0.000000
psid = 0.000000 sigd = 0.000000
Adsorbent Concentration (g/l): 3.442
Specific Surface Area (sq. meters/g): 600.00

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-2.019	[1.000] 150 [1.000] 140
5046000	ARTINITE	-7.497	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-5.059	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-1.862	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-3.011	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-9.470	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-18.231	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2

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3028101 MAGHEMITE       -9.953    [ -6.000] 330  [  2.000] 281  [  3.000]   2
5046002 MAGNESITE       -1.647    [  1.000] 460  [  1.000] 140
3028000 MAGNETITE      -17.723    [ -8.000] 330  [  2.000] 281  [  1.000] 280
                                  [  4.000]   2
3050000 NATRON         -11.542    [  2.000] 500  [  1.000] 140  [ 10.000]   2
5046003 NESQUEHONITE    -4.050    [  1.000] 460  [  1.000] 140  [  3.000]   2
5028000 SIDERITE       -20.914    [  1.000] 280  [  1.000] 140
5080000 STRONTIANITE    -2.747    [  1.000] 800  [  1.000] 140
5050001 THERMONATR     -13.243    [  2.000] 500  [  1.000] 140  [  1.000]   2
5010000 WITHERITE       -4.050    [  1.000] 100  [  1.000] 140
5023100 CUCO3           -9.307    [  1.000] 231  [  1.000] 140
2023100 CU(OH)2         -6.104    [ -2.000] 330  [  1.000] 231  [  2.000]   2
2023101 TENORITE        -5.084    [ -2.000] 330  [  1.000] 231  [  1.000]   2
3023100 CUPRICFERIT     -7.246    [ -8.000] 330  [  1.000] 231  [  2.000] 281
                                  [  4.000]   2
  95000 ZN METAL       -63.719    [  1.000] 950  [  2.000]   1
5095000 SMITHSONITE     -7.013    [  1.000] 950  [  1.000] 140
5095001 ZNCO3, 1H2O     -6.690    [  1.000] 950  [  1.000] 140  [  1.000]   2
2095000 ZN(OH)2 (A)     -7.710    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095001 ZN(OH)2 (C)     -7.460    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095002 ZN(OH)2 (B)     -7.010    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095003 ZN(OH)2 (G)     -6.970    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095004 ZN(OH)2 (E)     -6.760    [ -2.000] 330  [  1.000] 950  [  2.000]   2
2095005 ZNO(ACTIVE)     -6.570    [ -2.000] 330  [  1.000] 950  [  1.000]   2

  ID #      NAME       Sat. Index        Stoichiometry in [brackets]
2095006 ZINCITE         -6.712    [ -2.000] 330  [  1.000] 950  [  1.000]   2
  16000 CD METAL       -52.437    [  1.000] 160  [  2.000]   1
  16001 GAMMA CD       -52.539    [  1.000] 160  [  2.000]   1
5016000 OTAVITE         -4.472    [  1.000] 160  [  1.000] 140
2016000 CD(OH)2 (A)    -10.540    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016001 CD(OH)2 (C)    -10.163    [ -2.000] 330  [  1.000] 160  [  2.000]   2
2016002 MONTEPONITE    -11.987    [ -2.000] 330  [  1.000] 160  [  1.000]   2
  60000 PB METAL       -45.642    [  1.000] 600  [  2.000]   1
5060000 CERRUSITE       -7.692    [  1.000] 600  [  1.000] 140
2060000 MASSICOT       -12.350    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060001 LITHARGE       -12.155    [ -2.000] 330  [  1.000] 600  [  1.000]   2
2060002 PBO, .3H2O     -12.181    [ -2.000] 330  [  1.000] 600  [  1.330]   2
5060001 PB2OCO3        -19.756    [ -2.000] 330  [  2.000] 600  [  1.000]   2
                                  [  1.000] 140
5060002 PB3O2CO3       -30.690    [ -4.000] 330  [  3.000] 600  [  1.000] 140
                                  [  2.000]   2
2060003 PLATTNERITE     -7.334    [ -4.000] 330  [ -2.000]   1  [  1.000] 600
                                  [  2.000]   2
3060000 PB2O3          -17.264    [ -6.000] 330  [ -2.000]   1  [  2.000] 600
                                  [  3.000]   2
3060001 MINIUM         -30.583    [ -8.000] 330  [ -2.000]   1  [  3.000] 600
                                  [  4.000]   2
2060004 PB(OH)2 (C)     -7.551    [ -2.000] 330  [  1.000] 600  [  2.000]   2
5060003 HYDCERRUSITE   -23.523    [ -2.000] 330  [  3.000] 600  [  2.000] 140
                                  [  2.000]   2
2060005 PB2O(OH)2      -24.601    [ -4.000] 330  [  2.000] 600  [  3.000]   2
5054000 NICO3          -10.679    [  1.000] 540  [  1.000] 140
2054000 NI(OH)2         -6.052    [ -2.000] 330  [  1.000] 540  [  2.000]   2
2054001 BUNSENITE       -8.479    [ -2.000] 330  [  1.000] 540  [  1.000]   2
5023101 MALACHITE      -11.226    [  2.000] 231  [  2.000]   2  [  1.000] 140
                                  [ -2.000] 330
5023102 AZURITE        -18.539    [  3.000] 231  [  2.000]   2  [  2.000] 140
                                  [ -2.000] 330
2015000 LIME           -22.072    [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE    -11.727    [ -2.000] 330  [  1.000] 150  [  2.000]   2
2028000 WUSTITE        -20.377    [ -2.000] 330  [  0.947] 280  [  1.000]   2
2046001 PERICLASE       -9.924    [ -2.000] 330  [  1.000] 460  [  1.000]   2
3028001 HERCYNITE      -23.529    [ -8.000] 330  [  1.000] 280  [  2.000]  30
                                  [  4.000]   2
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3046000	SPINEL	-11.054	[-8.000]	330	[1.000]	460	[2.000]	30	
			[4.000]	2					
3046001	MAG-FERRITE	-9.182	[-8.000]	330	[1.000]	460	[2.000]	281	
			[4.000]	2					
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2	
3021100	FECR2O4	-12.371	[2.000]	211	[1.000]	280	[-4.000]	330	
3021101	MGCR2O4	-3.767	[2.000]	211	[1.000]	460	[-4.000]	330	
3021102	CR2O3	0.000	[2.000]	211	[-2.000]	330	[-1.000]	2	
2021102	CR(OH)3 (A)	-0.860	[1.000]	211	[1.000]	2	[-1.000]	330	
2021101	CR(OH)3 (C)	-3.412	[1.000]	211	[1.000]	2	[-1.000]	330	

6 – Modelling with pH = 8.5

PART 1 of OUTPUT FILE

Revuè river water-Site 14 – pH = 8.5

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair and adsorption

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.162E-09	-8.500	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 4.366E-04
PERCENT DIFFERENCE = 3.180E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	3.291E-09	3.162E-09	-8.50000	0.96076	0.017
30	Al+3	7.609E-19	5.307E-19	-18.27513	0.69751	0.156
100	Ba+2	1.871E-08	1.595E-08	-7.79736	0.85206	0.070
150	Ca+2	4.441E-06	3.784E-06	-5.42208	0.85206	0.070
160	Cd+2	4.479E-14	3.816E-14	-13.41840	0.85206	0.070
211	Cr(OH)2+	8.075E-11	7.758E-11	-10.11025	0.96076	0.017
231	Cu+2	7.885E-15	6.719E-15	-14.17272	0.85206	0.070
280	Fe+2	2.356E-27	2.008E-27	-26.69733	0.85206	0.070
410	K+1	6.647E-05	6.386E-05	-4.19476	0.96076	0.017
460	Mg+2	1.396E-04	1.190E-04	-3.92453	0.85206	0.070
500	Na+1	2.086E-04	2.004E-04	-3.69811	0.96076	0.017
540	Ni+2	2.938E-13	2.504E-13	-12.60142	0.85206	0.070

600	Pb+2	9.241E-17	7.874E-17	-16.10381	0.85206	0.070
800	Sr+2	5.707E-07	4.862E-07	-6.31314	0.85206	0.070
950	Zn+2	7.953E-13	6.776E-13	-12.16901	0.85206	0.070
811	ADS1TYP1	6.585E-05	6.585E-05	-4.18143	1.00000	0.000
140	CO3-2	2.394E-05	2.039E-05	-4.69048	0.85206	0.070
281	Fe+3	7.461E-28	5.204E-28	-27.28367	0.69751	0.156
812	ADS1TYP2	5.872E-03	5.872E-03	-2.23123	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	8.367E-09	8.367E-09	-8.07742	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.818E-09	1.819E-09	-8.74025	1.00030	-7.130
2113303	Cr(OH)4-	5.716E-12	5.492E-12	-11.26026	0.96076	-18.133
2113304	CrO2-	1.451E-11	1.394E-11	-10.85585	0.96076	-17.728
3300020	OH-	2.132E-06	2.048E-06	-5.68865	0.96076	-14.171
4603300	MgOH +	3.880E-08	3.728E-08	-7.42857	0.96076	-11.987
4601400	MgCO3 AQ	2.121E-06	2.122E-06	-5.67330	1.00030	2.942
4601401	MgHCO3 +	2.174E-06	2.089E-06	-5.68012	0.96076	11.452
1503300	CaOH +	1.948E-10	1.872E-10	-9.72773	0.96076	-12.788
1501400	CaHCO3 +	5.348E-08	5.139E-08	-7.28916	0.96076	11.341
1501401	CaCO3 AQ	9.742E-08	9.745E-08	-7.01120	1.00030	3.101
5001400	NaCO3 -	5.882E-08	5.651E-08	-7.24788	0.96076	1.158
5001401	NaHCO3 AQ	1.553E-07	1.554E-07	-6.80858	1.00030	10.080
303300	AlOH +2	1.363E-15	1.161E-15	-14.93512	0.85206	-5.090
303301	Al(OH)2 +	4.388E-12	4.216E-12	-11.37514	0.96076	-10.083
303302	Al(OH)4 -	1.297E-08	1.246E-08	-7.90459	0.96076	-23.612
303303	Al(OH)3 AQ	1.678E-09	1.678E-09	-8.77515	1.00030	-16.000
2803300	FeOH +	1.354E-28	1.300E-28	-27.88589	0.96076	-9.671
2803301	FeOH3 -1	2.439E-33	2.343E-33	-32.63021	0.96076	-31.415
2803302	FeOH2 AQ	2.111E-31	2.111E-31	-30.67542	1.00030	-20.978
2813300	FeOH +2	8.857E-22	7.547E-22	-21.12223	0.85206	-2.269
2813301	FeOH2 +	1.158E-16	1.113E-16	-15.95368	0.96076	-5.653
2813302	FeOH3 AQ	4.132E-16	4.133E-16	-15.38369	1.00030	-13.600
2813303	FeOH4 -	1.360E-15	1.307E-15	-14.88369	0.96076	-21.583
2813304	Fe2(OH)2+4	3.698E-41	1.949E-41	-40.71021	0.52707	-2.865
2813305	Fe3(OH)4+5	1.200E-54	4.413E-55	-54.35531	0.36764	-6.070
8003300	SrOH +	6.594E-12	6.335E-12	-11.19822	0.96076	-13.368
1003300	BaOH +	1.401E-13	1.346E-13	-12.87101	0.96076	-13.556
2311400	CuCO3 AQ	7.357E-13	7.359E-13	-12.13320	1.00030	6.730
2311401	Cu(CO3)2-2	2.217E-14	1.889E-14	-13.72367	0.85206	9.900
2313300	CuOH +	2.211E-14	2.125E-14	-13.67273	0.96076	-7.983
2313301	Cu(OH)2 AQ	1.403E-11	1.404E-11	-10.85273	1.00030	-13.680
2313302	Cu(OH)3 -	2.790E-16	2.681E-16	-15.57174	0.96076	-26.882
2313303	Cu(OH)4 -2	1.981E-20	1.688E-20	-19.77275	0.85206	-39.530
2313304	Cu2(OH)2+2	1.303E-22	1.110E-22	-21.95452	0.85206	-10.540
2311402	CuHCO3 +	4.510E-15	4.333E-15	-14.36320	0.96076	13.017
9503300	ZnOH +	1.574E-13	1.512E-13	-12.82043	0.96076	-9.134
9503301	Zn(OH)2 AQ	8.548E-13	8.550E-13	-12.06802	1.00030	-16.899
9503302	Zn(OH)3 -	8.899E-16	8.550E-16	-15.06803	0.96076	-28.382
9503303	Zn(OH)4 -2	5.029E-20	4.285E-20	-19.36803	0.85206	-41.129
9501400	ZnHCO3 +	1.143E-13	1.098E-13	-12.95949	0.96076	12.417
9501401	ZnCO3 AQ	2.757E-12	2.758E-12	-11.55948	1.00030	5.300
9501402	Zn(CO3)2-2	1.411E-12	1.202E-12	-11.91996	0.85206	9.700
1601400	Cd(CO3)3-4	1.019E-21	5.372E-22	-21.26983	0.52707	6.498
1603300	CdOH +	6.789E-16	6.523E-16	-15.18555	0.96076	-10.250
1603301	Cd(OH)2 AQ	1.704E-17	1.704E-17	-16.76841	1.00030	-20.350
1603302	Cd(OH)3 -	6.295E-22	6.048E-22	-21.21842	0.96076	-33.283
1603303	Cd(OH)4 -2	2.000E-27	1.704E-27	-26.76842	0.85206	-47.280
1603304	Cd2OH +3	1.879E-28	1.311E-28	-27.88250	0.69751	-9.389
1601400	CdHCO3 +	6.434E-15	6.182E-15	-14.20887	0.96076	12.417
1601401	CdCO3 AQ	1.950E-13	1.950E-13	-12.70987	1.00030	5.399
6001400	Pb(CO3)2-2	1.678E-15	1.430E-15	-14.84477	0.85206	10.710
6003300	PbOH +	5.053E-16	4.855E-16	-15.31382	0.96076	-7.693
6003301	Pb(OH)2 AQ	5.971E-17	5.973E-17	-16.22382	1.00030	-17.120

6003302	Pb(OH)3 -	2.257E-19	2.169E-19	-18.66383	0.96076	-28.043
6003303	Pb2OH +3	1.227E-30	8.558E-31	-30.06763	0.69751	-6.204
6003304	Pb3(OH)4+2	3.159E-39	2.691E-39	-38.57003	0.85206	-24.189
6001401	PbCO3 AQ	2.790E-14	2.791E-14	-13.55429	1.00030	7.240
6003305	Pb(OH)4 -2	1.848E-22	1.575E-22	-21.80284	0.85206	-39.629
6001402	PbHCO3 +	8.377E-17	8.048E-17	-16.09429	0.96076	13.217
5403300	NiOH +	7.560E-15	7.263E-15	-14.13886	0.96076	-10.020
5403301	Ni(OH)2 AQ	2.503E-15	2.504E-15	-14.60144	1.00030	-19.000
5403302	Ni(OH)3 -	8.240E-18	7.917E-18	-17.10145	0.96076	-29.983
5401400	NiHCO3 +	4.960E-14	4.765E-14	-13.32190	0.96076	12.487
5401401	NiCO3 AQ	3.784E-11	3.785E-11	-10.42190	1.00030	6.870
5401402	Ni(CO3)2-2	1.575E-12	1.342E-12	-11.87238	0.85206	10.180
3301400	HCO3 -	1.624E-03	1.560E-03	-2.80680	0.96076	10.401
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00030	16.713
2113300	Cr+3	8.994E-18	6.273E-18	-17.20252	0.69751	10.064
2113301	Cr(OH)+2	1.200E-13	1.023E-13	-12.99024	0.85206	5.690
8123301	=SO2-	1.031E-03	1.031E-03	-2.98681	1.00000	-8.930
8123302	=SO2H2+	7.662E-04	7.662E-04	-3.11564	1.00000	7.290
8113301	=SO1-	1.156E-05	1.156E-05	-4.93701	1.00000	-8.930
8113302	=SO1H2+	8.593E-06	8.593E-06	-5.06584	1.00000	7.290
8129500	=SO2Zn+	2.725E-08	2.725E-08	-7.56466	1.00000	-1.990
8119500	=SO1Zn+	2.787E-07	2.787E-07	-6.55485	1.00000	0.970
8121600	=SO2Cd+	1.888E-10	1.888E-10	-9.72405	1.00000	-2.900
8111600	=SO1Cd+	4.526E-09	4.526E-09	-8.34424	1.00000	0.430
8112310	=SO1Cu+	2.096E-07	2.096E-07	-6.67857	1.00000	2.850
8122310	=SO2Cu+	1.051E-07	1.051E-07	-6.97837	1.00000	0.600
8115400	=SO1Ni+	1.559E-08	1.559E-08	-7.80727	1.00000	0.150
8125400	=SO2Ni+	3.111E-09	3.111E-09	-8.50708	1.00000	-2.500
8116000	=SO1Pb+	1.780E-07	1.780E-07	-6.74966	1.00000	4.710
8126000	=SO2Pb+	6.174E-10	6.174E-10	-9.20946	1.00000	0.300
8121500	=SO2Ca+	2.100E-05	2.100E-05	-4.67773	1.00000	-5.850
8111500	=SO1HCa++	1.042E-04	1.042E-04	-3.98234	1.00000	4.970
8111000	=SO1HBa++	1.356E-06	1.356E-06	-5.86762	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-1.458E-03	-2.836	0.000	0.000
330	H+1	1.549E-03	-2.810	8.500	0.000
3301403	CO2 (g)	-1.244E-03	-2.905	21.690	-0.530
3300021	O2 (g)	1.001E-04	-4.000	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.804E-06	-5.318	-7.225	24.630
3021102	CR2O3	1.299E-08	-7.886	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

```
ADS1PSIo
              >1000.     PERCENT BOUND IN SPECIES #8123301   =SO2-
                33.3     PERCENT BOUND IN SPECIES #8113301   =SO1-
ADS1TYP2
                76.4     PERCENT BOUND IN SPECIES #    812   ADS1TYP2
                13.4     PERCENT BOUND IN SPECIES #8123301   =SO2-
                10.0     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
Ba+2
                 1.4     PERCENT BOUND IN SPECIES #    100   Ba+2
                98.0     PERCENT BOUND IN SPECIES #8111000   =SO1HBa++
Ca+2
                 3.4     PERCENT BOUND IN SPECIES #    150   Ca+2
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                16.2     PERCENT BOUND IN SPECIES #8121500   =SO2Ca+
                80.3     PERCENT BOUND IN SPECIES #8111500   =SO1HCa++
Cd+2
                 4.0     PERCENT BOUND IN SPECIES #8121600   =SO2Cd+
                96.0     PERCENT BOUND IN SPECIES #8111600   =SO1Cd+
Zn+2
                 8.9     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                91.1     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
Cu+2
                66.6     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                33.4     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
ADS1TYP1
                34.3     PERCENT BOUND IN SPECIES #    811   ADS1TYP1
                 6.0     PERCENT BOUND IN SPECIES #8113301   =SO1-
                 4.5     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
                54.2     PERCENT BOUND IN SPECIES #8111500   =SO1HCa++
K+1
               100.0     PERCENT BOUND IN SPECIES #    410   K+1
Mg+2
                97.0     PERCENT BOUND IN SPECIES #    460   Mg+2
                 1.5     PERCENT BOUND IN SPECIES #4601400   MgCO3 AQ
                 1.5     PERCENT BOUND IN SPECIES #4601401   MgHCO3 +
Na+1
                99.9     PERCENT BOUND IN SPECIES #    500   Na+1
Ni+2
                83.2     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                16.6     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
                99.7     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
               100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Cr(OH)2+
                 4.2     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
                94.7     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
Al+3
                88.5     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                11.5     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
                 1.4     PERCENT BOUND IN SPECIES #    140   CO3-2
                97.6     PERCENT BOUND IN SPECIES #3301400   HCO3 -
Fe+2
                94.6     PERCENT BOUND IN SPECIES #    280   Fe+2
                 5.4     PERCENT BOUND IN SPECIES #2803300   FeOH +
E-1
Fe+3
                 6.1     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                21.9     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                72.0     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
               119.8     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 1.6     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
                56.5     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
H2O
                69.8     PERCENT BOUND IN SPECIES #3300020   OH-
                 1.3     PERCENT BOUND IN SPECIES #4603300   MgOH +
                 1.7     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                 9.1     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                 6.9     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                 3.4     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                 5.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.871E-08	1.4	1.365E-06	98.6	0.000E-01	0.0
150	Ca+2	4.592E-06	3.5	1.252E-04	96.5	0.000E-01	0.0
160	Cd+2	2.469E-13	0.0	4.715E-09	100.0	0.000E-01	0.0
950	Zn+2	6.090E-12	0.0	3.060E-07	100.0	0.000E-01	0.0
231	Cu+2	1.483E-11	0.0	3.147E-07	100.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.977E-11	0.2	1.870E-08	99.8	0.000E-01	0.0
600	Pb+2	3.032E-14	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
211	Cr(OH)2+	1.919E-09	6.9	0.000E-01	0.0	2.599E-08	93.1
30	Al+3	1.465E-08	0.3	0.000E-01	0.0	4.804E-06	99.7
140	CO3-2	1.663E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.492E-27	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.889E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	1.645E-03	121.3	-2.894E-04	-21.3	0.000E-01	0.0
2	H2O	2.229E-06	73.0	8.227E-07	27.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 1.574E-03 Sum of ANIONS 2.716E-03
PERCENT DIFFERENCE = 2.662E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)
NON-CARBONATE ALKALINITY = 2.129E-06
EQUILIBRIUM IONIC STRENGTH (m) = 1.289E-03
EQUILIBRIUM pH = 8.500
EQUILIBRIUM pe = 12.589 or Eh = 730.45 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
**** Parameters For Adsorbent Number 1 ****
Electrostatic Variables: psi0 = -.018892 sig0 = -.001622
psib = 0.000000 sigb = 0.000000
psid = 0.000000 sigd = 0.000000
Adsorbent Concentration (g/l): 3.442
Specific Surface Area (sq. meters/g): 600.00

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-1.827	[1.000] 150 [1.000] 140
5046000	ARTINITE	-5.550	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-4.086	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-1.670	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-1.846	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-6.358	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-13.364	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2

3028101	MAGHEMITE	-9.953	[-6.000]	330	[2.000]	281	[3.000]	2			
5046002	MAGNESITE	-0.674	[1.000]	460	[1.000]	140					
3028000	MAGNETITE	-17.723	[-8.000]	330	[2.000]	281	[1.000]	280			
			[4.000]	2							
3050000	NATRON	-10.551	[2.000]	500	[1.000]	140	[10.000]	2			
5046003	NESQUEHONITE	-3.077	[1.000]	460	[1.000]	140	[3.000]	2			
5028000	SIDERITE	-20.914	[1.000]	280	[1.000]	140					
5080000	STRONTIANITE	-1.763	[1.000]	800	[1.000]	140					
5050001	THERMONATR	-12.252	[2.000]	500	[1.000]	140	[1.000]	2			
5010000	WITHERITE	-3.898	[1.000]	100	[1.000]	140					
5023100	CUCO3	-9.233	[1.000]	231	[1.000]	140					
2023100	CU(OH)2	-6.031	[-2.000]	330	[1.000]	231	[2.000]	2			
2023101	TENORITE	-5.010	[-2.000]	330	[1.000]	231	[1.000]	2			
3023100	CUPRICFERIT	-7.173	[-8.000]	330	[1.000]	231	[2.000]	281			
			[4.000]	2							
95000	ZN METAL	-63.628	[1.000]	950	[2.000]	1					
5095000	SMITHSONITE	-6.922	[1.000]	950	[1.000]	140					
5095001	ZNCO3, 1H2O	-6.599	[1.000]	950	[1.000]	140	[1.000]	2			
2095000	ZN(OH)2 (A)	-7.619	[-2.000]	330	[1.000]	950	[2.000]	2			
2095001	ZN(OH)2 (C)	-7.369	[-2.000]	330	[1.000]	950	[2.000]	2			
2095002	ZN(OH)2 (B)	-6.919	[-2.000]	330	[1.000]	950	[2.000]	2			
2095003	ZN(OH)2 (G)	-6.879	[-2.000]	330	[1.000]	950	[2.000]	2			
2095004	ZN(OH)2 (E)	-6.669	[-2.000]	330	[1.000]	950	[2.000]	2			
2095005	ZNO(ACTIVE)	-6.479	[-2.000]	330	[1.000]	950	[1.000]	2			

ID #	NAME	Sat. Index	Stoichiometry in [brackets]								
2095006	ZINCITE	-6.621	[-2.000]	330	[1.000]	950	[1.000]	2			
16000	CD METAL	-52.343	[1.000]	160	[2.000]	1					
16001	GAMMA CD	-52.445	[1.000]	160	[2.000]	1					
5016000	OTAVITE	-4.377	[1.000]	160	[1.000]	140					
2016000	CD(OH)2 (A)	-10.445	[-2.000]	330	[1.000]	160	[2.000]	2			
2016001	CD(OH)2 (C)	-10.068	[-2.000]	330	[1.000]	160	[2.000]	2			
2016002	MONTEPONITE	-11.892	[-2.000]	330	[1.000]	160	[1.000]	2			
60000	PB METAL	-45.545	[1.000]	600	[2.000]	1					
5060000	CERRUSITE	-7.595	[1.000]	600	[1.000]	140					
2060000	MASSICOT	-12.254	[-2.000]	330	[1.000]	600	[1.000]	2			
2060001	LITHARGE	-12.058	[-2.000]	330	[1.000]	600	[1.000]	2			
2060002	PBO, .3H2O	-12.084	[-2.000]	330	[1.000]	600	[1.330]	2			
5060001	PB2OCO3	-19.562	[-2.000]	330	[2.000]	600	[1.000]	2			
			[1.000]	140							
5060002	PB3O2CO3	-30.399	[-4.000]	330	[3.000]	600	[1.000]	140			
			[2.000]	2							
2060003	PLATTNERITE	-7.237	[-4.000]	330	[-2.000]	1	[1.000]	600			
			[2.000]	2							
3060000	PB2O3	-17.071	[-6.000]	330	[-2.000]	1	[2.000]	600			
			[3.000]	2							
3060001	MINIUM	-30.292	[-8.000]	330	[-2.000]	1	[3.000]	600			
			[4.000]	2							
2060004	PB(OH)2 (C)	-7.454	[-2.000]	330	[1.000]	600	[2.000]	2			
5060003	HYDCERRUSITE	-23.232	[-2.000]	330	[3.000]	600	[2.000]	140			
			[2.000]	2							
2060005	PB2O(OH)2	-24.408	[-4.000]	330	[2.000]	600	[3.000]	2			
5054000	NICO3	-10.594	[1.000]	540	[1.000]	140					
2054000	NI(OH)2	-5.966	[-2.000]	330	[1.000]	540	[2.000]	2			
2054001	BUNSENITE	-8.393	[-2.000]	330	[1.000]	540	[1.000]	2			
5023101	MALACHITE	-11.079	[2.000]	231	[2.000]	2	[1.000]	140			
			[-2.000]	330							
5023102	AZURITE	-18.319	[3.000]	231	[2.000]	2	[2.000]	140			
			[-2.000]	330							
2015000	LIME	-21.880	[-2.000]	330	[1.000]	150	[1.000]	2			
2015001	PORTLANDITE	-11.536	[-2.000]	330	[1.000]	150	[2.000]	2			
2028000	WUSTITE	-20.324	[-2.000]	330	[0.947]	280	[1.000]	2			
2046001	PERICLASE	-8.951	[-2.000]	330	[1.000]	460	[1.000]	2			
3028001	HERCYNITE	-23.529	[-8.000]	330	[1.000]	280	[2.000]	30			
			[4.000]	2							

```
3046000 SPINEL          -10.081    [ -8.000] 330  [  1.000] 460  [  2.000]  30
                                   [  4.000]   2
3046001 MAG-FERRITE      -8.209    [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                   [  4.000]   2
3028102 LEPIDOCROCIT     -3.155    [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021100 FECR2O4         -12.371    [  2.000] 211  [  1.000] 280  [ -4.000] 330
3021101 MGCR2O4          -2.794    [  2.000] 211  [  1.000] 460  [ -4.000] 330
3021102 CR2O3             0.000    [  2.000] 211  [ -2.000] 330  [ -1.000]   2
2021102 CR(OH)3 (A)      -0.860    [  1.000] 211  [  1.000]   2  [ -1.000] 330
2021101 CR(OH)3 (C)      -3.412    [  1.000] 211  [  1.000]   2  [ -1.000] 330
```

APPENDIX III

EFFECT OF DISSOLVED ORGANIC MATTER (DOM) CHANGES IN METALS ADSORPTION AND PRECIPITATION IN THE WATER OF THE CHICAMBA DAM (SITE 14): Output files of modelling with the Minteqa2 Program

Extended output files of the site 14 water quality modelling with different DOM values. The modelling was undertaken with the geochemical speciation program MINTEQA2 only for site 14 in order to see what would be the influence of DOM changes in the water quality supplied to Chimoio City from the Chicamba Dam. DOM values of 0.001 to 0.005 mol/l were introduced in the model after the four runs were undertaken. The output file has been reduced.

1 – Modelling with DOM = 0.001 mol/l

```
                              PART 1 of OUTPUT FILE
Revuè river water-Site 14 - DOM = 0.001 mol/l
Entered PCO2, PO2, fixed pH, solids allowed to precipitate, Fe redox pair,
adsorption and dissolved organic matter
-------------------------------------------------------------------------------
 Temperature (Celsius): 19.30
 Units of concentration: MG/L
 Ionic strength to be computed.
 Carbonate concentration represents carbonate alkalinity.
 Do not automatically terminate if charge imbalance exceeds 30%
 Precipitation is allowed for all solids in the thermodynamic database and
   the print option for solids is set to: 1
 The maximum number of iterations is: 200
 The method used to compute activity coefficients is: Davies equation
 Intermediate output file
 Adsorption model: Diffuse Layer
 Number of adsorbing surfaces: 1
-------------------------------------------------------------------------------

INPUT DATA BEFORE TYPE MODIFICATIONS
   ID        NAME       ACTIVITY GUESS     LOG GUESS    ANAL TOTAL
    330   H+1                 2.512E-08        -7.600    0.000E-01
     30   Al+3                4.786E-06        -5.320    1.300E-01
    100   Ba+2                1.380E-06        -5.860    1.900E-01
    150   Ca+2                1.288E-04        -3.890    5.200E+00
    160   Cd+2                4.677E-09        -8.330    5.300E-04
    211   Cr(OH)2+            2.818E-08        -7.550    2.400E-03
    231   Cu+2                3.162E-07        -6.500    2.000E-02
    280   Fe+2                5.370E-07        -6.270    3.000E-02
    410   K+1                 6.607E-05        -4.180    2.599E+00
    460   Mg+2                1.445E-04        -3.840    3.500E+00
    500   Na+1                2.089E-04        -3.680    4.800E+00
    540   Ni+2                1.862E-08        -7.730    1.100E-03
    600   Pb+2                1.778E-07        -6.750    3.700E-02
    800   Sr+2                5.754E-07        -6.240    5.000E-02
    950   Zn+2                3.090E-07        -6.510    2.000E-02
      1   E-1                 1.000E-16       -16.000    0.000E-01
    140   CO3-2               2.188E-04        -3.660    1.310E+01
    281   Fe+3                1.778E-21       -20.750    0.000E-01
    813   ADS1PSIo            1.000E+00         0.000    0.000E-01
    811   ADS1TYP1            1.905E-04        -3.720    1.922E-04
```

812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
145	DOM	1.000E-03	-3.000	1.000E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 3.237E-03
PERCENT DIFFERENCE = 5.864E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.686E-08	2.512E-08	-7.60000	0.93502	0.029
30	Al+3	4.869E-16	2.660E-16	-15.57513	0.54627	0.263
100	Ba+2	1.136E-07	8.685E-08	-7.06122	0.76435	0.117
150	Ca+2	1.798E-05	1.375E-05	-4.86184	0.76435	0.117
160	Cd+2	1.322E-12	1.010E-12	-11.99559	0.76435	0.117
211	Cr(OH)2+	6.591E-10	6.162E-10	-9.21025	0.93502	0.029
231	Cu+2	2.751E-13	2.102E-13	-12.67727	0.76435	0.117
280	Fe+2	1.657E-25	1.267E-25	-24.89733	0.76435	0.117
410	K+1	6.647E-05	6.215E-05	-4.20656	0.93502	0.029
460	Mg+2	9.480E-05	7.246E-05	-4.13989	0.76435	0.117
500	Na+1	2.088E-04	1.952E-04	-3.70950	0.93502	0.029
540	Ni+2	9.257E-12	7.075E-12	-11.15024	0.76435	0.117
600	Pb+2	2.687E-15	2.054E-15	-14.68741	0.76435	0.117
800	Sr+2	5.707E-07	4.362E-07	-6.36033	0.76435	0.117
950	Zn+2	2.413E-11	1.844E-11	-10.73416	0.76435	0.117
812	ADS1TYP2	5.901E-03	5.901E-03	-2.22906	1.00000	0.000
140	CO3-2	4.229E-07	3.232E-07	-6.49048	0.76435	0.117
281	Fe+3	4.774E-25	2.608E-25	-24.58367	0.54627	0.263
145	DOM	8.553E-04	5.051E-04	-3.29663	0.59055	0.229
811	ADS1TYP1	1.333E-04	1.333E-04	-3.87502	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	1.309E-10	1.309E-10	-9.88322	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.817E-09	1.819E-09	-8.74025	1.00089	-7.130
2113303	Cr(OH)4-	7.395E-13	6.914E-13	-12.16026	0.93502	-18.121
2113304	CrO2-	1.876E-12	1.755E-12	-11.75585	0.93502	-17.716
1453300	H DOM	1.887E-06	1.518E-06	-5.81881	0.80439	3.965
1450300	Al DOM	3.445E-13	3.436E-13	-12.46394	0.99732	5.201
1451000	Ba DOM	9.303E-07	8.912E-07	-6.05003	0.95791	3.119
1451500	Ca DOM	9.290E-05	8.899E-05	-4.05065	0.95791	2.919
1451600	Cd DOM	1.715E-11	1.643E-11	-10.78440	0.95791	3.319
1452110	Cr DOM	5.274E-12	5.259E-12	-11.27906	0.99732	15.221
1452310	Cu DOM	1.421E-10	1.361E-10	-9.86608	0.95791	4.919
1452810	Fe DOM	1.068E-19	1.065E-19	-18.97248	0.99732	7.701
1454600	Mg DOM	4.898E-05	4.691E-05	-4.32870	0.95791	1.919
1455400	Ni DOM	1.201E-10	1.151E-10	-9.93905	0.95791	3.319
1456000	Pb DOM	2.770E-12	2.653E-12	-11.57622	0.95791	5.219
1459500	Zn DOM	4.963E-10	4.754E-10	-9.32297	0.95791	3.519
3300020	OH-	2.758E-07	2.578E-07	-6.58865	0.93502	-14.159
4603300	MgOH +	3.057E-09	2.858E-09	-8.54393	0.93502	-11.975
4601400	MgCO3 AQ	2.046E-08	2.048E-08	-7.68866	1.00089	2.941
4601401	MgHCO3 +	1.713E-07	1.601E-07	-6.79547	0.93502	11.464
1503300	CaOH +	9.156E-11	8.561E-11	-10.06749	0.93502	-12.776
1501400	CaHCO3 +	2.513E-08	2.350E-08	-7.62892	0.93502	11.353
1501401	CaCO3 AQ	5.606E-09	5.611E-09	-8.25095	1.00089	3.101
5001400	NaCO3 -	9.330E-10	8.724E-10	-9.05928	0.93502	1.170
5001401	NaHCO3 AQ	1.904E-08	1.906E-08	-7.71998	1.00089	10.080
303300	AlOH +2	9.585E-14	7.326E-14	-13.13512	0.76435	-5.043
303301	Al(OH)2 +	3.581E-11	3.349E-11	-10.47514	0.93502	-10.071
303302	Al(OH)4 -	1.677E-09	1.568E-09	-8.80458	0.93502	-23.600
303303	Al(OH)3 AQ	1.677E-09	1.678E-09	-8.77515	1.00089	-16.000
2803300	FeOH +	1.105E-27	1.033E-27	-26.98589	0.93502	-9.659

2803301	FeOH3 -1	3.155E-34	2.950E-34	-33.53021	0.93502	-31.404
2803302	FeOH2 AQ	2.110E-31	2.111E-31	-30.67542	1.00089	-20.978
2813300	FeOH +2	6.230E-20	4.762E-20	-19.32223	0.76435	-2.222
2813301	FeOH2 +	9.451E-16	8.837E-16	-15.05368	0.93502	-5.641
2813302	FeOH3 AQ	4.130E-16	4.133E-16	-15.38369	1.00089	-13.600
2813303	FeOH4 -	1.760E-16	1.646E-16	-15.78369	0.93502	-21.571
2813304	Fe2(OH)2+4	2.273E-37	7.759E-38	-37.11021	0.34133	-2.676
2813305	Fe3(OH)4+5	7.483E-50	1.395E-50	-49.85531	0.18646	-5.775
8003300	SrOH +	7.652E-13	7.155E-13	-12.14541	0.93502	-13.356
1003300	BaOH +	9.870E-14	9.229E-14	-13.03487	0.93502	-13.544
2311400	CuCO3 AQ	3.646E-13	3.650E-13	-12.43774	1.00089	6.730
2311401	Cu(CO3)2-2	1.943E-16	1.485E-16	-15.82822	0.76435	9.947
2313300	CuOH +	8.952E-14	8.370E-14	-13.07727	0.93502	-7.971
2313301	Cu(OH)2 AQ	6.956E-12	6.962E-12	-11.15728	1.00089	-13.680
2313302	Cu(OH)3 -	1.790E-17	1.674E-17	-16.77629	0.93502	-26.870
2313303	Cu(OH)4 -2	1.735E-22	1.326E-22	-21.87729	0.76435	-39.483
2313304	Cu2(OH)2+2	2.255E-21	1.723E-21	-20.76361	0.76435	-10.492
2311402	CuHCO3 +	1.826E-14	1.707E-14	-13.76775	0.93502	13.029
9503300	ZnOH +	5.541E-13	5.181E-13	-12.28558	0.93502	-9.122
9503301	Zn(OH)2 AQ	3.685E-13	3.688E-13	-12.43317	1.00089	-16.899
9503302	Zn(OH)3 -	4.966E-17	4.643E-17	-16.33318	0.93502	-28.370
9503303	Zn(OH)4 -2	3.833E-22	2.930E-22	-21.53318	0.76435	-41.082
9501400	ZnHCO3 +	4.023E-13	3.762E-13	-12.42464	0.93502	12.429
9501401	ZnCO3 AQ	1.188E-12	1.190E-12	-11.92463	1.00089	5.300
9501402	Zn(CO3)2-2	1.075E-14	8.220E-15	-14.08511	0.76435	9.747
1601400	Cd(CO3)3-4	1.659E-25	5.662E-26	-25.24702	0.34133	6.687
1603300	CdOH +	2.325E-15	2.174E-15	-14.66274	0.93502	-10.238
1603301	Cd(OH)2 AQ	7.145E-18	7.152E-18	-17.14560	1.00089	-20.350
1603302	Cd(OH)3 -	3.416E-23	3.194E-23	-22.49561	0.93502	-33.271
1603303	Cd(OH)4 -2	1.483E-29	1.133E-29	-28.94561	0.76435	-47.233
1603304	Cd2OH +3	2.117E-26	1.156E-26	-25.93688	0.54627	-9.283
1601400	CdHCO3 +	2.203E-14	2.060E-14	-13.68607	0.93502	12.429
1601401	CdCO3 AQ	8.176E-14	8.183E-14	-13.08707	1.00089	5.399
6001400	Pb(CO3)2-2	1.226E-17	9.368E-18	-17.02836	0.76435	10.757
6003300	PbOH +	1.705E-15	1.594E-15	-14.79741	0.93502	-7.681
6003301	Pb(OH)2 AQ	2.467E-17	2.469E-17	-16.60742	1.00089	-17.120
6003302	Pb(OH)3 -	1.207E-20	1.129E-20	-19.94743	0.93502	-28.031
6003303	Pb2OH +3	1.342E-28	7.331E-29	-28.13482	0.54627	-6.097
6003304	Pb3(OH)4+2	1.570E-38	1.200E-38	-37.92082	0.76435	-24.142
6001401	PbCO3 AQ	1.153E-14	1.154E-14	-13.93789	1.00089	7.240
6003305	Pb(OH)4 -2	1.350E-24	1.032E-24	-23.98643	0.76435	-39.582
6001402	PbHCO3 +	2.827E-16	2.643E-16	-15.57789	0.93502	13.229
5403300	NiOH +	2.764E-14	2.584E-14	-13.58768	0.93502	-10.008
5403301	Ni(OH)2 AQ	1.120E-15	1.121E-15	-14.95026	1.00089	-19.000
5403302	Ni(OH)3 -	4.774E-19	4.464E-19	-18.35026	0.93502	-29.971
5401400	NiHCO3 +	1.813E-13	1.695E-13	-12.77072	0.93502	12.499
5401401	NiCO3 AQ	1.694E-11	1.695E-11	-10.77072	1.00089	6.870
5401402	Ni(CO3)2-2	1.246E-14	9.524E-15	-14.02120	0.76435	10.227
3301400	HCO3 -	2.101E-04	1.964E-04	-3.70680	0.93502	10.413
3301401	H2CO3 AQ	1.053E-05	1.053E-05	-4.97738	1.00089	16.713
2113300	Cr+3	5.755E-15	3.144E-15	-14.50252	0.54627	10.170
2113301	Cr(OH)+2	8.442E-12	6.453E-12	-11.19024	0.76435	5.737
8123301	=SO2-	8.658E-04	8.658E-04	-3.06258	1.00000	-8.930
8123302	=SO2H2+	9.214E-04	9.214E-04	-3.03553	1.00000	7.290
8113301	=SO1-	1.956E-05	1.956E-05	-4.70854	1.00000	-8.930
8113302	=SO1H2+	2.082E-05	2.082E-05	-4.68149	1.00000	7.290
8129500	=SO2Zn+	1.414E-08	1.414E-08	-7.84970	1.00000	-1.990
8119500	=SO1Zn+	2.913E-07	2.913E-07	-6.53566	1.00000	0.970
8121600	=SO2Cd+	9.525E-11	9.525E-11	-10.02113	1.00000	-2.900
8111600	=SO1Cd+	4.602E-09	4.602E-09	-8.33709	1.00000	0.430
8112310	=SO1Cu+	2.519E-07	2.519E-07	-6.59877	1.00000	2.850
8122310	=SO2Cu+	6.269E-08	6.269E-08	-7.20281	1.00000	0.600
8115400	=SO1Ni+	1.691E-08	1.691E-08	-7.77174	1.00000	0.150
8125400	=SO2Ni+	1.676E-09	1.676E-09	-8.77578	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74891	1.00000	4.710

8126000	=SO2Pb+	3.069E-10	3.069E-10	-9.51295	1.00000	0.300
8121500	=SO2Ca+	1.454E-06	1.454E-06	-5.83737	1.00000	-5.850
8111500	=SO1HCa++	1.739E-05	1.739E-05	-4.75980	1.00000	4.970
8111000	=SO1HBa++	3.395E-07	3.395E-07	-6.46918	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-1.423E-05	-4.847	0.000	0.000
330	H+1	-2.661E-04	-3.575	7.600	0.000
3301403	CO2 (g)	2.252E-04	-3.647	21.690	-0.530
3300021	O2 (g)	1.139E-04	-3.943	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.271E-08	-7.896	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP1			
	69.4	PERCENT BOUND IN SPECIES # 811	ADS1TYP1
	10.2	PERCENT BOUND IN SPECIES #8113301	=SO1-
	10.8	PERCENT BOUND IN SPECIES #8113302	=SO1H2+
	9.0	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++
ADS1TYP2			
	76.7	PERCENT BOUND IN SPECIES # 812	ADS1TYP2
	11.3	PERCENT BOUND IN SPECIES #8123301	=SO2-
	12.0	PERCENT BOUND IN SPECIES #8123302	=SO2H2+
Ba+2			
	8.2	PERCENT BOUND IN SPECIES # 100	Ba+2
	67.2	PERCENT BOUND IN SPECIES #1451000	Ba DOM
	24.5	PERCENT BOUND IN SPECIES #8111000	=SO1HBa++
Ca+2			
	13.9	PERCENT BOUND IN SPECIES # 150	Ca+2
	71.6	PERCENT BOUND IN SPECIES #1451500	Ca DOM
	1.1	PERCENT BOUND IN SPECIES #8121500	=SO2Ca+
	13.4	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++
Cd+2			
	2.0	PERCENT BOUND IN SPECIES #8121600	=SO2Cd+
	97.6	PERCENT BOUND IN SPECIES #8111600	=SO1Cd+
ADS1PSIo			
	973.8	PERCENT BOUND IN SPECIES #8123302	=SO2H2+
	22.0	PERCENT BOUND IN SPECIES #8113302	=SO1H2+
	1.5	PERCENT BOUND IN SPECIES #8121500	=SO2Ca+
	36.7	PERCENT BOUND IN SPECIES #8111500	=SO1HCa++
Cu+2			
	80.0	PERCENT BOUND IN SPECIES #8112310	=SO1Cu+
	19.9	PERCENT BOUND IN SPECIES #8122310	=SO2Cu+
DOM			
	85.5	PERCENT BOUND IN SPECIES # 145	DOM
	9.3	PERCENT BOUND IN SPECIES #1451500	Ca DOM
	4.9	PERCENT BOUND IN SPECIES #1454600	Mg DOM
K+1			
	100.0	PERCENT BOUND IN SPECIES # 410	K+1
Mg+2			
	65.8	PERCENT BOUND IN SPECIES # 460	Mg+2
	34.0	PERCENT BOUND IN SPECIES #1454600	Mg DOM
Na+1			
	100.0	PERCENT BOUND IN SPECIES # 500	Na+1
Ni+2			

```
                90.3     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                 8.9     PERCENT BOUND IN SPECIES #8125400   =SO2Ni+
Pb+2
                99.8     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
Sr+2
               100.0     PERCENT BOUND IN SPECIES #    800   Sr+2
Zn+2
                 4.6     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                95.2     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
Cr(OH)2+
                26.4     PERCENT BOUND IN SPECIES #    211   Cr(OH)2+
                72.9     PERCENT BOUND IN SPECIES #2113302   Cr(OH)3 AQ
Al+3
                 1.1     PERCENT BOUND IN SPECIES # 303301   Al(OH)2 +
                49.5     PERCENT BOUND IN SPECIES # 303302   Al(OH)4 -
                49.5     PERCENT BOUND IN SPECIES # 303303   Al(OH)3 AQ
CO3-2
                94.9     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 4.8     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
                99.3     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
                61.6     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                26.9     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                11.5     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
                73.0     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 7.3     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
               320.4     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                 7.2     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                24.7     PERCENT BOUND IN SPECIES #3300020   OH-
                 1.3     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                26.1     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                22.6     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                 5.6     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                 1.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                16.0     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED		SORBED		PRECIPITATED	
		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
100	Ba+2	1.044E-06	75.5	3.396E-07	24.5	0.000E-01	0.0
150	Ca+2	1.109E-04	85.5	1.884E-05	14.5	0.000E-01	0.0
160	Cd+2	1.858E-11	0.4	4.697E-09	99.6	0.000E-01	0.0
231	Cu+2	1.498E-10	0.0	3.146E-07	100.0	0.000E-01	0.0
145	DOM	1.000E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.465E-10	0.8	1.859E-08	99.2	0.000E-01	0.0
600	Pb+2	2.786E-12	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	5.229E-10	0.2	3.054E-07	99.8	0.000E-01	0.0
211	Cr(OH)2+	2.492E-09	8.9	0.000E-01	0.0	2.541E-08	91.1
30	Al+3	3.390E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.213E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	1.668E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.534E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.330E-04	81.0	5.462E-05	19.0	0.000E-01	0.0
2	H2O	2.925E-07	26.2	8.219E-07	73.8	0.000E-01	0.0

```
     Charge Balance: SPECIATED
       Sum of CATIONS =  1.482E-03 Sum of ANIONS   3.609E-03
       PERCENT DIFFERENCE =   4.177E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =   2.490E-07
     EQUILIBRIUM IONIC STRENGTH (m) =   3.872E-03
     EQUILIBRIUM pH                 =   7.600
     EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.028808     sig0 = 0.004421
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
```

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-3.067	[1.000] 150 [1.000] 140
5046000	ARTINITE	-9.581	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.101	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-2.910	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-5.101	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-13.643	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-23.441	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-2.689	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.374	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.092	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.611	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.075	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-4.962	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.538	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.335	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.315	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.477	[-8.000] 330 [1.000] 231 [2.000] 281 [4.000] 2
95000	ZN METAL	-63.994	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.287	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-6.965	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-7.984	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.734	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.284	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.244	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-7.034	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.844	[-2.000] 330 [1.000] 950 [1.000] 2

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2095006	ZINCITE	-6.986	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.720	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.822	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.754	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-10.822	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-10.446	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-12.269	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-45.929	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-7.978	[1.000] 600 [1.000] 140
2060000	MASSICOT	-12.637	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-12.441	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-12.467	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-20.329	[-2.000] 330 [2.000] 600 [1.000] 2
			[1.000] 140
5060002	PB3O2CO3	-31.550	[-4.000] 330 [3.000] 600 [1.000] 140
			[2.000] 2
2060003	PLATTNERITE	-7.621	[-4.000] 330 [-2.000] 1 [1.000] 600
			[2.000] 2
3060000	PB2O3	-17.838	[-6.000] 330 [-2.000] 1 [2.000] 600
			[3.000] 2
3060001	MINIUM	-31.443	[-8.000] 330 [-2.000] 1 [3.000] 600
			[4.000] 2
2060004	PB(OH)2 (C)	-7.837	[-2.000] 330 [1.000] 600 [2.000] 2
5060003	HYDCERRUSITE	-24.383	[-2.000] 330 [3.000] 600 [2.000] 140
			[2.000] 2
2060005	PB2O(OH)2	-25.175	[-4.000] 330 [2.000] 600 [3.000] 2
5054000	NICO3	-10.943	[1.000] 540 [1.000] 140
2054000	NI(OH)2	-6.315	[-2.000] 330 [1.000] 540 [2.000] 2
2054001	BUNSENITE	-8.742	[-2.000] 330 [1.000] 540 [1.000] 2
5023101	MALACHITE	-11.688	[2.000] 231 [2.000] 2 [1.000] 140
			[-2.000] 330
5023102	AZURITE	-19.232	[3.000] 231 [2.000] 2 [2.000] 140
			[-2.000] 330
2015000	LIME	-23.120	[-2.000] 330 [1.000] 150 [1.000] 2
2015001	PORTLANDITE	-12.775	[-2.000] 330 [1.000] 150 [2.000] 2
2028000	WUSTITE	-20.420	[-2.000] 330 [0.947] 280 [1.000] 2
2046001	PERICLASE	-10.966	[-2.000] 330 [1.000] 460 [1.000] 2
3028001	HERCYNITE	-23.529	[-8.000] 330 [1.000] 280 [2.000] 30
			[4.000] 2
3046000	SPINEL	-12.096	[-8.000] 330 [1.000] 460 [2.000] 30
			[4.000] 2
3046001	MAG-FERRITE	-10.224	[-8.000] 330 [1.000] 460 [2.000] 281
			[4.000] 2
3028102	LEPIDOCROCIT	-3.155	[-3.000] 330 [1.000] 281 [2.000] 2
3021100	FECR2O4	-12.371	[2.000] 211 [1.000] 280 [-4.000] 330
3021101	MGCR2O4	-4.809	[2.000] 211 [1.000] 460 [-4.000] 330
3021102	CR2O3	0.000	[2.000] 211 [-2.000] 330 [-1.000] 2
2021102	CR(OH)3 (A)	-0.860	[1.000] 211 [1.000] 2 [-1.000] 330
2021101	CR(OH)3 (C)	-3.412	[1.000] 211 [1.000] 2 [-1.000] 330

2 – Modelling with DOM = 0.002 mol/l

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - DOM = 0.002 mol/l

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair, adsorption and dissolved organic matter

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
145	DOM	1.995E-03	-2.700	2.000E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 6.037E-03
PERCENT DIFFERENCE = 7.547E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.751E-08	2.512E-08	-7.60000	0.91323	0.039
30	Al+3	6.021E-16	2.660E-16	-15.57513	0.44181	0.355
100	Ba+2	5.296E-08	3.683E-08	-7.43375	0.69555	0.158
150	Ca+2	8.112E-06	5.642E-06	-5.24856	0.69555	0.158
160	Cd+2	1.330E-12	9.254E-13	-12.03369	0.69555	0.158
211	Cr(OH)2+	6.748E-10	6.162E-10	-9.21025	0.91323	0.039
231	Cu+2	2.810E-13	1.955E-13	-12.70890	0.69555	0.158
280	Fe+2	1.821E-25	1.267E-25	-24.89733	0.69555	0.158
410	K+1	6.647E-05	6.070E-05	-4.21680	0.91323	0.039
460	Mg+2	6.010E-05	4.181E-05	-4.37877	0.69555	0.158
500	Na+1	2.088E-04	1.907E-04	-3.71974	0.91323	0.039

540	Ni+2	9.308E-12	6.474E-12	-11.18882	0.69555	0.158
600	Pb+2	2.719E-15	1.891E-15	-14.72321	0.69555	0.158
800	Sr+2	5.707E-07	3.969E-07	-6.40129	0.69555	0.158
950	Zn+2	2.441E-11	1.698E-11	-10.77016	0.69555	0.158
812	ADS1TYP2	5.900E-03	5.900E-03	-2.22914	1.00000	0.000
140	CO3-2	4.647E-07	3.232E-07	-6.49048	0.69555	0.158
281	Fe+3	5.903E-25	2.608E-25	-24.58367	0.44181	0.355
145	DOM	1.796E-03	8.816E-04	-3.05471	0.49086	0.309
811	ADS1TYP1	1.407E-04	1.407E-04	-3.85183	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	5.881E-11	5.881E-11	-10.23055	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.816E-09	1.819E-09	-8.74025	1.00173	-7.131
2113303	Cr(OH)4-	7.571E-13	6.914E-13	-12.16026	0.91323	-18.111
2113304	CrO2-	1.921E-12	1.755E-12	-11.75585	0.91323	-17.706
1453300	H DOM	5.946E-06	4.431E-06	-5.35346	0.74522	3.998
1450300	Al DOM	1.007E-12	1.003E-12	-11.99859	0.99638	5.202
1451000	Ba DOM	1.170E-06	1.104E-06	-5.95721	0.94357	3.125
1451500	Ca DOM	1.130E-04	1.067E-04	-3.97202	0.94357	2.925
1451600	Cd DOM	4.657E-11	4.394E-11	-10.35715	0.94357	3.325
1452110	Cr DOM	1.541E-11	1.536E-11	-10.81371	0.99638	15.222
1452310	Cu DOM	3.916E-10	3.695E-10	-9.43237	0.94357	4.925
1452810	Fe DOM	3.122E-19	3.111E-19	-18.50713	0.99638	7.702
1454600	Mg DOM	8.375E-05	7.903E-05	-4.10223	0.94357	1.925
1455400	Ni DOM	3.258E-10	3.074E-10	-9.51229	0.94357	3.325
1456000	Pb DOM	7.561E-12	7.134E-12	-11.14668	0.94357	5.225
1459500	Zn DOM	1.354E-09	1.278E-09	-8.89362	0.94357	3.525
3300020	OH-	2.823E-07	2.578E-07	-6.58865	0.91323	-14.149
4603300	MgOH +	1.806E-09	1.649E-09	-8.78281	0.91323	-11.965
4601400	MgCO3 AQ	1.180E-08	1.182E-08	-7.92754	1.00173	2.941
4601401	MgHCO3 +	1.012E-07	9.239E-08	-7.03436	0.91323	11.474
1503300	CaOH +	3.848E-11	3.514E-11	-10.45421	0.91323	-12.766
1501400	CaHCO3 +	1.056E-08	9.646E-09	-8.01564	0.91323	11.363
1501401	CaCO3 AQ	2.299E-09	2.303E-09	-8.63768	1.00173	3.101
5001400	NaCO3 -	9.330E-10	8.521E-10	-9.06952	0.91323	1.180
5001401	NaHCO3 AQ	1.858E-08	1.861E-08	-7.73022	1.00173	10.079
303300	AlOH +2	1.053E-13	7.326E-14	-13.13512	0.69555	-5.002
303301	Al(OH)2 +	3.667E-11	3.349E-11	-10.47514	0.91323	-10.061
303302	Al(OH)4 -	1.717E-09	1.568E-09	-8.80458	0.91323	-23.590
303303	Al(OH)3 AQ	1.675E-09	1.678E-09	-8.77515	1.00173	-16.001
2803300	FeOH +	1.131E-27	1.033E-27	-26.98589	0.91323	-9.649
2803301	FeOH3 -1	3.230E-34	2.950E-34	-33.53021	0.91323	-31.393
2803302	FeOH2 AQ	2.108E-31	2.111E-31	-30.67542	1.00173	-20.979
2813300	FeOH +2	6.846E-20	4.762E-20	-19.32223	0.69555	-2.181
2813301	FeOH2 +	9.677E-16	8.837E-16	-15.05368	0.91323	-5.631
2813302	FeOH3 AQ	4.126E-16	4.133E-16	-15.38369	1.00173	-13.601
2813303	FeOH4 -	1.802E-16	1.646E-16	-15.78369	0.91323	-21.561
2813304	Fe2(OH)2+4	3.315E-37	7.759E-38	-37.11021	0.23405	-2.512
2813305	Fe3(OH)4+5	1.349E-49	1.395E-50	-49.85531	0.10341	-5.519
8003300	SrOH +	7.129E-13	6.511E-13	-12.18637	0.91323	-13.346
1003300	BaOH +	4.286E-14	3.914E-14	-13.40740	0.91323	-13.534
2311400	CuCO3 AQ	3.387E-13	3.393E-13	-12.46938	1.00173	6.729
2311401	Cu(CO3)2-2	1.985E-16	1.381E-16	-15.85986	0.69555	9.988
2313300	CuOH +	8.521E-14	7.782E-14	-13.10891	0.91323	-7.961
2313301	Cu(OH)2 AQ	6.462E-12	6.473E-12	-11.18892	1.00173	-13.681
2313302	Cu(OH)3 -	1.704E-17	1.556E-17	-16.80792	0.91323	-26.860
2313303	Cu(OH)4 -2	1.773E-22	1.233E-22	-21.90893	0.69555	-39.442
2313304	Cu2(OH)2+2	2.142E-21	1.490E-21	-20.82688	0.69555	-10.451
2311402	CuHCO3 +	1.738E-14	1.587E-14	-13.79938	0.91323	13.039
9503300	ZnOH +	5.222E-13	4.769E-13	-12.32158	0.91323	-9.112
9503301	Zn(OH)2 AQ	3.389E-13	3.395E-13	-12.46917	1.00173	-16.900
9503302	Zn(OH)3 -	4.680E-17	4.274E-17	-16.36918	0.91323	-28.360
9503303	Zn(OH)4 -2	3.877E-22	2.697E-22	-21.56918	0.69555	-41.041

9501400	ZnHCO3 +	3.791E-13	3.462E-13	-12.46064	0.91323	12.439
9501401	ZnCO3 AQ	1.093E-12	1.095E-12	-11.96064	1.00173	5.299
9501402	Zn(CO3)2-2	1.088E-14	7.566E-15	-14.12111	0.69555	9.788
1601400	Cd(CO3)3-4	2.216E-25	5.187E-26	-25.28512	0.23405	6.851
1603300	CdOH +	2.181E-15	1.991E-15	-14.70084	0.91323	-10.228
1603301	Cd(OH)2 AQ	6.540E-18	6.551E-18	-17.18370	1.00173	-20.351
1603302	Cd(OH)3 -	3.204E-23	2.926E-23	-22.53371	0.91323	-33.261
1603303	Cd(OH)4 -2	1.493E-29	1.038E-29	-28.98371	0.69555	-47.192
1603304	Cd2OH +3	2.196E-26	9.703E-27	-26.01308	0.44181	-9.191
1601400	CdHCO3 +	2.067E-14	1.887E-14	-13.72417	0.91323	12.439
1601401	CdCO3 AQ	7.483E-14	7.496E-14	-13.12516	1.00173	5.398
6001400	Pb(CO3)2-2	1.240E-17	8.626E-18	-17.06417	0.69555	10.798
6003300	PbOH +	1.608E-15	1.468E-15	-14.83322	0.91323	-7.671
6003301	Pb(OH)2 AQ	2.270E-17	2.274E-17	-16.64322	1.00173	-17.121
6003302	Pb(OH)3 -	1.138E-20	1.039E-20	-19.98323	0.91323	-28.021
6003303	Pb2OH +3	1.407E-28	6.217E-29	-28.20643	0.44181	-6.005
6003304	Pb3(OH)4+2	1.347E-38	9.371E-39	-38.02823	0.69555	-24.101
6001401	PbCO3 AQ	1.061E-14	1.062E-14	-13.97369	1.00173	7.239
6003305	Pb(OH)4 -2	1.366E-24	9.501E-25	-24.02224	0.69555	-39.541
6001402	PbHCO3 +	2.665E-16	2.434E-16	-15.61369	0.91323	13.239
5403300	NiOH +	2.589E-14	2.365E-14	-13.62626	0.91323	-9.998
5403301	Ni(OH)2 AQ	1.024E-15	1.026E-15	-14.98884	1.00173	-19.001
5403302	Ni(OH)3 -	4.473E-19	4.085E-19	-18.38885	0.91323	-29.961
5401400	NiHCO3 +	1.699E-13	1.551E-13	-12.80930	0.91323	12.509
5401401	NiCO3 AQ	1.549E-11	1.551E-11	-10.80930	1.00173	6.869
5401402	Ni(CO3)2-2	1.253E-14	8.714E-15	-14.05978	0.69555	10.268
3301400	HCO3 -	2.151E-04	1.964E-04	-3.70680	0.91323	10.423
3301401	H2CO3 AQ	1.052E-05	1.053E-05	-4.97738	1.00173	16.712
2113300	Cr+3	7.116E-15	3.144E-15	-14.50252	0.44181	10.262
2113301	Cr(OH)+2	9.278E-12	6.453E-12	-11.19024	0.69555	5.778
8123301	=SO2-	8.408E-04	8.408E-04	-3.07532	1.00000	-8.930
8123302	=SO2H2+	9.485E-04	9.485E-04	-3.02297	1.00000	7.290
8113301	=SO1-	2.004E-05	2.004E-05	-4.69801	1.00000	-8.930
8113302	=SO1H2+	2.261E-05	2.261E-05	-4.64566	1.00000	7.290
8129500	=SO2Zn+	1.339E-08	1.339E-08	-7.87314	1.00000	-1.990
8119500	=SO1Zn+	2.912E-07	2.912E-07	-6.53583	1.00000	0.970
8121600	=SO2Cd+	8.981E-11	8.981E-11	-10.04667	1.00000	-2.900
8111600	=SO1Cd+	4.578E-09	4.578E-09	-8.33936	1.00000	0.430
8112310	=SO1Cu+	2.543E-07	2.543E-07	-6.59457	1.00000	2.850
8122310	=SO2Cu+	6.000E-08	6.000E-08	-7.22188	1.00000	0.600
8115400	=SO1Ni+	1.681E-08	1.681E-08	-7.77449	1.00000	0.150
8125400	=SO2Ni+	1.578E-09	1.578E-09	-8.80180	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74888	1.00000	4.710
8126000	=SO2Pb+	2.909E-10	2.909E-10	-9.53619	1.00000	0.300
8121500	=SO2Ca+	6.144E-07	6.144E-07	-6.21153	1.00000	-5.850
8111500	=SO1HCa++	7.979E-06	7.979E-06	-5.09805	1.00000	4.970
8111000	=SO1HBa++	1.610E-07	1.610E-07	-6.79324	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-1.918E-05	-4.717	0.000	0.000
330	H+1	-3.194E-04	-3.496	7.600	0.000
3301403	CO2 (g)	2.202E-04	-3.657	21.690	-0.530
3300021	O2 (g)	1.139E-04	-3.943	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.269E-08	-7.896	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP1			
73.2	PERCENT BOUND IN SPECIES #	811	ADS1TYP1
10.4	PERCENT BOUND IN SPECIES #	8113301	=SO1-
11.8	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
4.2	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
ADS1TYP2			
76.7	PERCENT BOUND IN SPECIES #	812	ADS1TYP2
10.9	PERCENT BOUND IN SPECIES #	8123301	=SO2-
12.3	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
Ba+2			
3.8	PERCENT BOUND IN SPECIES #	100	Ba+2
84.5	PERCENT BOUND IN SPECIES #	1451000	Ba DOM
11.6	PERCENT BOUND IN SPECIES #	8111000	=SO1HBa++
Ca+2			
6.3	PERCENT BOUND IN SPECIES #	150	Ca+2
87.1	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
6.1	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cd+2			
1.9	PERCENT BOUND IN SPECIES #	8121600	=SO2Cd+
97.1	PERCENT BOUND IN SPECIES #	8111600	=SO1Cd+
ADS1PSIo			
741.1	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
17.7	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
12.5	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cu+2			
80.8	PERCENT BOUND IN SPECIES #	8112310	=SO1Cu+
19.1	PERCENT BOUND IN SPECIES #	8122310	=SO2Cu+
DOM			
89.8	PERCENT BOUND IN SPECIES #	145	DOM
5.7	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
4.2	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
K+1			
100.0	PERCENT BOUND IN SPECIES #	410	K+1
Mg+2			
41.7	PERCENT BOUND IN SPECIES #	460	Mg+2
58.2	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
Na+1			
100.0	PERCENT BOUND IN SPECIES #	500	Na+1
Ni+2			
1.7	PERCENT BOUND IN SPECIES #	1455400	Ni DOM
89.7	PERCENT BOUND IN SPECIES #	8115400	=SO1Ni+
8.4	PERCENT BOUND IN SPECIES #	8125400	=SO2Ni+
Pb+2			
99.8	PERCENT BOUND IN SPECIES #	8116000	=SO1Pb+
Sr+2			
100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
Zn+2			
4.4	PERCENT BOUND IN SPECIES #	8129500	=SO2Zn+
95.2	PERCENT BOUND IN SPECIES #	8119500	=SO1Zn+
Cr(OH)2+			
26.8	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
72.1	PERCENT BOUND IN SPECIES #	2113302	Cr(OH)3 AQ
Al+3			
1.1	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
50.1	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
48.8	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
CO3-2			
95.1	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
4.6	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ
Fe+2			
99.4	PERCENT BOUND IN SPECIES #	280	Fe+2

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E-1
Fe+3
                62.0     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
                26.4     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
                11.5     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
                 1.7     PERCENT BOUND IN SPECIES #1453300   H DOM
                61.3     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                 6.0     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
               270.4     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                 6.4     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
                25.2     PERCENT BOUND IN SPECIES #3300020   OH-
                 1.2     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
                26.0     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
                22.7     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                 5.4     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                 1.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
                15.9     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.223E-06	88.4	1.610E-07	11.6	0.000E-01	0.0
150	Ca+2	1.212E-04	93.4	8.593E-06	6.6	0.000E-01	0.0
160	Cd+2	4.799E-11	1.0	4.667E-09	99.0	0.000E-01	0.0
231	Cu+2	3.988E-10	0.1	3.143E-07	99.9	0.000E-01	0.0
145	DOM	2.000E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	3.508E-10	1.9	1.839E-08	98.1	0.000E-01	0.0
600	Pb+2	7.576E-12	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	1.381E-09	0.5	3.046E-07	99.5	0.000E-01	0.0
211	Cr(OH)2+	2.518E-09	9.0	0.000E-01	0.0	2.539E-08	91.0
30	Al+3	3.430E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.262E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	1.832E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.561E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.419E-04	69.0	1.088E-04	31.0	0.000E-01	0.0
2	H2O	2.979E-07	26.6	8.206E-07	73.4	0.000E-01	0.0

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     Charge Balance: SPECIATED
       Sum of CATIONS =  1.402E-03 Sum of ANIONS   6.275E-03
       PERCENT DIFFERENCE =   6.348E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =   2.549E-07
     EQUILIBRIUM IONIC STRENGTH (m) =   7.498E-03
     EQUILIBRIUM pH                 =   7.600
     EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.028075     sig0 = 0.005979
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-3.453	[1.000] 150 [1.000] 140
5046000	ARTINITE	-10.059	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.340	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-3.297	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-5.727	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-14.747	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-24.636	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-2.928	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.394	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.331	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.652	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.095	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-5.334	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.569	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.367	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.347	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.509	[-8.000] 330 [1.000] 231 [2.000] 281 [4.000] 2
95000	ZN METAL	-64.030	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.323	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-7.001	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-8.020	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.770	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.320	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.280	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-7.070	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.880	[-2.000] 330 [1.000] 950 [1.000] 2

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2095006	ZINCITE	-7.022	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.758	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.860	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.792	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-10.860	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-10.484	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-12.307	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-45.965	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-8.014	[1.000] 600 [1.000] 140
2060000	MASSICOT	-12.673	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-12.477	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-12.503	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-20.401	[-2.000] 330 [2.000] 600 [1.000] 2 [1.000] 140
5060002	PB3O2CO3	-31.658	[-4.000] 330 [3.000] 600 [1.000] 140 [2.000] 2

2060003	PLATTNERITE	-7.657	[-4.000]	330	[-2.000]	1	[1.000]	600		
			[2.000]	2						
3060000	PB2O3	-17.909	[-6.000]	330	[-2.000]	1	[2.000]	600		
			[3.000]	2						
3060001	MINIUM	-31.551	[-8.000]	330	[-2.000]	1	[3.000]	600		
			[4.000]	2						
2060004	PB(OH)2 (C)	-7.873	[-2.000]	330	[1.000]	600	[2.000]	2		
5060003	HYDCERRUSITE	-24.491	[-2.000]	330	[3.000]	600	[2.000]	140		
			[2.000]	2						
2060005	PB2O(OH)2	-25.246	[-4.000]	330	[2.000]	600	[3.000]	2		
5054000	NICO3	-10.981	[1.000]	540	[1.000]	140				
2054000	NI(OH)2	-6.354	[-2.000]	330	[1.000]	540	[2.000]	2		
2054001	BUNSENITE	-8.781	[-2.000]	330	[1.000]	540	[1.000]	2		
5023101	MALACHITE	-11.751	[2.000]	231	[2.000]	2	[1.000]	140		
			[-2.000]	330						
5023102	AZURITE	-19.327	[3.000]	231	[2.000]	2	[2.000]	140		
			[-2.000]	330						
2015000	LIME	-23.506	[-2.000]	330	[1.000]	150	[1.000]	2		
2015001	PORTLANDITE	-13.162	[-2.000]	330	[1.000]	150	[2.000]	2		
2028000	WUSTITE	-20.420	[-2.000]	330	[0.947]	280	[1.000]	2		
2046001	PERICLASE	-11.205	[-2.000]	330	[1.000]	460	[1.000]	2		
3028001	HERCYNITE	-23.529	[-8.000]	330	[1.000]	280	[2.000]	30		
			[4.000]	2						
3046000	SPINEL	-12.335	[-8.000]	330	[1.000]	460	[2.000]	30		
			[4.000]	2						
3046001	MAG-FERRITE	-10.463	[-8.000]	330	[1.000]	460	[2.000]	281		
			[4.000]	2						
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2		
3021100	FECR2O4	-12.371	[2.000]	211	[1.000]	280	[-4.000]	330		
3021101	MGCR2O4	-5.048	[2.000]	211	[1.000]	460	[-4.000]	330		
3021102	CR2O3	0.000	[2.000]	211	[-2.000]	330	[-1.000]	2		
2021102	CR(OH)3 (A)	-0.860	[1.000]	211	[1.000]	2	[-1.000]	330		
2021101	CR(OH)3 (C)	-3.412	[1.000]	211	[1.000]	2	[-1.000]	330		

3 – Modelling with DOM = 0.003 mol/l

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - DOM = 0.003 mol/l

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair, adsorption and dissolved organic matter

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
145	DOM	3.020E-03	-2.520	3.000E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 8.837E-03
PERCENT DIFFERENCE = 8.257E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.800E-08	2.512E-08	-7.60000	0.89701	0.047
30	Al+3	7.074E-16	2.660E-16	-15.57513	0.37599	0.425
100	Ba+2	3.219E-08	2.084E-08	-7.68107	0.64743	0.189
150	Ca+2	4.870E-06	3.153E-06	-5.50126	0.64743	0.189
160	Cd+2	1.368E-12	8.859E-13	-12.05264	0.64743	0.189
211	Cr(OH)2+	6.870E-10	6.162E-10	-9.21025	0.89701	0.047
231	Cu+2	2.920E-13	1.891E-13	-12.72342	0.64743	0.189
280	Fe+2	1.957E-25	1.267E-25	-24.89733	0.64743	0.189
410	K+1	6.647E-05	5.962E-05	-4.22458	0.89701	0.047
460	Mg+2	4.159E-05	2.692E-05	-4.56986	0.64743	0.189
500	Na+1	2.088E-04	1.873E-04	-3.72752	0.89701	0.047

540	Ni+2	9.525E-12	6.167E-12	-11.20994	0.64743	0.189
600	Pb+2	2.819E-15	1.825E-15	-14.73876	0.64743	0.189
800	Sr+2	5.707E-07	3.695E-07	-6.43243	0.64743	0.189
950	Zn+2	2.523E-11	1.633E-11	-10.78696	0.64743	0.189
812	ADS1TYP2	5.899E-03	5.899E-03	-2.22926	1.00000	0.000
140	CO3-2	4.993E-07	3.232E-07	-6.49048	0.64743	0.189
281	Fe+3	6.937E-25	2.608E-25	-24.58367	0.37599	0.425
145	DOM	2.765E-03	1.179E-03	-2.92841	0.42651	0.370
811	ADS1TYP1	1.432E-04	1.432E-04	-3.84412	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	3.449E-11	3.449E-11	-10.46232	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.814E-09	1.819E-09	-8.74025	1.00260	-7.131
2113303	Cr(OH)4-	7.708E-13	6.914E-13	-12.16026	0.89701	-18.103
2113304	CrO2-	1.956E-12	1.755E-12	-11.75585	0.89701	-17.698
1453300	H DOM	1.182E-05	8.310E-06	-5.08042	0.70318	4.023
1450300	Al DOM	1.889E-12	1.881E-12	-11.72555	0.99566	5.202
1451000	Ba DOM	1.255E-06	1.171E-06	-5.93149	0.93280	3.130
1451500	Ca DOM	1.198E-04	1.118E-04	-3.95168	0.93280	2.930
1451600	Cd DOM	8.456E-11	7.888E-11	-10.10306	0.93280	3.330
1452110	Cr DOM	2.892E-11	2.880E-11	-10.54067	0.99566	15.222
1452310	Cu DOM	7.184E-10	6.701E-10	-9.17384	0.93280	4.930
1452810	Fe DOM	5.859E-19	5.833E-19	-18.23409	0.99566	7.702
1454600	Mg DOM	1.023E-04	9.544E-05	-4.02028	0.93280	1.930
1455400	Ni DOM	5.886E-10	5.491E-10	-9.26037	0.93280	3.330
1456000	Pb DOM	1.384E-11	1.291E-11	-10.88918	0.93280	5.230
1459500	Zn DOM	2.471E-09	2.305E-09	-8.63738	0.93280	3.530
3300020	OH-	2.874E-07	2.578E-07	-6.58865	0.89701	-14.141
4603300	MgOH +	1.184E-09	1.062E-09	-8.97390	0.89701	-11.957
4601400	MgCO3 AQ	7.590E-09	7.610E-09	-8.11863	1.00260	2.941
4601401	MgHCO3 +	6.634E-08	5.950E-08	-7.22545	0.89701	11.482
1503300	CaOH +	2.189E-11	1.964E-11	-10.70691	0.89701	-12.758
1501400	CaHCO3 +	6.010E-09	5.391E-09	-8.26834	0.89701	11.371
1501401	CaCO3 AQ	1.284E-09	1.287E-09	-8.89038	1.00260	3.100
5001400	NaCO3 -	9.330E-10	8.369E-10	-9.07730	0.89701	1.188
5001401	NaHCO3 AQ	1.823E-08	1.828E-08	-7.73800	1.00260	10.079
303300	AlOH +2	1.132E-13	7.326E-14	-13.13512	0.64743	-4.971
303301	Al(OH)2 +	3.733E-11	3.349E-11	-10.47514	0.89701	-10.053
303302	Al(OH)4 -	1.748E-09	1.568E-09	-8.80458	0.89701	-23.582
303303	Al(OH)3 AQ	1.674E-09	1.678E-09	-8.77515	1.00260	-16.001
2803300	FeOH +	1.152E-27	1.033E-27	-26.98589	0.89701	-9.641
2803301	FeOH3 -1	3.288E-34	2.950E-34	-33.53021	0.89701	-31.386
2803302	FeOH2 AQ	2.106E-31	2.111E-31	-30.67542	1.00260	-20.979
2813300	FeOH +2	7.355E-20	4.762E-20	-19.32223	0.64743	-2.150
2813301	FeOH2 +	9.852E-16	8.837E-16	-15.05368	0.89701	-5.623
2813302	FeOH3 AQ	4.123E-16	4.133E-16	-15.38369	1.00260	-13.601
2813303	FeOH4 -	1.834E-16	1.646E-16	-15.78369	0.89701	-21.553
2813304	Fe2(OH)2+4	4.416E-37	7.759E-38	-37.11021	0.17570	-2.388
2813305	Fe3(OH)4+5	2.112E-49	1.395E-50	-49.85531	0.06606	-5.324
8003300	SrOH +	6.756E-13	6.060E-13	-12.21751	0.89701	-13.338
1003300	BaOH +	2.469E-14	2.215E-14	-13.65472	0.89701	-13.526
2311400	CuCO3 AQ	3.273E-13	3.282E-13	-12.48389	1.00260	6.729
2311401	Cu(CO3)2-2	2.063E-16	1.335E-16	-15.87437	0.64743	10.019
2313300	CuOH +	8.390E-14	7.526E-14	-13.12342	0.89701	-7.953
2313301	Cu(OH)2 AQ	6.244E-12	6.260E-12	-11.20343	1.00260	-13.681
2313302	Cu(OH)3 -	1.678E-17	1.505E-17	-16.82244	0.89701	-26.852
2313303	Cu(OH)4 -2	1.842E-22	1.193E-22	-21.92344	0.64743	-39.411
2313304	Cu2(OH)2+2	2.152E-21	1.393E-21	-20.85591	0.64743	-10.420
2311402	CuHCO3 +	1.711E-14	1.535E-14	-13.81390	0.89701	13.047
9503300	ZnOH +	5.115E-13	4.588E-13	-12.33838	0.89701	-9.104
9503301	Zn(OH)2 AQ	3.258E-13	3.266E-13	-12.48597	1.00260	-16.900
9503302	Zn(OH)3 -	4.584E-17	4.112E-17	-16.38598	0.89701	-28.352
9503303	Zn(OH)4 -2	4.007E-22	2.594E-22	-21.58599	0.64743	-41.010

9501400	ZnHCO3 +	3.713E-13	3.331E-13	-12.47744	0.89701	12.447
9501401	ZnCO3 AQ	1.051E-12	1.053E-12	-11.97744	1.00260	5.299
9501402	Zn(CO3)2-2	1.124E-14	7.279E-15	-14.13791	0.64743	9.819
1601400	Cd(CO3)3-4	2.826E-25	4.965E-26	-25.30407	0.17570	6.975
1603300	CdOH +	2.125E-15	1.906E-15	-14.71979	0.89701	-10.220
1603301	Cd(OH)2 AQ	6.255E-18	6.271E-18	-17.20265	1.00260	-20.351
1603302	Cd(OH)3 -	3.123E-23	2.801E-23	-22.55266	0.89701	-33.253
1603303	Cd(OH)4 -2	1.535E-29	9.939E-30	-29.00266	0.64743	-47.161
1603304	Cd2OH +3	2.365E-26	8.892E-27	-26.05098	0.37599	-9.121
1601400	CdHCO3 +	2.014E-14	1.807E-14	-13.74311	0.89701	12.447
1601401	CdCO3 AQ	7.157E-14	7.176E-14	-13.14411	1.00260	5.398
6001400	Pb(CO3)2-2	1.286E-17	8.323E-18	-17.07971	0.64743	10.829
6003300	PbOH +	1.579E-15	1.417E-15	-14.84877	0.89701	-7.663
6003301	Pb(OH)2 AQ	2.188E-17	2.194E-17	-16.65877	1.00260	-17.121
6003302	Pb(OH)3 -	1.118E-20	1.003E-20	-19.99878	0.89701	-28.013
6003303	Pb2OH +3	1.539E-28	5.787E-29	-28.23752	0.37599	-5.935
6003304	Pb3(OH)4+2	1.300E-38	8.416E-39	-38.07488	0.64743	-24.070
6001401	PbCO3 AQ	1.022E-14	1.025E-14	-13.98924	1.00260	7.239
6003305	Pb(OH)4 -2	1.416E-24	9.167E-25	-24.03779	0.64743	-39.510
6001402	PbHCO3 +	2.618E-16	2.348E-16	-15.62924	0.89701	13.247
5403300	NiOH +	2.511E-14	2.252E-14	-13.64738	0.89701	-9.990
5403301	Ni(OH)2 AQ	9.748E-16	9.773E-16	-15.00996	1.00260	-19.001
5403302	Ni(OH)3 -	4.337E-19	3.891E-19	-18.40996	0.89701	-29.953
5401400	NiHCO3 +	1.647E-13	1.478E-13	-12.83042	0.89701	12.517
5401401	NiCO3 AQ	1.474E-11	1.478E-11	-10.83042	1.00260	6.869
5401402	Ni(CO3)2-2	1.282E-14	8.300E-15	-14.08090	0.64743	10.299
3301400	HCO3 -	2.190E-04	1.964E-04	-3.70680	0.89701	10.431
3301401	H2CO3 AQ	1.051E-05	1.053E-05	-4.97738	1.00260	16.712
2113300	Cr+3	8.362E-15	3.144E-15	-14.50252	0.37599	10.333
2113301	Cr(OH)+2	9.967E-12	6.453E-12	-11.19024	0.64743	5.809
8123301	=SO2-	8.255E-04	8.255E-04	-3.08326	1.00000	-8.930
8123302	=SO2H2+	9.655E-04	9.655E-04	-3.01525	1.00000	7.290
8113301	=SO1-	2.004E-05	2.004E-05	-4.69813	1.00000	-8.930
8113302	=SO1H2+	2.344E-05	2.344E-05	-4.63012	1.00000	7.290
8129500	=SO2Zn+	1.312E-08	1.312E-08	-7.88222	1.00000	-1.990
8119500	=SO1Zn+	2.903E-07	2.903E-07	-6.53708	1.00000	0.970
8121600	=SO2Cd+	8.752E-11	8.752E-11	-10.05789	1.00000	-2.900
8111600	=SO1Cd+	4.542E-09	4.542E-09	-8.34276	1.00000	0.430
8112310	=SO1Cu+	2.550E-07	2.550E-07	-6.59354	1.00000	2.850
8122310	=SO2Cu+	5.906E-08	5.906E-08	-7.22867	1.00000	0.600
8115400	=SO1Ni+	1.659E-08	1.659E-08	-7.78007	1.00000	0.150
8125400	=SO2Ni+	1.530E-09	1.530E-09	-8.81520	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74888	1.00000	4.710
8126000	=SO2Pb+	2.857E-10	2.857E-10	-9.54402	1.00000	0.300
8121500	=SO2Ca+	3.495E-07	3.495E-07	-6.45651	1.00000	-5.850
8111500	=SO1HCa++	4.706E-06	4.706E-06	-5.32737	1.00000	4.970
8111000	=SO1HBa++	9.612E-08	9.612E-08	-7.01718	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-2.306E-05	-4.637	0.000	0.000
330	H+1	-3.547E-04	-3.450	7.600	0.000
3301403	CO2 (g)	2.163E-04	-3.665	21.690	-0.530
3300021	O2 (g)	1.139E-04	-3.944	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.268E-08	-7.897	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP1			
74.5	PERCENT BOUND IN SPECIES #	811	ADS1TYP1
10.4	PERCENT BOUND IN SPECIES #	8113301	=SO1-
12.2	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
2.4	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
ADS1TYP2			
76.7	PERCENT BOUND IN SPECIES #	812	ADS1TYP2
10.7	PERCENT BOUND IN SPECIES #	8123301	=SO2-
12.6	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
Ba+2			
2.3	PERCENT BOUND IN SPECIES #	100	Ba+2
90.7	PERCENT BOUND IN SPECIES #	1451000	Ba DOM
6.9	PERCENT BOUND IN SPECIES #	8111000	=SO1HBa++
Ca+2			
3.8	PERCENT BOUND IN SPECIES #	150	Ca+2
92.3	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
3.6	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cd+2			
1.8	PERCENT BOUND IN SPECIES #	1451600	Cd DOM
1.9	PERCENT BOUND IN SPECIES #	8121600	=SO2Cd+
96.3	PERCENT BOUND IN SPECIES #	8111600	=SO1Cd+
ADS1PSIo			
626.5	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
15.2	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
6.1	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cu+2			
81.0	PERCENT BOUND IN SPECIES #	8112310	=SO1Cu+
18.8	PERCENT BOUND IN SPECIES #	8122310	=SO2Cu+
DOM			
92.2	PERCENT BOUND IN SPECIES #	145	DOM
4.0	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
3.4	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
K+1			
100.0	PERCENT BOUND IN SPECIES #	410	K+1
Mg+2			
28.9	PERCENT BOUND IN SPECIES #	460	Mg+2
71.1	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
Na+1			
100.0	PERCENT BOUND IN SPECIES #	500	Na+1
Ni+2			
3.1	PERCENT BOUND IN SPECIES #	1455400	Ni DOM
88.6	PERCENT BOUND IN SPECIES #	8115400	=SO1Ni+
8.2	PERCENT BOUND IN SPECIES #	8125400	=SO2Ni+
Pb+2			
99.8	PERCENT BOUND IN SPECIES #	8116000	=SO1Pb+
Sr+2			
100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
Zn+2			
4.3	PERCENT BOUND IN SPECIES #	8129500	=SO2Zn+
94.9	PERCENT BOUND IN SPECIES #	8119500	=SO1Zn+
Cr(OH)2+			
27.0	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
71.3	PERCENT BOUND IN SPECIES #	2113302	Cr(OH)3 AQ
1.1	PERCENT BOUND IN SPECIES #	1452110	Cr DOM
Al+3			
1.1	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
50.5	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
48.4	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
CO3-2			
95.2	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
4.6	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ

```
Fe+2
              99.4     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
              62.3     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
              26.1     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
              11.6     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
               3.0     PERCENT BOUND IN SPECIES #1453300   H DOM
              55.6     PERCENT BOUND IN SPECIES #3301400   HCO3 -
               5.3     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
             245.2     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
               6.0     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
              25.6     PERCENT BOUND IN SPECIES #3300020   OH-
               1.2     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
              25.9     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
              22.7     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
               5.3     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
               1.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
              15.9     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
```

PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.287E-06	93.1	9.615E-08	6.9	0.000E-01	0.0
150	Ca+2	1.247E-04	96.1	5.055E-06	3.9	0.000E-01	0.0
160	Cd+2	8.602E-11	1.8	4.629E-09	98.2	0.000E-01	0.0
231	Cu+2	7.254E-10	0.2	3.140E-07	99.8	0.000E-01	0.0
145	DOM	3.000E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	6.131E-10	3.3	1.812E-08	96.7	0.000E-01	0.0
600	Pb+2	1.385E-11	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	2.498E-09	0.8	3.035E-07	99.2	0.000E-01	0.0
211	Cr(OH)2+	2.543E-09	9.1	0.000E-01	0.0	2.536E-08	90.9
30	Al+3	3.462E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.301E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	1.968E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.582E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.516E-04	63.9	1.422E-04	36.1	0.000E-01	0.0
2	H2O	3.025E-07	27.0	8.188E-07	73.0	0.000E-01	0.0

```
     Charge Balance: SPECIATED
       Sum of CATIONS =  1.369E-03 Sum of ANIONS   9.007E-03
       PERCENT DIFFERENCE =   7.361E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =   2.595E-07
     EQUILIBRIUM IONIC STRENGTH (m) =   1.127E-02
     EQUILIBRIUM pH                 =   7.600
     EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.027620     sig0 = 0.007201
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
```

PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-3.706	[1.000] 150 [1.000] 140
5046000	ARTINITE	-10.441	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.531	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-3.549	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-6.171	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-15.573	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-25.591	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-3.119	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.410	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.522	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.683	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.111	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-5.581	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.584	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.381	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.361	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.523	[-8.000] 330 [1.000] 231 [2.000] 281 [4.000] 2
95000	ZN METAL	-64.046	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.340	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-7.017	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-8.037	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.787	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.337	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.297	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-7.087	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.897	[-2.000] 330 [1.000] 950 [1.000] 2

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2095006	ZINCITE	-7.039	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.777	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.879	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.811	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-10.879	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-10.503	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-12.326	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-45.980	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-8.030	[1.000] 600 [1.000] 140
2060000	MASSICOT	-12.688	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-12.493	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-12.519	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-20.432	[-2.000] 330 [2.000] 600 [1.000] 2 [1.000] 140
5060002	PB3O2CO3	-31.704	[-4.000] 330 [3.000] 600 [1.000] 140 [2.000] 2

2060003	PLATTNERITE	-7.672	[-4.000]	330	[-2.000]	1	[1.000]	600		
			[2.000]	2						
3060000	PB2O3	-17.941	[-6.000]	330	[-2.000]	1	[2.000]	600		
			[3.000]	2						
3060001	MINIUM	-31.597	[-8.000]	330	[-2.000]	1	[3.000]	600		
			[4.000]	2						
2060004	PB(OH)2 (C)	-7.889	[-2.000]	330	[1.000]	600	[2.000]	2		
5060003	HYDCERRUSITE	-24.537	[-2.000]	330	[3.000]	600	[2.000]	140		
			[2.000]	2						
2060005	PB2O(OH)2	-25.278	[-4.000]	330	[2.000]	600	[3.000]	2		
5054000	NICO3	-11.002	[1.000]	540	[1.000]	140				
2054000	NI(OH)2	-6.375	[-2.000]	330	[1.000]	540	[2.000]	2		
2054001	BUNSENITE	-8.802	[-2.000]	330	[1.000]	540	[1.000]	2		
5023101	MALACHITE	-11.780	[2.000]	231	[2.000]	2	[1.000]	140		
			[-2.000]	330						
5023102	AZURITE	-19.371	[3.000]	231	[2.000]	2	[2.000]	140		
			[-2.000]	330						
2015000	LIME	-23.759	[-2.000]	330	[1.000]	150	[1.000]	2		
2015001	PORTLANDITE	-13.415	[-2.000]	330	[1.000]	150	[2.000]	2		
2028000	WUSTITE	-20.420	[-2.000]	330	[0.947]	280	[1.000]	2		
2046001	PERICLASE	-11.396	[-2.000]	330	[1.000]	460	[1.000]	2		
3028001	HERCYNITE	-23.529	[-8.000]	330	[1.000]	280	[2.000]	30		
			[4.000]	2						
3046000	SPINEL	-12.526	[-8.000]	330	[1.000]	460	[2.000]	30		
			[4.000]	2						
3046001	MAG-FERRITE	-10.654	[-8.000]	330	[1.000]	460	[2.000]	281		
			[4.000]	2						
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2		
3021100	FECR2O4	-12.371	[2.000]	211	[1.000]	280	[-4.000]	330		
3021101	MGCR2O4	-5.239	[2.000]	211	[1.000]	460	[-4.000]	330		
3021102	CR2O3	0.000	[2.000]	211	[-2.000]	330	[-1.000]	2		
2021102	CR(OH)3 (A)	-0.860	[1.000]	211	[1.000]	2	[-1.000]	330		
2021101	CR(OH)3 (C)	-3.412	[1.000]	211	[1.000]	2	[-1.000]	330		

4 – Modelling with DOM = 0.004 mol/l

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - DOM = 0.004 mol/l

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair, adsorption and dissolved organic matter

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
145	DOM	3.981E-03	-2.400	4.000E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 1.164E-02
PERCENT DIFFERENCE = 8.648E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.842E-08	2.512E-08	-7.60000	0.88399	0.054
30	Al+3	8.070E-16	2.660E-16	-15.57513	0.32961	0.482
100	Ba+2	2.268E-08	1.385E-08	-7.85854	0.61063	0.214
150	Ca+2	3.412E-06	2.083E-06	-5.68122	0.61063	0.214
160	Cd+2	1.407E-12	8.592E-13	-12.06592	0.61063	0.214
211	Cr(OH)2+	6.971E-10	6.162E-10	-9.21025	0.88399	0.054
231	Cu+2	3.031E-13	1.851E-13	-12.73259	0.61063	0.214
280	Fe+2	2.074E-25	1.267E-25	-24.89733	0.61063	0.214
410	K+1	6.647E-05	5.876E-05	-4.23093	0.88399	0.054
460	Mg+2	3.128E-05	1.910E-05	-4.71900	0.61063	0.214
500	Na+1	2.088E-04	1.846E-04	-3.73388	0.88399	0.054

540	Ni+2	9.732E-12	5.943E-12	-11.22601	0.61063	0.214
600	Pb+2	2.925E-15	1.786E-15	-14.74809	0.61063	0.214
800	Sr+2	5.707E-07	3.485E-07	-6.45784	0.61063	0.214
950	Zn+2	2.608E-11	1.592E-11	-10.79795	0.61063	0.214
812	ADS1TYP2	5.897E-03	5.897E-03	-2.22937	1.00000	0.000
140	CO3-2	5.293E-07	3.232E-07	-6.49048	0.61063	0.214
281	Fe+3	7.913E-25	2.608E-25	-24.58367	0.32961	0.482
145	DOM	3.744E-03	1.424E-03	-2.84652	0.38030	0.420
811	ADS1TYP1	1.443E-04	1.443E-04	-3.84072	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	2.355E-11	2.355E-11	-10.62806	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.812E-09	1.819E-09	-8.74025	1.00348	-7.132
2113303	Cr(OH)4-	7.822E-13	6.914E-13	-12.16026	0.88399	-18.096
2113304	CrO2-	1.985E-12	1.755E-12	-11.75585	0.88399	-17.692
1453300	H DOM	1.905E-05	1.278E-05	-4.89356	0.67063	4.044
1450300	Al DOM	2.907E-12	2.893E-12	-11.53869	0.99508	5.202
1451000	Ba DOM	1.295E-06	1.196E-06	-5.92211	0.92411	3.134
1451500	Ca DOM	1.229E-04	1.136E-04	-3.94479	0.92411	2.934
1451600	Cd DOM	1.273E-10	1.176E-10	-9.92948	0.92411	3.334
1452110	Cr DOM	4.450E-11	4.428E-11	-10.35381	0.99508	15.222
1452310	Cu DOM	1.092E-09	1.009E-09	-8.99616	0.92411	4.934
1452810	Fe DOM	9.014E-19	8.970E-19	-18.04723	0.99508	7.702
1454600	Mg DOM	1.126E-04	1.041E-04	-3.98257	0.92411	1.934
1455400	Ni DOM	8.804E-10	8.136E-10	-9.08957	0.92411	3.334
1456000	Pb DOM	2.102E-11	1.942E-11	-10.71165	0.92411	5.234
1459500	Zn DOM	3.739E-09	3.455E-09	-8.46151	0.92411	3.534
3300020	OH-	2.917E-07	2.578E-07	-6.58865	0.88399	-14.135
4603300	MgOH +	8.521E-10	7.533E-10	-9.12305	0.88399	-11.950
4601400	MgCO3 AQ	5.379E-09	5.398E-09	-8.26777	1.00348	2.940
4601401	MgHCO3 +	4.775E-08	4.221E-08	-7.37459	0.88399	11.488
1503300	CaOH +	1.468E-11	1.298E-11	-10.88687	0.88399	-12.752
1501400	CaHCO3 +	4.030E-09	3.562E-09	-8.44830	0.88399	11.377
1501401	CaCO3 AQ	8.475E-10	8.505E-10	-9.07034	1.00348	3.100
5001400	NaCO3 -	9.330E-10	8.248E-10	-9.08365	0.88399	1.194
5001401	NaHCO3 AQ	1.795E-08	1.802E-08	-7.74435	1.00348	10.078
303300	AlOH +2	1.200E-13	7.326E-14	-13.13512	0.61063	-4.946
303301	Al(OH)2 +	3.788E-11	3.349E-11	-10.47514	0.88399	-10.046
303302	Al(OH)4 -	1.774E-09	1.568E-09	-8.80458	0.88399	-23.576
303303	Al(OH)3 AQ	1.672E-09	1.678E-09	-8.77515	1.00348	-16.002
2803300	FeOH +	1.169E-27	1.033E-27	-26.98589	0.88399	-9.635
2803301	FeOH3 -1	3.337E-34	2.950E-34	-33.53021	0.88399	-31.379
2803302	FeOH2 AQ	2.104E-31	2.111E-31	-30.67542	1.00348	-20.980
2813300	FeOH +2	7.798E-20	4.762E-20	-19.32223	0.61063	-2.124
2813301	FeOH2 +	9.997E-16	8.837E-16	-15.05368	0.88399	-5.616
2813302	FeOH3 AQ	4.119E-16	4.133E-16	-15.38369	1.00348	-13.602
2813303	FeOH4 -	1.861E-16	1.646E-16	-15.78369	0.88399	-21.546
2813304	Fe2(OH)2+4	5.580E-37	7.759E-38	-37.11021	0.13903	-2.286
2813305	Fe3(OH)4+5	3.045E-49	1.395E-50	-49.85531	0.04583	-5.165
8003300	SrOH +	6.466E-13	5.716E-13	-12.24292	0.88399	-13.332
1003300	BaOH +	1.665E-14	1.472E-14	-13.83219	0.88399	-13.520
2311400	CuCO3 AQ	3.202E-13	3.213E-13	-12.49307	1.00348	6.728
2311401	Cu(CO3)2-2	2.141E-16	1.308E-16	-15.88355	0.61063	10.044
2313300	CuOH +	8.336E-14	7.369E-14	-13.13260	0.88399	-7.946
2313301	Cu(OH)2 AQ	6.108E-12	6.129E-12	-11.21261	1.00348	-13.682
2313302	Cu(OH)3 -	1.667E-17	1.474E-17	-16.83161	0.88399	-26.845
2313303	Cu(OH)4 -2	1.912E-22	1.168E-22	-21.93262	0.61063	-39.386
2313304	Cu2(OH)2+2	2.188E-21	1.336E-21	-20.87426	0.61063	-10.395
2311402	CuHCO3 +	1.700E-14	1.503E-14	-13.82307	0.88399	13.054
9503300	ZnOH +	5.060E-13	4.473E-13	-12.34937	0.88399	-9.098
9503301	Zn(OH)2 AQ	3.173E-13	3.185E-13	-12.49696	1.00348	-16.901
9503302	Zn(OH)3 -	4.535E-17	4.009E-17	-16.39697	0.88399	-28.345
9503303	Zn(OH)4 -2	4.142E-22	2.529E-22	-21.59697	0.61063	-40.985

9501400	ZnHCO3 +	3.674E-13	3.248E-13	-12.48842	0.88399	12.454
9501401	ZnCO3 AQ	1.023E-12	1.027E-12	-11.98842	1.00348	5.298
9501402	Zn(CO3)2-2	1.162E-14	7.097E-15	-14.14890	0.61063	9.844
1601400	Cd(CO3)3-4	3.464E-25	4.816E-26	-25.31735	0.13903	7.077
1603300	CdOH +	2.092E-15	1.849E-15	-14.73307	0.88399	-10.214
1603301	Cd(OH)2 AQ	6.061E-18	6.082E-18	-17.21593	1.00348	-20.352
1603302	Cd(OH)3 -	3.073E-23	2.717E-23	-22.56594	0.88399	-33.246
1603303	Cd(OH)4 -2	1.579E-29	9.640E-30	-29.01594	0.61063	-47.136
1603304	Cd2OH +3	2.538E-26	8.365E-27	-26.07754	0.32961	-9.064
1601400	CdHCO3 +	1.982E-14	1.752E-14	-13.75640	0.88399	12.454
1601401	CdCO3 AQ	6.936E-14	6.960E-14	-13.15739	1.00348	5.397
6001400	Pb(CO3)2-2	1.334E-17	8.146E-18	-17.08904	0.61063	10.854
6003300	PbOH +	1.568E-15	1.386E-15	-14.85809	0.88399	-7.656
6003301	Pb(OH)2 AQ	2.140E-17	2.147E-17	-16.66810	1.00348	-17.122
6003302	Pb(OH)3 -	1.110E-20	9.815E-21	-20.00811	0.88399	-28.006
6003303	Pb2OH +3	1.682E-28	5.544E-29	-28.25618	0.32961	-5.878
6003304	Pb3(OH)4+2	1.292E-38	7.891E-39	-38.10286	0.61063	-24.044
6001401	PbCO3 AQ	9.998E-15	1.003E-14	-13.99857	1.00348	7.238
6003305	Pb(OH)4 -2	1.469E-24	8.972E-25	-24.04711	0.61063	-39.485
6001402	PbHCO3 +	2.600E-16	2.298E-16	-15.63857	0.88399	13.254
5403300	NiOH +	2.455E-14	2.170E-14	-13.66344	0.88399	-9.984
5403301	Ni(OH)2 AQ	9.386E-16	9.418E-16	-15.02602	1.00348	-19.002
5403302	Ni(OH)3 -	4.242E-19	3.749E-19	-18.42603	0.88399	-29.946
5401400	NiHCO3 +	1.611E-13	1.424E-13	-12.84649	0.88399	12.524
5401401	NiCO3 AQ	1.419E-11	1.424E-11	-10.84648	1.00348	6.868
5401402	Ni(CO3)2-2	1.310E-14	7.999E-15	-14.09696	0.61063	10.324
3301400	HCO3 -	2.222E-04	1.964E-04	-3.70680	0.88399	10.437
3301401	H2CO3 AQ	1.050E-05	1.053E-05	-4.97738	1.00348	16.712
2113300	Cr+3	9.538E-15	3.144E-15	-14.50252	0.32961	10.390
2113301	Cr(OH)+2	1.057E-11	6.453E-12	-11.19024	0.61063	5.834
8123301	=SO2-	8.142E-04	8.142E-04	-3.08929	1.00000	-8.930
8123302	=SO2H2+	9.785E-04	9.785E-04	-3.00944	1.00000	7.290
8113301	=SO1-	1.992E-05	1.992E-05	-4.70065	1.00000	-8.930
8113302	=SO1H2+	2.394E-05	2.394E-05	-4.62080	1.00000	7.290
8129500	=SO2Zn+	1.296E-08	1.296E-08	-7.88739	1.00000	-1.990
8119500	=SO1Zn+	2.892E-07	2.892E-07	-6.53875	1.00000	0.970
8121600	=SO2Cd+	8.603E-11	8.603E-11	-10.06537	1.00000	-2.900
8111600	=SO1Cd+	4.501E-09	4.501E-09	-8.34672	1.00000	0.430
8112310	=SO1Cu+	2.550E-07	2.550E-07	-6.59340	1.00000	2.850
8122310	=SO2Cu+	5.861E-08	5.861E-08	-7.23204	1.00000	0.600
8115400	=SO1Ni+	1.634E-08	1.634E-08	-7.78681	1.00000	0.150
8125400	=SO2Ni+	1.495E-09	1.495E-09	-8.82546	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74890	1.00000	4.710
8126000	=SO2Pb+	2.834E-10	2.834E-10	-9.54754	1.00000	0.300
8121500	=SO2Ca+	2.341E-07	2.341E-07	-6.63067	1.00000	-5.850
8111500	=SO1HCa++	3.220E-06	3.220E-06	-5.49210	1.00000	4.970
8111000	=SO1HBa++	6.616E-08	6.616E-08	-7.17942	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-2.628E-05	-4.580	0.000	0.000
330	H+1	-3.838E-04	-3.416	7.600	0.000
3301403	CO2 (g)	2.130E-04	-3.672	21.690	-0.530
3300021	O2 (g)	1.139E-04	-3.944	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.267E-08	-7.897	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP1			
75.1	PERCENT BOUND IN SPECIES #	811	ADS1TYP1
10.4	PERCENT BOUND IN SPECIES #	8113301	=SO1-
12.5	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
1.7	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
ADS1TYP2			
76.7	PERCENT BOUND IN SPECIES #	812	ADS1TYP2
10.6	PERCENT BOUND IN SPECIES #	8123301	=SO2-
12.7	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
Ba+2			
1.6	PERCENT BOUND IN SPECIES #	100	Ba+2
93.6	PERCENT BOUND IN SPECIES #	1451000	Ba DOM
4.8	PERCENT BOUND IN SPECIES #	8111000	=SO1HBa++
Ca+2			
2.6	PERCENT BOUND IN SPECIES #	150	Ca+2
94.7	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
2.5	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cd+2			
2.7	PERCENT BOUND IN SPECIES #	1451600	Cd DOM
1.8	PERCENT BOUND IN SPECIES #	8121600	=SO2Cd+
95.4	PERCENT BOUND IN SPECIES #	8111600	=SO1Cd+
ADS1PSIo			
556.0	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
13.6	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
3.7	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cu+2			
81.0	PERCENT BOUND IN SPECIES #	8112310	=SO1Cu+
18.6	PERCENT BOUND IN SPECIES #	8122310	=SO2Cu+
DOM			
93.6	PERCENT BOUND IN SPECIES #	145	DOM
3.1	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
2.8	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
K+1			
100.0	PERCENT BOUND IN SPECIES #	410	K+1
Mg+2			
21.7	PERCENT BOUND IN SPECIES #	460	Mg+2
78.2	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
Na+1			
100.0	PERCENT BOUND IN SPECIES #	500	Na+1
Ni+2			
4.7	PERCENT BOUND IN SPECIES #	1455400	Ni DOM
87.2	PERCENT BOUND IN SPECIES #	8115400	=SO1Ni+
8.0	PERCENT BOUND IN SPECIES #	8125400	=SO2Ni+
Pb+2			
99.8	PERCENT BOUND IN SPECIES #	8116000	=SO1Pb+
Sr+2			
100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
Zn+2			
1.2	PERCENT BOUND IN SPECIES #	1459500	Zn DOM
4.2	PERCENT BOUND IN SPECIES #	8129500	=SO2Zn+
94.5	PERCENT BOUND IN SPECIES #	8119500	=SO1Zn+
Cr(OH)2+			
27.2	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
70.6	PERCENT BOUND IN SPECIES #	2113302	Cr(OH)3 AQ
1.7	PERCENT BOUND IN SPECIES #	1452110	Cr DOM
Al+3			
1.1	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
50.9	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
48.0	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
CO3-2			
95.2	PERCENT BOUND IN SPECIES #	3301400	HCO3 -

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                4.5     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
               99.4     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
               62.5     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
               25.8     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
               11.6     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
                4.4     PERCENT BOUND IN SPECIES #1453300   H DOM
               51.8     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                4.9     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
              227.9     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                5.6     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
               26.0     PERCENT BOUND IN SPECIES #3300020   OH-
                1.2     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
               25.7     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
               22.7     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                5.2     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                1.5     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
               15.9     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.317E-06	95.2	6.618E-08	4.8	0.000E-01	0.0
150	Ca+2	1.263E-04	97.3	3.454E-06	2.7	0.000E-01	0.0
160	Cd+2	1.288E-10	2.7	4.587E-09	97.3	0.000E-01	0.0
231	Cu+2	1.099E-09	0.3	3.136E-07	99.7	0.000E-01	0.0
145	DOM	4.000E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	9.046E-10	4.8	1.783E-08	95.2	0.000E-01	0.0
600	Pb+2	2.103E-11	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	3.767E-09	1.2	3.022E-07	98.8	0.000E-01	0.0
211	Cr(OH)2+	2.567E-09	9.2	0.000E-01	0.0	2.534E-08	90.8
30	Al+3	3.487E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.333E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.086E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.599E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.620E-04	61.0	1.673E-04	39.0	0.000E-01	0.0
2	H2O	3.065E-07	27.3	8.168E-07	72.7	0.000E-01	0.0

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    Charge Balance: SPECIATED
      Sum of CATIONS =  1.356E-03 Sum of ANIONS   1.176E-02
      PERCENT DIFFERENCE =   7.933E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
    NON-CARBONATE ALKALINITY       =   2.633E-07
    EQUILIBRIUM IONIC STRENGTH (m) =   1.510E-02
    EQUILIBRIUM pH                 =   7.600
    EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.027277     sig0 = 0.008222
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-3.886	[1.000] 150 [1.000] 140
5046000	ARTINITE	-10.739	[-2.000] 330 [2.000] 460 [1.000] 140
			[5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.680	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-3.729	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-6.500	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280
			[8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-16.200	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-26.337	[5.000] 460 [4.000] 140 [-2.000] 330
			[6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-3.269	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280
			[4.000] 2
3050000	NATRON	-12.422	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.671	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.708	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.123	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-5.759	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.593	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.390	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.370	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.533	[-8.000] 330 [1.000] 231 [2.000] 281
			[4.000] 2
95000	ZN METAL	-64.057	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.351	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-7.028	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-8.048	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.798	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.348	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.308	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-7.098	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.908	[-2.000] 330 [1.000] 950 [1.000] 2

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2095006	ZINCITE	-7.050	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.790	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.892	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.825	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-10.893	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-10.516	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-12.340	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-45.989	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-8.039	[1.000] 600 [1.000] 140
2060000	MASSICOT	-12.698	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-12.502	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-12.528	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-20.450	[-2.000] 330 [2.000] 600 [1.000] 2
			[1.000] 140
5060002	PB3O2CO3	-31.732	[-4.000] 330 [3.000] 600 [1.000] 140
			[2.000] 2

2060003	PLATTNERITE	-7.681	[-4.000]	330	[-2.000]	1	[1.000]	600		
			[2.000]	2						
3060000	PB2O3	-17.959	[-6.000]	330	[-2.000]	1	[2.000]	600		
			[3.000]	2						
3060001	MINIUM	-31.625	[-8.000]	330	[-2.000]	1	[3.000]	600		
			[4.000]	2						
2060004	PB(OH)2 (C)	-7.898	[-2.000]	330	[1.000]	600	[2.000]	2		
5060003	HYDCERRUSITE	-24.565	[-2.000]	330	[3.000]	600	[2.000]	140		
			[2.000]	2						
2060005	PB2O(OH)2	-25.296	[-4.000]	330	[2.000]	600	[3.000]	2		
5054000	NICO3	-11.018	[1.000]	540	[1.000]	140				
2054000	NI(OH)2	-6.391	[-2.000]	330	[1.000]	540	[2.000]	2		
2054001	BUNSENITE	-8.818	[-2.000]	330	[1.000]	540	[1.000]	2		
5023101	MALACHITE	-11.799	[2.000]	231	[2.000]	2	[1.000]	140		
			[-2.000]	330						
5023102	AZURITE	-19.398	[3.000]	231	[2.000]	2	[2.000]	140		
			[-2.000]	330						
2015000	LIME	-23.939	[-2.000]	330	[1.000]	150	[1.000]	2		
2015001	PORTLANDITE	-13.595	[-2.000]	330	[1.000]	150	[2.000]	2		
2028000	WUSTITE	-20.420	[-2.000]	330	[0.947]	280	[1.000]	2		
2046001	PERICLASE	-11.545	[-2.000]	330	[1.000]	460	[1.000]	2		
3028001	HERCYNITE	-23.529	[-8.000]	330	[1.000]	280	[2.000]	30		
			[4.000]	2						
3046000	SPINEL	-12.675	[-8.000]	330	[1.000]	460	[2.000]	30		
			[4.000]	2						
3046001	MAG-FERRITE	-10.803	[-8.000]	330	[1.000]	460	[2.000]	281		
			[4.000]	2						
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2		
3021100	FECR2O4	-12.371	[2.000]	211	[1.000]	280	[-4.000]	330		
3021101	MGCR2O4	-5.389	[2.000]	211	[1.000]	460	[-4.000]	330		
3021102	CR2O3	0.000	[2.000]	211	[-2.000]	330	[-1.000]	2		
2021102	CR(OH)3 (A)	-0.860	[1.000]	211	[1.000]	2	[-1.000]	330		
2021101	CR(OH)3 (C)	-3.412	[1.000]	211	[1.000]	2	[-1.000]	330		

5 – Modelling with DOM = 0.005 mol/l

PART 1 of OUTPUT FILE

Revuè river water-Site 14 - DOM = 0.005 mol/l

Entered PCO_2, PO_2, fixed pH, solids allowed to precipitate, Fe redox pair, adsorption and dissolved organic matter

Temperature (Celsius): 19.30
Units of concentration: MG/L
Ionic strength to be computed.
Carbonate concentration represents carbonate alkalinity.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and the print option for solids is set to: 1
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Diffuse Layer
Number of adsorbing surfaces: 1

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	2.512E-08	-7.600	0.000E-01
30	Al+3	4.786E-06	-5.320	1.300E-01
100	Ba+2	1.380E-06	-5.860	1.900E-01
150	Ca+2	1.288E-04	-3.890	5.200E+00
160	Cd+2	4.677E-09	-8.330	5.300E-04
211	Cr(OH)2+	2.818E-08	-7.550	2.400E-03
231	Cu+2	3.162E-07	-6.500	2.000E-02
280	Fe+2	5.370E-07	-6.270	3.000E-02
410	K+1	6.607E-05	-4.180	2.599E+00
460	Mg+2	1.445E-04	-3.840	3.500E+00
500	Na+1	2.089E-04	-3.680	4.800E+00
540	Ni+2	1.862E-08	-7.730	1.100E-03
600	Pb+2	1.778E-07	-6.750	3.700E-02
800	Sr+2	5.754E-07	-6.240	5.000E-02
950	Zn+2	3.090E-07	-6.510	2.000E-02
1	E-1	1.000E-16	-16.000	0.000E-01
140	CO3-2	2.188E-04	-3.660	1.310E+01
281	Fe+3	1.778E-21	-20.750	0.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E-01
811	ADS1TYP1	1.905E-04	-3.720	1.922E-04
812	ADS1TYP2	7.762E-03	-2.110	7.690E-03
145	DOM	5.012E-03	-2.300	5.000E-03
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED
Sum of CATIONS= 8.438E-04 Sum of ANIONS = 1.444E-02
PERCENT DIFFERENCE = 8.896E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	2.877E-08	2.512E-08	-7.60000	0.87306	0.059
30	Al+3	9.025E-16	2.660E-16	-15.57513	0.29473	0.531
100	Ba+2	1.750E-08	1.017E-08	-7.99288	0.58101	0.236
150	Ca+2	2.624E-06	1.524E-06	-5.81691	0.58101	0.236
160	Cd+2	1.442E-12	8.379E-13	-12.07680	0.58101	0.236
211	Cr(OH)2+	7.058E-10	6.162E-10	-9.21025	0.87306	0.059
231	Cu+2	3.136E-13	1.822E-13	-12.73946	0.58101	0.236
280	Fe+2	2.180E-25	1.267E-25	-24.89733	0.58101	0.236
410	K+1	6.647E-05	5.803E-05	-4.23633	0.87306	0.059
460	Mg+2	2.505E-05	1.455E-05	-4.83707	0.58101	0.236
500	Na+1	2.088E-04	1.823E-04	-3.73927	0.87306	0.059

540	Ni+2	9.907E-12	5.756E-12	-11.23989	0.58101	0.236
600	Pb+2	3.027E-15	1.759E-15	-14.75477	0.58101	0.236
800	Sr+2	5.707E-07	3.316E-07	-6.47943	0.58101	0.236
950	Zn+2	2.688E-11	1.561E-11	-10.80646	0.58101	0.236
812	ADS1TYP2	5.896E-03	5.896E-03	-2.22947	1.00000	0.000
140	CO3-2	5.563E-07	3.232E-07	-6.49048	0.58101	0.236
281	Fe+3	8.849E-25	2.608E-25	-24.58367	0.29473	0.531
145	DOM	4.728E-03	1.631E-03	-2.78752	0.34499	0.462
811	ADS1TYP1	1.449E-04	1.449E-04	-3.83895	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
8121000	=SO2Ba+	1.767E-11	1.767E-11	-10.75273	1.00000	-7.200
2113302	Cr(OH)3 AQ	1.811E-09	1.819E-09	-8.74025	1.00438	-7.132
2113303	Cr(OH)4-	7.919E-13	6.914E-13	-12.16026	0.87306	-18.091
2113304	CrO2-	2.010E-12	1.755E-12	-11.75585	0.87306	-17.687
1453300	H DOM	2.726E-05	1.756E-05	-4.75554	0.64416	4.061
1450300	Al DOM	3.997E-12	3.975E-12	-11.40067	0.99458	5.202
1451000	Ba DOM	1.316E-06	1.207E-06	-5.91842	0.91679	3.138
1451500	Ca DOM	1.245E-04	1.142E-04	-3.94245	0.91679	2.938
1451600	Cd DOM	1.719E-10	1.576E-10	-9.80234	0.91679	3.338
1452110	Cr DOM	6.118E-11	6.084E-11	-10.21578	0.99458	15.222
1452310	Cu DOM	1.488E-09	1.365E-09	-8.86499	0.91679	4.938
1452810	Fe DOM	1.239E-18	1.233E-18	-17.90921	0.99458	7.702
1454600	Mg DOM	1.189E-04	1.090E-04	-3.96260	0.91679	1.938
1455400	Ni DOM	1.181E-09	1.083E-09	-8.96543	0.91679	3.338
1456000	Pb DOM	2.867E-11	2.628E-11	-10.58031	0.91679	5.238
1459500	Zn DOM	5.078E-09	4.656E-09	-8.33200	0.91679	3.538
3300020	OH-	2.953E-07	2.578E-07	-6.58865	0.87306	-14.130
4603300	MgOH +	6.574E-10	5.740E-10	-9.24111	0.87306	-11.945
4601400	MgCO3 AQ	4.095E-09	4.113E-09	-8.38583	1.00438	2.940
4601401	MgHCO3 +	3.684E-08	3.216E-08	-7.49265	0.87306	11.494
1503300	CaOH +	1.087E-11	9.494E-12	-11.02256	0.87306	-12.747
1501400	CaHCO3 +	2.985E-09	2.606E-09	-8.58399	0.87306	11.382
1501401	CaCO3 AQ	6.195E-10	6.223E-10	-9.20603	1.00438	3.099
5001400	NaCO3 -	9.330E-10	8.146E-10	-9.08905	0.87306	1.200
5001401	NaHCO3 AQ	1.772E-08	1.779E-08	-7.74975	1.00438	10.078
303300	AlOH +2	1.261E-13	7.326E-14	-13.13512	0.58101	-4.924
303301	Al(OH)2 +	3.835E-11	3.349E-11	-10.47514	0.87306	-10.041
303302	Al(OH)4 -	1.796E-09	1.568E-09	-8.80458	0.87306	-23.570
303303	Al(OH)3 AQ	1.671E-09	1.678E-09	-8.77515	1.00438	-16.002
2803300	FeOH +	1.183E-27	1.033E-27	-26.98589	0.87306	-9.630
2803301	FeOH3 -1	3.379E-34	2.950E-34	-33.53021	0.87306	-31.374
2803302	FeOH2 AQ	2.102E-31	2.111E-31	-30.67542	1.00438	-20.980
2813300	FeOH +2	8.196E-20	4.762E-20	-19.32223	0.58101	-2.103
2813301	FeOH2 +	1.012E-15	8.837E-16	-15.05368	0.87306	-5.611
2813302	FeOH3 AQ	4.115E-16	4.133E-16	-15.38369	1.00438	-13.602
2813303	FeOH4 -	1.885E-16	1.646E-16	-15.78369	0.87306	-21.541
2813304	Fe2(OH)2+4	6.808E-37	7.759E-38	-37.11021	0.11396	-2.200
2813305	Fe3(OH)4+5	4.155E-49	1.395E-50	-49.85531	0.03359	-5.030
8003300	SrOH +	6.229E-13	5.439E-13	-12.26451	0.87306	-13.326
1003300	BaOH +	1.237E-14	1.080E-14	-13.96653	0.87306	-13.515
2311400	CuCO3 AQ	3.149E-13	3.163E-13	-12.49993	1.00438	6.728
2311401	Cu(CO3)2-2	2.215E-16	1.287E-16	-15.89041	0.58101	10.066
2313300	CuOH +	8.308E-14	7.253E-14	-13.13946	0.87306	-7.941
2313301	Cu(OH)2 AQ	6.007E-12	6.033E-12	-11.21947	1.00438	-13.682
2313302	Cu(OH)3 -	1.661E-17	1.451E-17	-16.83848	0.87306	-26.840
2313303	Cu(OH)4 -2	1.978E-22	1.150E-22	-21.93948	0.58101	-39.364
2313304	Cu2(OH)2+2	2.228E-21	1.294E-21	-20.88799	0.58101	-10.373
2311402	CuHCO3 +	1.694E-14	1.479E-14	-13.82993	0.87306	13.059
9503300	ZnOH +	5.024E-13	4.387E-13	-12.35788	0.87306	-9.092
9503301	Zn(OH)2 AQ	3.109E-13	3.123E-13	-12.50547	1.00438	-16.901
9503302	Zn(OH)3 -	4.503E-17	3.931E-17	-16.40548	0.87306	-28.340
9503303	Zn(OH)4 -2	4.269E-22	2.480E-22	-21.60548	0.58101	-40.963

9501400	ZnHCO3 +	3.648E-13	3.185E-13	-12.49694	0.87306	12.459
9501401	ZnCO3 AQ	1.003E-12	1.007E-12	-11.99694	1.00438	5.298
9501402	Zn(CO3)2-2	1.198E-14	6.960E-15	-14.15741	0.58101	9.866
1601400	Cd(CO3)3-4	4.121E-25	4.696E-26	-25.32823	0.11396	7.163
1603300	CdOH +	2.065E-15	1.803E-15	-14.74395	0.87306	-10.208
1603301	Cd(OH)2 AQ	5.906E-18	5.932E-18	-17.22681	1.00438	-20.352
1603302	Cd(OH)3 -	3.035E-23	2.650E-23	-22.57682	0.87306	-33.241
1603303	Cd(OH)4 -2	1.618E-29	9.401E-30	-29.02682	0.58101	-47.114
1603304	Cd2OH +3	2.699E-26	7.956E-27	-26.09930	0.29473	-9.015
1601400	CdHCO3 +	1.957E-14	1.709E-14	-13.76728	0.87306	12.459
1601401	CdCO3 AQ	6.758E-14	6.788E-14	-13.16827	1.00438	5.397
6001400	Pb(CO3)2-2	1.381E-17	8.022E-18	-17.09572	0.58101	10.876
6003300	PbOH +	1.564E-15	1.365E-15	-14.86477	0.87306	-7.651
6003301	Pb(OH)2 AQ	2.105E-17	2.115E-17	-16.67478	1.00438	-17.122
6003302	Pb(OH)3 -	1.107E-20	9.665E-21	-20.01479	0.87306	-28.001
6003303	Pb2OH +3	1.824E-28	5.376E-29	-28.26954	0.29473	-5.829
6003304	Pb3(OH)4+2	1.297E-38	7.535E-39	-38.12290	0.58101	-24.023
6001401	PbCO3 AQ	9.837E-15	9.880E-15	-14.00524	1.00438	7.238
6003305	Pb(OH)4 -2	1.521E-24	8.835E-25	-24.05379	0.58101	-39.463
6001402	PbHCO3 +	2.592E-16	2.263E-16	-15.64525	0.87306	13.259
5403300	NiOH +	2.408E-14	2.102E-14	-13.67733	0.87306	-9.978
5403301	Ni(OH)2 AQ	9.082E-16	9.122E-16	-15.03990	1.00438	-19.002
5403302	Ni(OH)3 -	4.159E-19	3.632E-19	-18.43991	0.87306	-29.941
5401400	NiHCO3 +	1.580E-13	1.379E-13	-12.86037	0.87306	12.529
5401401	NiCO3 AQ	1.373E-11	1.379E-11	-10.86037	1.00438	6.868
5401402	Ni(CO3)2-2	1.333E-14	7.747E-15	-14.11085	0.58101	10.346
3301400	HCO3 -	2.250E-04	1.964E-04	-3.70680	0.87306	10.443
3301401	H2CO3 AQ	1.049E-05	1.053E-05	-4.97738	1.00438	16.711
2113300	Cr+3	1.067E-14	3.144E-15	-14.50252	0.29473	10.438
2113301	Cr(OH)+2	1.111E-11	6.453E-12	-11.19024	0.58101	5.856
8123301	=SO2-	8.048E-04	8.048E-04	-3.09429	1.00000	-8.930
8123302	=SO2H2+	9.893E-04	9.893E-04	-3.00466	1.00000	7.290
8113301	=SO1-	1.978E-05	1.978E-05	-4.70376	1.00000	-8.930
8113302	=SO1H2+	2.431E-05	2.431E-05	-4.61414	1.00000	7.290
8129500	=SO2Zn+	1.285E-08	1.285E-08	-7.89113	1.00000	-1.990
8119500	=SO1Zn+	2.880E-07	2.880E-07	-6.54060	1.00000	0.970
8121600	=SO2Cd+	8.483E-11	8.483E-11	-10.07146	1.00000	-2.900
8111600	=SO1Cd+	4.457E-09	4.457E-09	-8.35094	1.00000	0.430
8112310	=SO1Cu+	2.549E-07	2.549E-07	-6.59360	1.00000	2.850
8122310	=SO2Cu+	5.833E-08	5.833E-08	-7.23412	1.00000	0.600
8115400	=SO1Ni+	1.607E-08	1.607E-08	-7.79403	1.00000	0.150
8125400	=SO2Ni+	1.464E-09	1.464E-09	-8.83456	1.00000	-2.500
8116000	=SO1Pb+	1.783E-07	1.783E-07	-6.74891	1.00000	4.710
8126000	=SO2Pb+	2.822E-10	2.822E-10	-9.54943	1.00000	0.300
8121500	=SO2Ca+	1.732E-07	1.732E-07	-6.76157	1.00000	-5.850
8111500	=SO1HCa++	2.420E-06	2.420E-06	-5.61624	1.00000	4.970
8111000	=SO1HBa++	4.987E-08	4.987E-08	-7.30220	1.00000	5.460

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-2.907E-05	-4.537	0.000	0.000
330	H+1	-4.099E-04	-3.387	7.600	0.000
3301403	CO2 (g)	2.102E-04	-3.677	21.690	-0.530
3300021	O2 (g)	1.138E-04	-3.944	-84.354	133.830
2802810	Fe+2/Fe+3	-5.372E-07	-6.270	13.175	-10.000

Type IV - FINITE SOLIDS (present at equilibrium)

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
3028100	HEMATITE	2.686E-07	-6.571	3.567	30.845
2003002	DIASPORE	4.815E-06	-5.317	-7.225	24.630
3021102	CR2O3	1.266E-08	-7.898	3.220	12.125

PART 4 of OUTPUT FILE

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS1TYP1			
75.4	PERCENT BOUND IN SPECIES #	811	ADS1TYP1
10.3	PERCENT BOUND IN SPECIES #	8113301	=SO1-
12.7	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
1.3	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
ADS1TYP2			
76.7	PERCENT BOUND IN SPECIES #	812	ADS1TYP2
10.5	PERCENT BOUND IN SPECIES #	8123301	=SO2-
12.9	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
Ba+2			
1.3	PERCENT BOUND IN SPECIES #	100	Ba+2
95.1	PERCENT BOUND IN SPECIES #	1451000	Ba DOM
3.6	PERCENT BOUND IN SPECIES #	8111000	=SO1HBa++
Ca+2			
2.0	PERCENT BOUND IN SPECIES #	150	Ca+2
96.0	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
1.9	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cd+2			
3.6	PERCENT BOUND IN SPECIES #	1451600	Cd DOM
1.8	PERCENT BOUND IN SPECIES #	8121600	=SO2Cd+
94.5	PERCENT BOUND IN SPECIES #	8111600	=SO1Cd+
ADS1PSIo			
507.5	PERCENT BOUND IN SPECIES #	8123302	=SO2H2+
12.5	PERCENT BOUND IN SPECIES #	8113302	=SO1H2+
2.5	PERCENT BOUND IN SPECIES #	8111500	=SO1HCa++
Cu+2			
81.0	PERCENT BOUND IN SPECIES #	8112310	=SO1Cu+
18.5	PERCENT BOUND IN SPECIES #	8122310	=SO2Cu+
DOM			
94.6	PERCENT BOUND IN SPECIES #	145	DOM
2.5	PERCENT BOUND IN SPECIES #	1451500	Ca DOM
2.4	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
K+1			
100.0	PERCENT BOUND IN SPECIES #	410	K+1
Mg+2			
17.4	PERCENT BOUND IN SPECIES #	460	Mg+2
82.6	PERCENT BOUND IN SPECIES #	1454600	Mg DOM
Na+1			
100.0	PERCENT BOUND IN SPECIES #	500	Na+1
Ni+2			
6.3	PERCENT BOUND IN SPECIES #	1455400	Ni DOM
85.8	PERCENT BOUND IN SPECIES #	8115400	=SO1Ni+
7.8	PERCENT BOUND IN SPECIES #	8125400	=SO2Ni+
Pb+2			
99.8	PERCENT BOUND IN SPECIES #	8116000	=SO1Pb+
Sr+2			
100.0	PERCENT BOUND IN SPECIES #	800	Sr+2
Zn+2			
1.7	PERCENT BOUND IN SPECIES #	1459500	Zn DOM
4.2	PERCENT BOUND IN SPECIES #	8129500	=SO2Zn+
94.1	PERCENT BOUND IN SPECIES #	8119500	=SO1Zn+
Cr(OH)2+			
27.2	PERCENT BOUND IN SPECIES #	211	Cr(OH)2+
69.9	PERCENT BOUND IN SPECIES #	2113302	Cr(OH)3 AQ
2.4	PERCENT BOUND IN SPECIES #	1452110	Cr DOM
Al+3			
1.1	PERCENT BOUND IN SPECIES #	303301	Al(OH)2 +
51.2	PERCENT BOUND IN SPECIES #	303302	Al(OH)4 -
47.6	PERCENT BOUND IN SPECIES #	303303	Al(OH)3 AQ
CO3-2			
95.3	PERCENT BOUND IN SPECIES #	3301400	HCO3 -

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                4.4     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
Fe+2
               99.5     PERCENT BOUND IN SPECIES #    280   Fe+2
E-1
Fe+3
               62.7     PERCENT BOUND IN SPECIES #2813301   FeOH2 +
               25.5     PERCENT BOUND IN SPECIES #2813302   FeOH3 AQ
               11.7     PERCENT BOUND IN SPECIES #2813303   FeOH4 -
H+1
                5.9     PERCENT BOUND IN SPECIES #1453300   H DOM
               48.8     PERCENT BOUND IN SPECIES #3301400   HCO3 -
                4.6     PERCENT BOUND IN SPECIES #3301401   H2CO3 AQ
              214.6     PERCENT BOUND IN SPECIES #8123302   =SO2H2+
                5.3     PERCENT BOUND IN SPECIES #8113302   =SO1H2+
H2O
               26.3     PERCENT BOUND IN SPECIES #3300020   OH-
                1.1     PERCENT BOUND IN SPECIES #8129500   =SO2Zn+
               25.6     PERCENT BOUND IN SPECIES #8119500   =SO1Zn+
               22.7     PERCENT BOUND IN SPECIES #8112310   =SO1Cu+
                5.2     PERCENT BOUND IN SPECIES #8122310   =SO2Cu+
                1.4     PERCENT BOUND IN SPECIES #8115400   =SO1Ni+
               15.9     PERCENT BOUND IN SPECIES #8116000   =SO1Pb+
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PART 5 of OUTPUT FILE

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
100	Ba+2	1.334E-06	96.4	4.988E-08	3.6	0.000E-01	0.0
150	Ca+2	1.272E-04	98.0	2.593E-06	2.0	0.000E-01	0.0
160	Cd+2	1.735E-10	3.7	4.542E-09	96.3	0.000E-01	0.0
231	Cu+2	1.495E-09	0.5	3.132E-07	99.5	0.000E-01	0.0
145	DOM	5.000E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	6.647E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	1.440E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	2.088E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
540	Ni+2	1.205E-09	6.4	1.753E-08	93.6	0.000E-01	0.0
600	Pb+2	2.868E-11	0.0	1.786E-07	100.0	0.000E-01	0.0
800	Sr+2	5.707E-07	100.0	0.000E-01	0.0	0.000E-01	0.0
950	Zn+2	5.108E-09	1.7	3.009E-07	98.3	0.000E-01	0.0
211	Cr(OH)2+	2.592E-09	9.3	0.000E-01	0.0	2.531E-08	90.7
30	Al+3	3.510E-09	0.1	0.000E-01	0.0	4.815E-06	99.9
140	CO3-2	2.361E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
280	Fe+2	2.192E-25	100.0	0.000E-01	0.0	0.000E-01	0.0
1	E-1	0.000E-01	0.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.614E-15	0.0	0.000E-01	0.0	5.372E-07	100.0
330	H+1	2.730E-04	59.2	1.880E-04	40.8	0.000E-01	0.0
2	H2O	3.100E-07	27.6	8.147E-07	72.4	0.000E-01	0.0

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     Charge Balance: SPECIATED
       Sum of CATIONS =  1.351E-03 Sum of ANIONS   1.453E-02
       PERCENT DIFFERENCE =   8.299E+01  (ANIONS - CATIONS)/(ANIONS + CATIONS)
     NON-CARBONATE ALKALINITY       =   2.666E-07
     EQUILIBRIUM IONIC STRENGTH (m) =   1.896E-02
     EQUILIBRIUM pH                 =   7.600
     EQUILIBRIUM pe                 =  13.489   or Eh  =   782.67 mv

******* DIFFUSE LAYER ADSORPTION MODEL ********
 **** Parameters For Adsorbent Number 1 ****
  Electrostatic Variables:  psi0 = 0.026993     sig0 = 0.009108
                            psib = 0.000000     sigb = 0.000000
                            psid = 0.000000     sigd = 0.000000
  Adsorbent Concentration (g/l):   3.442
  Specific Surface Area (sq. meters/g):  600.00
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PART 6 of OUTPUT FILE

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2003000	ALOH3(A)	-3.542	[1.000] 30 [3.000] 2 [-3.000] 330
5015000	ARAGONITE	-4.022	[1.000] 150 [1.000] 140
5046000	ARTINITE	-10.975	[-2.000] 330 [2.000] 460 [1.000] 140 [5.000] 2
2003001	BOEHMITE	-1.755	[-3.000] 330 [1.000] 30 [2.000] 2
2046000	BRUCITE	-6.798	[1.000] 460 [2.000] 2 [-2.000] 330
5015001	CALCITE	-3.865	[1.000] 150 [1.000] 140
2003002	DIASPORE	0.000	[-3.000] 330 [1.000] 30 [2.000] 2
5015002	DOLOMITE	-6.753	[1.000] 150 [1.000] 460 [2.000] 140
2028100	FERRIHYDRITE	-6.675	[-3.000] 330 [1.000] 281 [3.000] 2
2028101	FE3(OH)8	-33.487	[-8.000] 330 [2.000] 281 [1.000] 280 [8.000] 2
2003003	GIBBSITE (C)	-1.871	[-3.000] 330 [1.000] 30 [3.000] 2
3003000	Al2O3	-8.530	[2.000] 30 [3.000] 2 [-6.000] 330
2028102	GOETHITE	-2.491	[-3.000] 330 [1.000] 281 [2.000] 2
3028100	HEMATITE	0.000	[-6.000] 330 [2.000] 281 [3.000] 2
5015003	HUNTITE	-16.690	[3.000] 460 [1.000] 150 [4.000] 140
5046001	HYDRMAGNESIT	-26.927	[5.000] 460 [4.000] 140 [-2.000] 330 [6.000] 2
3028101	MAGHEMITE	-9.953	[-6.000] 330 [2.000] 281 [3.000] 2
5046002	MAGNESITE	-3.387	[1.000] 460 [1.000] 140
3028000	MAGNETITE	-17.723	[-8.000] 330 [2.000] 281 [1.000] 280 [4.000] 2
3050000	NATRON	-12.433	[2.000] 500 [1.000] 140 [10.000] 2
5046003	NESQUEHONITE	-5.789	[1.000] 460 [1.000] 140 [3.000] 2
5028000	SIDERITE	-20.914	[1.000] 280 [1.000] 140
5080000	STRONTIANITE	-3.730	[1.000] 800 [1.000] 140
5050001	THERMONATR	-14.134	[2.000] 500 [1.000] 140 [1.000] 2
5010000	WITHERITE	-5.893	[1.000] 100 [1.000] 140
5023100	CUCO3	-9.600	[1.000] 231 [1.000] 140
2023100	CU(OH)2	-6.397	[-2.000] 330 [1.000] 231 [2.000] 2
2023101	TENORITE	-5.377	[-2.000] 330 [1.000] 231 [1.000] 2
3023100	CUPRICFERIT	-7.540	[-8.000] 330 [1.000] 231 [2.000] 281 [4.000] 2
95000	ZN METAL	-64.066	[1.000] 950 [2.000] 1
5095000	SMITHSONITE	-7.359	[1.000] 950 [1.000] 140
5095001	ZNCO3, 1H2O	-7.037	[1.000] 950 [1.000] 140 [1.000] 2
2095000	ZN(OH)2 (A)	-8.056	[-2.000] 330 [1.000] 950 [2.000] 2
2095001	ZN(OH)2 (C)	-7.806	[-2.000] 330 [1.000] 950 [2.000] 2
2095002	ZN(OH)2 (B)	-7.356	[-2.000] 330 [1.000] 950 [2.000] 2
2095003	ZN(OH)2 (G)	-7.316	[-2.000] 330 [1.000] 950 [2.000] 2
2095004	ZN(OH)2 (E)	-7.106	[-2.000] 330 [1.000] 950 [2.000] 2
2095005	ZNO(ACTIVE)	-6.916	[-2.000] 330 [1.000] 950 [1.000] 2

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
2095006	ZINCITE	-7.059	[-2.000] 330 [1.000] 950 [1.000] 2
16000	CD METAL	-52.801	[1.000] 160 [2.000] 1
16001	GAMMA CD	-52.903	[1.000] 160 [2.000] 1
5016000	OTAVITE	-4.836	[1.000] 160 [1.000] 140
2016000	CD(OH)2 (A)	-10.904	[-2.000] 330 [1.000] 160 [2.000] 2
2016001	CD(OH)2 (C)	-10.527	[-2.000] 330 [1.000] 160 [2.000] 2
2016002	MONTEPONITE	-12.351	[-2.000] 330 [1.000] 160 [1.000] 2
60000	PB METAL	-45.996	[1.000] 600 [2.000] 1
5060000	CERRUSITE	-8.046	[1.000] 600 [1.000] 140
2060000	MASSICOT	-12.704	[-2.000] 330 [1.000] 600 [1.000] 2
2060001	LITHARGE	-12.509	[-2.000] 330 [1.000] 600 [1.000] 2
2060002	PBO, .3H2O	-12.535	[-2.000] 330 [1.000] 600 [1.330] 2
5060001	PB2OCO3	-20.464	[-2.000] 330 [2.000] 600 [1.000] 2 [1.000] 140
5060002	PB3O2CO3	-31.752	[-4.000] 330 [3.000] 600 [1.000] 140 [2.000] 2

2060003	PLATTNERITE	-7.688	[-4.000]	330	[-2.000]	1	[1.000]	600			
			[2.000]	2							
3060000	PB2O3	-17.973	[-6.000]	330	[-2.000]	1	[2.000]	600			
			[3.000]	2							
3060001	MINIUM	-31.645	[-8.000]	330	[-2.000]	1	[3.000]	600			
			[4.000]	2							
2060004	PB(OH)2 (C)	-7.905	[-2.000]	330	[1.000]	600	[2.000]	2			
5060003	HYDCERRUSITE	-24.585	[-2.000]	330	[3.000]	600	[2.000]	140			
			[2.000]	2							
2060005	PB2O(OH)2	-25.310	[-4.000]	330	[2.000]	600	[3.000]	2			
5054000	NICO3	-11.032	[1.000]	540	[1.000]	140					
2054000	NI(OH)2	-6.405	[-2.000]	330	[1.000]	540	[2.000]	2			
2054001	BUNSENITE	-8.832	[-2.000]	330	[1.000]	540	[1.000]	2			
5023101	MALACHITE	-11.812	[2.000]	231	[2.000]	2	[1.000]	140			
			[-2.000]	330							
5023102	AZURITE	-19.419	[3.000]	231	[2.000]	2	[2.000]	140			
			[-2.000]	330							
2015000	LIME	-24.075	[-2.000]	330	[1.000]	150	[1.000]	2			
2015001	PORTLANDITE	-13.730	[-2.000]	330	[1.000]	150	[2.000]	2			
2028000	WUSTITE	-20.420	[-2.000]	330	[0.947]	280	[1.000]	2			
2046001	PERICLASE	-11.663	[-2.000]	330	[1.000]	460	[1.000]	2			
3028001	HERCYNITE	-23.529	[-8.000]	330	[1.000]	280	[2.000]	30			
			[4.000]	2							
3046000	SPINEL	-12.793	[-8.000]	330	[1.000]	460	[2.000]	30			
			[4.000]	2							
3046001	MAG-FERRITE	-10.921	[-8.000]	330	[1.000]	460	[2.000]	281			
			[4.000]	2							
3028102	LEPIDOCROCIT	-3.155	[-3.000]	330	[1.000]	281	[2.000]	2			
3021100	FECR2O4	-12.371	[2.000]	211	[1.000]	280	[-4.000]	330			
3021101	MGCR2O4	-5.507	[2.000]	211	[1.000]	460	[-4.000]	330			
3021102	CR2O3	0.000	[2.000]	211	[-2.000]	330	[-1.000]	2			
2021102	CR(OH)3 (A)	-0.860	[1.000]	211	[1.000]	2	[-1.000]	330			
2021101	CR(OH)3 (C)	-3.412	[1.000]	211	[1.000]	2	[-1.000]	330			