The Application of Water Pinch Analysis at AECI Bioproducts

A thesis submitted to the

University of Natal School of Chemical Engineering

for the degree of

Master of Science in Engineering (MscEng)

by

Janos Pal Zsigmond Schneider

under the joint supervision of

Professor Christopher Buckley

and

Mr. Christopher Brouckaert

Pollution Research Group
University of Natal
Durban 4014

February 2002

I hereby declare that all work submitted within this thesis, except where specifically acknowledged or referenced, is my own

Signed : ………………… Name : ……………………… Date : …………………

As the candidate's supervisor I have/have not approved this thesis/dissertation for submission

Signed : ………………… Name : ……………………… Date : …………………

Summary

AECI Bioproducts (Bioproducts) is part of an industrial complex located at Umbogintwini, approximately 26 km south of Durban, Kwazulu-Natal. This system was selected for water pinch investigation, as it is one of the major users of freshwater on the complex and hence discharges a related quantity of wastewater, amounting to approximately 400 ML per annum. Bioproducts is a manufacturer of l-lysine, which is an animal feed additive.

Water stream flowrate and purity data, as well as operating cost information, were obtained from plant records at AECI Bioproducts. Limiting flowrate and purity conditions for the water-using operations were established from a mass balance over the entire system using the Linnhoff-March software, WaterTracker. Subject to the specified constraints and operating costs, the problem was to determine the design of the water-using subsystem. No treatment plants were included in the study, as none exist at the facility.

Three scenarios were investigated, which examined the operating variability of one of the evaporators on the site (the AS evaporator), which produces a condensate source of variable purity. The operating cost target and network design for each scenario was determined using the Linnhoff-March software, WaterPinch. Alterations from current operating practice were identified and associated savings (water-using network operating cost and freshwater flowrate) were highlighted.

A robust optimal design was identified, with a recycle, which was consistent for all scenarios investigated. The degree of reuse of the AS evaporator condensate source was determined to be dependent on the purity of the source. The limiting constraint was identified at the sea pipeline, for suspended solids (SS): a prohibitively low discharge concentration constraint was identified as posing the major obstacle for saving. The potential for saving was investigated by incrementing the SS concentration constraint and subsequently the free and saline ammonia (FSA) constraint and allowing for the broth effluent to be discharged via the sea pipeline (which was previously disallowed by an effluent exemption). Although relatively small savings were identified through process integration (from 0.61% to 1.56% of the water-using network operating cost), the analysis identified a potential saving of over 70% of the water-using network operating cost, with relaxation of the sea pipeline SS and FSA constraint.

Acknowledgements

The completion of this thesis would not have been possible without the contributions and support of many people. I would like to mention the following people and institutions who played a part:

From the Pollution Research Group, I thank my supervisors, Chris Buckley and Chris Brouckaert for their insight and guidance, and my fellow ‘pincher’ Paolo Gianadda for his assistance in finding the important (and not so important) literature and countless discussions of ideas. I thank too, the satellite students involved with industry projects who provided a source of new perspectives.

From AECI Bioproducts, I thank Mark Thompson, Lenny Govender, Gavin Barnard, and Martin Perling for their insights into the lysine manufacturing process and their time devoted to obtaining plant data.

I thank the Linnhoff-March company for the use of their data reconciliation and optimisation software suite, WaterTarget.

I express my gratitude to institutions that provided financial support: the WRC and the NRF.

Finally, I wish to thank my friends for their encouragement and patience and especially my family for providing a source of inspiration and tireless support.

Zsig Schneider

8 February, 2002

TABLE OF CONTENTS

Page

Abbreviations .... **xvi**
Preface: Thesis Outline .... **xviii**
Chapter 1: Introduction **1.1**
1.1 Water Resources 1.1
1.2 Water Use and Management in South Africa 1.2
1.3 Industrial Water Use 1.2
1.3.1 Industrial Wastewater 1.3
1.4 Industrial Water Management 1.3
1.5 Water Usage Impact and Cost Reduction 1.4
1.6 Process Integration 1.7
1.6.1 Conceptual Design Techniques 1.7
1.6.2 Pinch Analysis 1.8
1.7 The Application of Water Pinch Analysis in Industry 1.8
1.7.1 Previous Work 1.8
1.7.2 The Application of Water Pinch Analysis at AECI Bioproducts 1.9
1.7.2.1 Project Aims 1.9
1.8 References 1.10
Chapter 2: Literature Review **2.1**
2.1 Introduction 2.1
2.1.1 Mass Exchange Networks 2.1
2.1.2 Water Pinch Analysis 2.1
2.1.3 Optimal Water Allocation 2.1
2.1.4 Mathematical Programming 2.1
2.2 Data 2.2
2.2.1 Auditing Techniques and Requirements 2.2
2.2.2 Data Reconciliation 2.2
2.2.3 Project Feasibility 2.3
2.3 Modelling the Water-Using Network 2.3
2.3.1 Elements of the Water-Using Network 2.4
2.3.2 Mass Transfer and Flow Model 2.4
2.3.2.1 Water-Using Subsystem 2.5

2.3.2.2 Treatment and Regeneration 2.6
2.3.3 Concentration and Flowrate Constraints 2.6
2.3.3.1 Concentration 2.6
2.3.3.2 Flowrate 2.7
2.4 Targeting for Minimum Water Flowrate 2.8
2.4.1 Mass Interval Composite Curves 2.8
2.4.1.1 Effluent Treatment...2.12
2.4.1.2 Regeneration 2.14
2.4.1.3 Geographical Constraints 2.16
2.4.2 Flow Interval Composite Curves 2.16
2.4.3 Multiple Contaminants 2.18
2.5 Mathematical Programming Techniques 2.18
2.5.1 Background 2.18
2.5.2 Regional Water Distribution and Reuse 2.19
2.5.3 Industrial Water Distribution, Reuse and Treatment 2.19
2.5.4 Wastewater Minimisation and Optimal Design of Treatment Plants 2.20
2.5.4.1 Heuristic Procedures 2.22
2.6 Mathematical Programming Software 2.23
2.6.1 GAMS 2.23
2.6.2 WaterTarget 2.23
2.7 Optimisation and Water Reuse in the L-Lysine Manufacturing Industry 2.23
2.7.1 Ion Exchange Modelling 2.23
2.7.2 Process Water Reuse 2.24
2.8 References 2.24
Chapter 3: Investigation at AECI Bioproducts 3.1
3.1 Introduction 3.1
3.2 Process Overview 3.2
3.2.1 Process Water 3.3
3.2.2 Effluent Dilution from UOS 3.3
3.2.3 Raw Materials 3.3
3.2.4 Fermentation..3.4
3.2.4.1 Sterilisation 3.4
3.2.5 Primary Ion Exchange 3.5
3.2.5.1 Adsorption Phase 3.5

3.2.5.2 Backwash Phase 3.6
3.2.5.3 Strip Phase 3.6
3.2.6 Ammonium Stripper and Lysine Evaporator Train 3.6
3.2.7 Secondary Ion Exchange 3.6
3.2.8 Ammonium Sulphate Evaporator 3.7
3.2.9 Steam Condensate....................3.7
3.2.10 Granulation and Bagging 3.7
3.2.11 Cleaning and Cooling Utilities and Pump Seal Water 3.7
3.2.11.1 Clean In Place System 3.8
3.2.11.2 Pump Seals 3.8
3.2.11.3 Cooling Tower 3.8
3.3 Current and Potential Water Reuse and Recycle Opportunities 3.8
3.3.1 PIX: Broth Effluent 3.8
3.3.2 PIX: Backwash Effluent 3.9
3.3.3 Condensate 3.9
3.3.4 PIX: Adsorption and Strip Phase 3.9
3.3.5 Pump Seals 3.10
3.3.6 Clean In Place 3.10
3.3.7 Cooling Tower 3.10
3.4 Model Constraints and Parameters....................3.10
3.4.1 Mathematical Programming Model 3.11
3.4.2 Model Constraints 3.11
3.4.2.1 Mass Balance 3.11
3.4.2.2 Contaminant Concentration and Mass Flowrate 3.11
3.4.2.3 Water Availability 3.12
3.4.2.4 User Demand Constraints 3.12
3.4.3 Objective Function 3.12
3.4.3.1 Freshwater 3.13
3.4.3.2 Piping 3.13
3.4.3.3 Water Treatment and Discharge 3.13
3.4.3.4 Connectivity 3.14
3.4.3.5 Objective Function 3.14
3.4.4 Sensitivity Analysis....................3.14
3.5 Water Using System Model....................3.14

3.5.1 Key Contaminants 3.14
3.5.1.1 Free and Saline Ammonia...3.15
3.5.1.2 Suspended Solids 3.15
3.5.1.3 Chloride 3.15
3.5.2 Elements of the Water-Using System and Model Assumptions.........................3.16
3.5.2.1 PIX Strip 3.16
3.5.2.2 Evaporators and Condensate 3.18
3.5.2.3 SIX 3.18
3.5.2.4 Clean In Place 3.18
3.5.2.5 Pump Seals 3.19
3.5.3 Water Users 3.19
3.6 Water-Using System Model Analysis 3.23
3.6.1 Scenario A 3.23
3.6.1.1 Initial Sensitivity Analysis 3.28
3.6.2 Scenario B 3.29
3.6.2.1 Initial Sensitivity Analysis 3.30
3.6.3 Scenario C 3.30
3.6.3.1 Initial Sensitivity Analysis 3.31
3.7 Model Sensitivity...3.32
3.7.1 Freshwater 3.32
3.7.2 Inlet Constraints 3.33
3.7.2.1 PIX Backwash Sensitivity 3.33
3.7.2.2 Sea Pipeline Sensitivity 3.35
3.7.3 AS Condensate Sensitivity 3.40
3.8 References 3.42
Chapter 4: Discussion and Conclusion 4.1
4.1 Discussion 4.1
4.1.1 Scenario A 4.1
4.1.1.1 PIX Recycle..4.1
4.1.2 Scenario B 4.2
4.1.3 Scenario C 4.2
4.1.4 AS Evaporator Condensate Reuse 4.2
4.1.5 Sea Pipeline Constraint 4.5
4.1.5.1 SS Mass-Flowrate Constraint 4.5

4.1.5.2 FSA Constraint 4.5
4.1.5.3 Unconstrained Sea Pipeline 4.6
4.1.6 Overall Saving 4.6
4.1.7 Barriers to Saving 4.7
4.1.7.1 Obstacle to Process Integration 4.7
4.1.7.2 Broth Effluent Discharge Legislation 4.8
4.1.8 Summary 4.8
4.2 Conclusion 4.9
4.2.1 Recent Developments 4.9
4.2.2 Future Work 4.9
4.3 References 4.10
Appendix A: Nomenclature A.1
Appendix B: Sample Calculations B.1
B.1 Data Conversions B.1
B.1.1 Standard Deviation, Mean and Confidence Interval B.1
B.1.2 Flow Data B.1
B.1.2.1 Mass Flowrate from Volumetric Flowrate B.1
B.2 Mass Loads B.2
B.3 Piping and Installation Costs B.2
B.3.1 Hourly Costs B.2
B.3.2 Sea Pipeline Hourly Usage Cost B.3
Appendix C: Statistical Analysis C.1
C.1 Sample Points C.1
Appendix D: Case Study …................................. D.1
D.1 Introduction D.1
D.1.1 Case Study D.1
D.1.2 Outline of a Water Pinch Investigation D.1
D.1.3 WaterTarget D.1
D.1.4 Elements of the Water-Using System D.3
D.1.5 WaterTracker D.4
D.1.5.1 Types of Data D.4
D.1.5.2 Metering Analysis....................D.4
D.1.5.3 Data Entry and Reconciliation D.4
D.1.6 WaterPinch D.5

D.1.6.1 Inlet and Outlet Classification D.5
D.1.6.2 Contaminant Mass Addition and Removal..D.6
D.1.6.3 Environmental and Discharge Constraints D.7
D.1.6.4 Costs D.7
D.1.6.5 Bounds D.8
D.1.6.6 Optimisation D.9
D.1.6.7 Sensitivity Analysis D.9
D.2 AECI Bioproducts Model D.9
D.2.1 Key Contaminants D.11
D.2.1.1 Free and Saline Ammonia..D.11
D.2.1.2 Suspended Solids D.12
D.2.1.3 Chlorides D.12
D.3 Building a WaterPinch Model D.13
D.3.1 Source and Sink Elimination (Inlet and Outlet Classification) D.13
D.3.2 Processes and Utilities D.14
D.3.2.1 Dummy Utilities D.16
D.3.2.2 Base Case Water-Using System D.16
D.3.3 Mass Loading Properties D.16
D.3.4 Piping Costs D.17
D.3.4.1 Geographical Positions D.17
D.3.5 Structural Constraints D.18
D.3.6 Optimal Water-Using Strategy D.19
D.3.6.1 Connectivity D.19
D.3.6.2 Sensitivity Analysis D.20
D.4 Summary D.20
D.5 Data D.22
D.5.1 Water-Using Network (WaterTracker Mass Balance) D.22
D.5.2 WaterTracker Flowrate and Contaminant Data D.22
D.5.3 Source and Sink Elimination D.31
D.5.4 Illustrations of Water-Using Networks D.32
Appendix E: Data E.1
E.1 Mass Balance Data E.1
E.1.1 Connectivity Data E.1
E.1.2 Flow Data E.2

E.1.3 Concentration Data E.3
E.2 Pipe Capacities E.8
E.3 Solution Flow Data E.9
E.4 Scenario A, B, and C Solution Concentration Data E.10
E.5 Sensitivity Analysis Data E.13
E.5.1 Initial Sensitivity Values E.13
E.5.2 Data for Model Sensitivity Analysis E.14

LIST OF FIGURES

Page

Figure 1.1 Water usage distribution in South Africa 1.1
Figure 1.2 Typical water use on a chemical site 1.4
Figure 1.3 Water minimisation through reuse, regeneration reuse, and regeneration recycling 1.6
Figure 1.4 The onion diagram 1.7
Figure 2.1 System for industrial water use and treatment 2.4
Figure 2.2 Fundamental Model of a water-using operation 2.5
Figure 2.3 Mass transfer model for water-using operations and treatment plants 2.6
Figure 2.4 Network designs for conceptual solution techniques 2.8
Figure 2.5 Limiting water profile for a water-using operation 2.9
Figure 2.6 Composite curves for determining minimum freshwater requirement 2.10
Figure 2.7 Single contaminant design grid procedure 2.10
Figure 2.8 Loop breaking procedure 2.11
Figure 2.9 Incorporating multiple sources and processes with a flow loss 2.12
Figure 2.10 Effluent treatment flowrate targeting method 2.13
Figure 2.11 General industrial water flow scheme 2.13
Figure 2.12 Procedure for simultaneously identifying freshwater targets and regeneration targets 2.14
Figure 2.13 Generating a treatment curve from the wastewater composite curve 2.15
Figure 2.14 Composite curve for five water sources and four water sinks 2.17
Figure 2.15 Superstructure of all possible inter-operational connections 2.20
Figure 3.1 Flowsheet outlining water and raw material distribution, and process streams in the manufacture of l-lysine at Bioproducts 3.2
Figure 3.2 The set of water-using operations used for the pinch analysis model....... 3.17
Figure 3.3 Base-case water-using subsystem configuration for the AECI Bioproducts system 3.20
Figure 3.4 Configuration of the water-using network for Scenario A 3.28
Figure 3.5 Inlet and outlet sensitivity values for Scenario A 3.29
Figure 3.6 Scenario B: Configuration of the water-using system with pure AS evaporator condensate 3.31
Figure 3.7 Inlet and outlet sensitivity value for Scenario B 3.32

Figure 3.8 Scenario C: Configuration of the water-using system with the AS evaporator condensate reuse prohibited 3.33
Figure 3.9 Sensitivity of the objective cost to freshwater costs 3.34
Figure 3.10 Sensitivity of the freshwater flow to freshwater costs 3.35
Figure 3.11 Sensitivity of the objective cost to relaxation of the inlet SS constraint to the PIX backwash 3.36
Figure 3.12 Overall freshwater flowrate as a function of SS inlet concentration constraint to the PIX backwash 3.36
Figure 3.13 Objective cost sensitivity to SS concentration in the sea pipeline 3.37
Figure 3.14 FSA concentration in the sea pipeline as a function of SS mass-flowrate 3.38
Figure 3.15 Objective cost sensitivity to FSA concentration in the sea pipeline 3.38
Figure 3.16 SS mass-flowrate as a function of the FSA constraint in the sea pipeline 3.39
Figure 3.17 Sensitivity of the design to FSA concentration in the sea pipeline (in terms of freshwater and effluent flowrate) 3.39
Figure 3.18 Scenario A: Configuration of the water-using system with the FSA purity constraint in the sea pipeline relaxed to 5000ppm and SS unconstrained 3.40
Figure 3.19 Sensitivity of the objective cost to AS evaporator condensate SS concentration 3.41
Figure 3.20 Sensitivity of reuse flowrate to AS evaporator condensate SS concentration 3.42
Figure 4.1 Configuration of the base-case with the three scenarios A, B, and C....... 4.3
Figure 4.2 AS evaporator condensate reuse as a function of outlet concentration..... 4.4
Figure 4.3 Comparison of the optimal design cost with the current water-using network operating cost 4.7
Figure D.1 Outline of a pinch investigation carried out using WaterTarget D.2
Figure D.2 A conceptual view of the water-using system D.3
Figure D.3 Illustration of feasible and infeasible related measured information........D.5
Figure D.4 Process and utility unit operation models..D.7
Figure D.5 Illustration of source / sink elimination...D.13
Figure D.6 Initial inlet and outlet sensitivity values..D.20
Figure D.8 The water-using network drawn on WaterTracker D.22

Figure D.9 Base-case water-using system design for the AECI Bioproducts system D.32
Figure D.10 Design of the water-using network for optimal connectivity in table D.8 ....D.33
Figure E.1 The water-using network drawn on WaterTracker E.1

LIST OF TABLES

Page

TABLE 1.1 Important wastewater contaminants..1.3
TABLE 1.2 Examples of wastewater savings using water pinch analysis.................1.9
TABLE 3.1 Inter-operation flowrates for base-case configuration 3.21
TABLE 3.2 Mass loading relationships and flowrates for the water-using operations 3.22
TABLE 3.3 Source flowrates and concentrations 3.22
TABLE 3.4 Approximate positions of the operations at AECI Bioproducts 3.23
TABLE 3.5 Economic parameters 3.23
TABLE 3.6 Matrix of existing capacities, and allowed and prohibited flows for Scenario A 3.25
TABLE 3.7 Conditions for the AS evaporator (Scenario A) 3.25
TABLE 3.8 Sea pipeline discharge constraints for Scenario A 3.26
TABLE 3.9 Inlet and outlet flowrate and maximum inlet and outlet concentration constraints for Scenario A 3.27
TABLE 3.10 Matrix of inter-operation flows for the configuration of the Scenario A water system 3.29
TABLE 3.11 Conditions for the AS evaporator (Scenario B) 3.30
TABLE 4.1 Summary of economic and freshwater savings at Bioproducts 4.7
TABLE D.1 (a) Process sink constraints D.15
TABLE D.1 (b) Process source conditions D.15
TABLE D.2 (a) Utility source conditions and costs D.16
TABLE D.2 (b) Utility sink constraints and costs D.16
TABLE D.3 Mass loading relationships for the water-using operations D.17
TABLE D.4 Additional economic parameters...D.17
TABLE D.5 Geographical positions of the operations at AECI Bioproducts D.18
TABLE D.6 Bounds for connections between all sources and sinks (all bounds shown) D.18
TABLE D.7 Results summary D.19
TABLE D.8 Inter-operation flowrates (network design) D.19
TABLE D.9 (a) Flowrate data specifications as they appear on WaterTracker D.23
TABLE D.9 (b) Flowrate data specifications as they appear on WaterTracker D.24

TABLE D.10 (a) SS concentration data specifications as they appear on WaterTracker D.25
TABLE D.10 (b) SS concentration data specifications as they appear on WaterTracker D.26
TABLE D.11 (a) FSA concentration data specifications as they appear on WaterTracker D.27
TABLE D.11 (b) FSA concentration data specifications as they appear on WaterTracker D.28
TABLE D.12 (a) Cl concentration data specifications as they appear on WaterTracker D.29
TABLE D.12 (b) Cl concentration data specifications as they appear on WaterTracker D.30
TABLE D.13 Classification of WaterTracker streams for determining the WaterPinch model D.31
TABLE E.1 Calculated and user-specified stream flowrates E.2
TABLE E.2 Calculated and user-specified SS concentration E.3
TABLE E.3 Calculated and user-specified FSA concentration E.5
TABLE E.4 Calculated and user-specified Cl concentration E.6
TABLE E.5 Pipe diameters and capacities for existing connections E.8
TABLE E.6 Pipe diameters and capacities for existing connections from condensate tank E.8
TABLE E.7 Matrix of inter-operation flows for the configuration of the Scenario B water system .... E.9.
TABLE E.8 Matrix of inter-operation flows for the configuration of the Scenario C water system E.10
TABLE E.9 Matrix of inter-operation flows for the configuration of the water system with SS unconstrained in the sea pipeline and FSA ≤ 5000ppm E.10
TABLE E.10 Scenario A sink conditions E.11
TABLE E.11 Scenario A source conditions E.11
TABLE E.12 Scenario B sink conditions E.11
TABLE E.13 Scenario B source conditions E.12
TABLE E.14 Scenario C sink conditions. E.12
TABLE E.15 Scenario C source conditions E.12

TABLE E.16 Initial objective cost sensitivity values for Scenario A inlet constraints E.13
TABLE E.17 Initial objective cost sensitivity values for Scenario A outlet concentrations E.13
TABLE E.18 Initial objective cost sensitivity values for Scenario B inlet constraints E.13
TABLE E.19 Initial objective cost sensitivity values for Scenario B outlet concentrations E.13
TABLE E.20 Initial objective cost sensitivity values for Scenario C inlet constraints E.14
TABLE E.21 Initial objective cost sensitivity values for Scenario C outlet concentrations E.14
TABLE E.22 Sensitivity of the objective cost, and FW flowrate to the FW cost E.14
TABLE E.23 Sensitivity of the objective cost, and FW flowrate SS concentration constraint for the inlet to the PIX backwash .... E.15.
TABLE E.24 Sensitivity of the objective cost to SS concentration in the sea pipeline E.15
TABLE E.25 Sensitivity of the objective cost, FW flowrate and sea pipeline flowrate to FSA concentration in the sea pipeline .... E.16.
TABLE E.26 Sensitivity of the objective cost, and AS cond. reuse flowrate to the SS concentration in the AS evaporator condensate E.16

Abbreviations

AECI – African Explosives and Chemical Industries

AS – Ammonium Sulphate

AS EVAP. – Ammonium Sulphate Evaporator

BFW – Boiler Feed Water

Bioproducts – AECI Bioproducts

BOD – Biological Oxygen Demand

BW – Backwash

CFS – Cattle Feed Supplement

CIP – Clean in Place System

Cl – Chloride

COD – Chemical Oxygen Demand

COOL TOWER – Cooling Tower

Cond. – Condensate

CSL – Corn Steep Liquor

Dil. – Dilution

Distr. - Distribution

DRY – Drying and Granulation

DWAF – Department of Water Affairs and Forestry

Evap. – Evaporation / Evaporator

FERM. – Fermenters

FSA – Free and Saline Ammonia

FW – Freshwater

g – gram

h – Hours

HTM – High Test Molasses

JNC – Junction

kg – kilogram

Lys. – Lysine

m – metre

MEN – Mass Exchange Network

MSA – Mass Separating Agent

PIX – Primary Ion Exchange

ppm – Parts per million

PRG – Pollution Research Group

PSW – Pump Seal Water

R – Rands

SIX – Secondary Ion Exchange

SOGs – Sorbs, Oils, and Greases

SOP – Sea Outfall Pipeline

SS – Suspended Solids

STEAM COND. – Pure Steam Condensate

STRIP. / EVAP. – Ammonia Stripper and Lysine Evaporator

SWW – Southern Wastewater Works

t – tons

UOS – Umbogintwini Operating Services

UND – University of Natal, Durban

WDCS – Waste Discharge Charge System

WRC – Water Research Commission

Preface: Thesis Outline

The structure and content of the body this thesis entitled *The Application of Water Pinch Analysis at AECI Bioproducts* may be outlined as follows:

Chapter 1 looks at the current state of water and legislation in South Africa. A case is made for the need to reduce industrial water use and associated wastewater production. Methodologies for accomplishing this are introduced.

Chapter 2, the Literature Review, looks mainly at techniques for reducing freshwater consumption and associated costs. This methodology is broadly classified into two areas: the first is conceptual, or graphical techniques, the second is mathematical programming techniques. As a starting point, modelling characteristics of the elements of the water-using system, which are common to both techniques, are discussed (section 2.3). After this point (section 2.4) the review diverges and the discussion focuses on the conceptual technique for reducing freshwater consumption. Subsequently, in section 2.5, the mathematical programming technique is discussed. Other relevant elements of the literature that are associated with conducting a pinch analysis and process optimisation are reviewed: in section 2.2 data gathering and mass-balance techniques are assessed. Section 2.6 looks at the popular software available for optimisation and data reconciliation. In the final section of the review, process optimisation in the lysine manufacturing industry is discussed.

Chapter 3 examines the process at AECI Bioproducts (section 3.2), focusing on the water-using network and operations. Reuse opportunities are proposed in section 3.3. Section 3.4 diverges from discussing the process and looks at the relevant model constraints and parameters that were used for modelling the water-using network. Section 3.5 decomposes the process network presented in the beginning of the chapter, to form the water pinch supply and demand model. Other related model parameters such as key contaminants as well as model assumptions are discussed in this section. In Section 3.6 potential savings were identified by examining three operating models of the water-using network. The configurations that achieved the saving were drawn for each case, and the limiting constraint for each model was identified. Section 3.7 looks at the extent to which the limiting constraints, identified in the previous section, may be relaxed in order to achieve further potential savings. Regeneration opportunities are also discussed in this section.

Chapter 4 discusses the implications of the result. Improvements in current operating conditions are proposed along with the associated saving. The thesis is concluded with a discussion of improvements at AECI Bioproducts that transpired before the completion of this work. Future work in the field of water pinch analysis is also discussed here.

The application of the WaterTarget software is discussed in Appendix D, which is a case-study of the investigation at AECI Bioproducts, with specific reference to the main features of the software.

CHAPTER 1: Introduction

1.1 Water Resources

Based on new data and analysis, the U.N. report of 2000 [1] asserts 2.3 billion people face water shortages. Human beings use 54 % of the Earth's rainfall, and 70 % of this amount goes to agriculture. Recent decades have witnessed an annual increase in water withdrawal of between 4 and 8 percent, with the highest rates of growth occurring in developing countries.

South Africa, which may be defined as an arid county, receives an average of 502 mm of rain per annum [2]. The total renewable supply of freshwater for the country is approximately 50 km^3, which includes the 10 km^3 imported from Lesotho [3]. Recent initiatives in improving the standard of living for previously disadvantaged communities has seen an increase in the distribution of potable water to these communities. Over the next 20 years, the government predicts that the per capita demand for domestic water will increase from the current daily average of 30 litres to 500 litres. Based on this projected growth in demand for freshwater, it is anticipated that the total demand will equal the supply (of suitable quality water) during the decade of 2020 to 2030 [4]. From this it may be deduced that economic, and therefore industrial growth in South Africa, will be seriously affected by the availability of water in the near future.

The current total annual water demand in South Africa is approximately 20 km^3 [2]. Although the industrial sector uses only 8 % [5] of this total (figure 1.1), it is one of the major polluters of natural water resources.

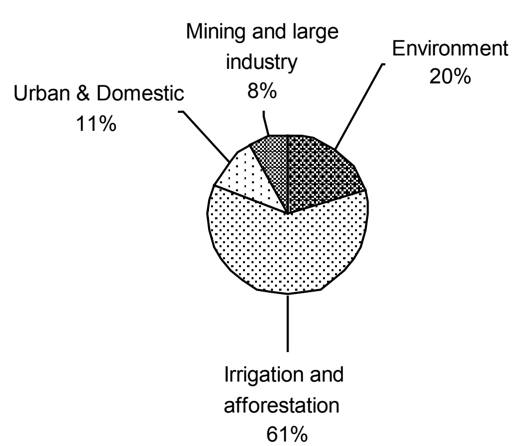

Figure 1.1
Water usage distribution in South Africa (1996).

1.2 Water Use and Management in South Africa

The underlying principle of the National Water Act (Act 36 of 1998) is the sustainability of water resources: Provisions have been made to provide for the continued availability of sufficient water for basic human and ecological needs. It must be noted that for the first time, the rights of non-human water users have been considered [2]. This Water Act makes provisions for the way in which water resources are to be developed, managed and allocated and provides for the use of economic instruments (incentives and disincentives) to encourage water conservation and reduction of waste. The Department of Water Affairs and Forestry (DWAF) [5] is in the process of developing water conservation strategies for the water user sectors (figure 1.1). The Waste Discharge Charge System (WDCS) [5] is one such strategy, which will provide a framework for charging water users who dispose of their waste into water. The WDCS has four main aims of which two are mentioned below. These are to:

(i) promote sustainable development and the efficient use of water resources, and

(ii) create *financial incentives* for dischargers to reduce waste and use water in a more optimal way.

Organisations that will be affected by the WDCS are those who emit waste directly or indirectly into a water resource or coastal marine waters.

1.3 Industrial Water Use

Activities that constitute water use are well defined in the National Water Act, 1998. Industrial water use is subject to the granting of a license, the nature of which will take into account the impact of the water use on the reserve. The reserve is defined as the human and ecological requirements in terms of the purity and quantity of the water resource [2]. The value of water with regards to its use in industry arises due to its excellent heat and mass transfer properties combined with its seemingly limitless, low-cost abundance. Hence the main uses for water in industry are related to these functions, which may be broadly classified for the industrial sector as follows [5]:

- *Process*. One of the major uses of water in the industrial sector is that related to the actual manufacturing processes and the end product. Water use may be *consumptive*, such as the water used to manufacture a product in a bottling factory that is then distributed for consumption. It may also be *non-consumptive*, such as water used to dye fabrics in a textile industry that is then discharged to the wastewater system.

- *Cleaning*. Although water use for cleaning can be related to a process, it is also used for non-cleaning purposes, such as the washing down of floors of a premises.
- *Cooling*. Cooling is often process related, such as heat-transfer operations and cooling towers.

1.3.1 Industrial Waste-Water

Industrial wastewater is characterised by the volume and the contaminant load carried [6]. Conventional pollutants (as established by the EPA) include biological oxygen demand (BOD), total suspended solids (TSS), pH and faecal coliform. Non-conventional pollutants are pollutants such as iron and ammonia [7].

A list of contaminants commonly found in wastewater, along with their sources and environmental consequences is given in table 1.1 [8].

TABLE 1.1
Important wastewater contaminants

Contaminant	Source	Environmental significance
Suspended solids	Domestic use, industrial wastes, erosion by infiltration / inflow	Cause sludge deposits and anaerobic conditions in aquatic environment
Biodegradable organics	Domestic and industrial waste	Cause biological degradation, which may use up oxygen in receiving water and result in undesirable conditions
Pathogens	Domestic waste	Transmit communicable diseases
Nutrients	Domestic and industrial waste	May cause eutrophication
Refractory organics	Industrial waste	May cause taste and odour problems, may be toxic or carcinogenic
Heavy metals	Industrial waste, mining, etc.	Are toxic, may interfere with effluent reuse
Dissolved inorganic solids	Increases above level in water supply by domestic and / or industrial use	May interfere with effluent reuse.

1.4 Industrial Water Management

Traditional industrial practice is to attempt to address the problem of pollution at the end-of-pipe [9]. This often has negative repercussions, as polluters are unable to meet the constraints placed upon them by the regulatory bodies and, at the same time, remain profitable. The shortcut is to dilute controlled wastes before discharge to the resource. Even in cases where treatment is affordable, the environmental burden created by the manufacture of the necessary treatment chemicals and the burden of the electrical demands of the treatment operations, results in an even greater negative impact on the environment in some cases.

Smith [6] gave a generalised illustration of water use on a typical process site (figure 1.2). Raw water is pre-treated before use in various processes such as washing, (e.g. vessel cleaning). In these processes water comes into contact with process materials, becomes contaminated, and is sent to wastewater treatment. Freshwater (treated raw water) may be upgraded in boiler feed water (BFW) treatment for use in the steam system. Wastewater is generated by ion-exchange regeneration, boiler blowdown and condensate loss. Another source of wastewater is the cooling tower blowdown. The various wastewater streams are then typically mixed, along with contaminated storm water, and sent to treatment.

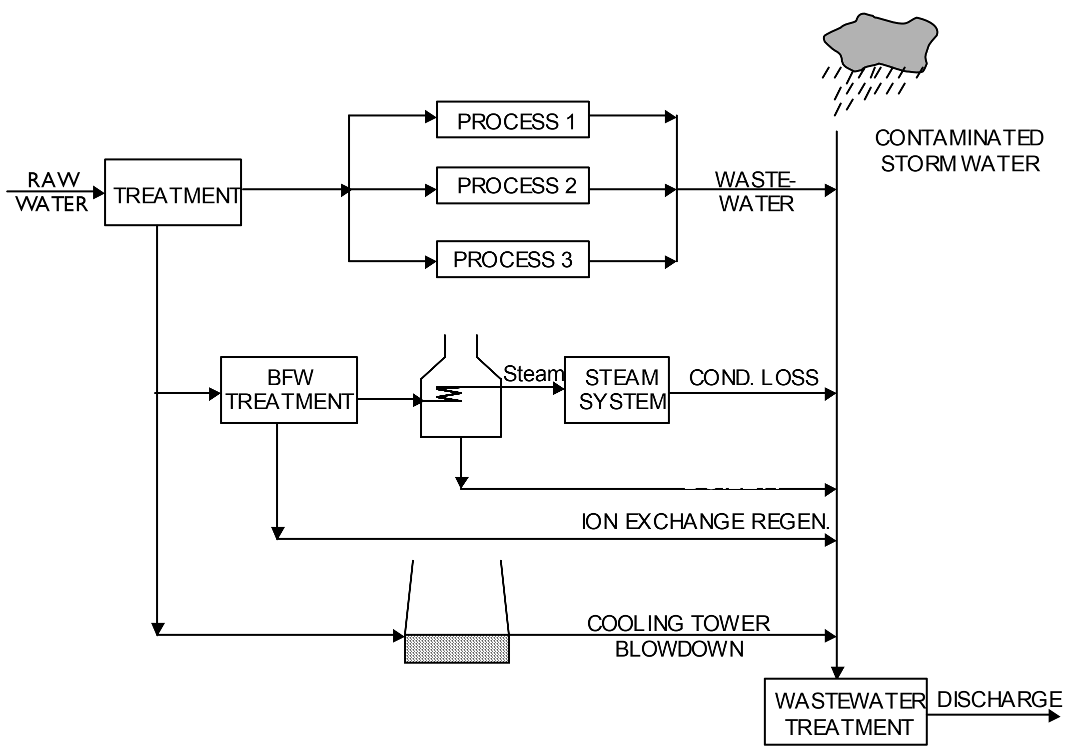

Figure 1.2
Typical water use on a chemical process site [6].

1.5 Water Usage Impact and Cost Reduction

The challenge is to find ways to reduce or eliminate pollution, which are both profitable to the industry concerned and environmentally friendly. Therefore, in order for the industry to remain viable, it is evident that steps must be taken to ensure that the usage strategy for natural resources in particular, must use techniques that employ the best available methods. The following general principles should be applied to control releases to water [10]:

i. Any use of water should be minimised, thereby minimising the amount of contaminated water to be dealt with,

ii. Methods of avoiding or reducing contamination, or risk thereof, of process or surface water should be considered,

iii. Water should be recycled within the process from which it issues, by treating it first if necessary. Where it is not practicable it should be recycled to another part of the process which has a lower water quality requirement (reuse),

iv. Ultimately, water is likely to need treatment to meet the environmental requirements. Generally any physicochemical treatment will be more efficient on the more concentrated individual or similar effluent streams than treating the whole mixed effluent. However, the inherent properties of dissimilar waste streams can be usefully employed to avoid adding further chemicals, for example by balancing waste acid and alkaline streams to control the resultant pH. An exception to the preference for treating waste streams individually would be when biological treatment is proposed and treatment of the whole mixed effluent overcomes an inhibitory effect of any individual waste stream.

Wang and Smith [11] proposed four general approaches to water and wastewater minimisation:

i. *Process changes*. Process changes can reduce their inherent demand for water. For example, wet-cooling towers can be changed to air coolers, or extraction operations can have a number of stages increased, etc.

ii. *Reuse*. Wastewater can be re-used directly in other operations (figure 1.3 (a)) providing the level of previous contamination does not interfere with the operation. When water is re-used it does not re-enter operations in which it has previously been used. Some operations can be split into parts such as multi-stage washing and supplied with different sources of water. Here, reuse implies that water cannot re-enter part operations in which it has already been used. Re-use might require wastewater being blended with wastewater from other operations (or part operations) and/or freshwater.

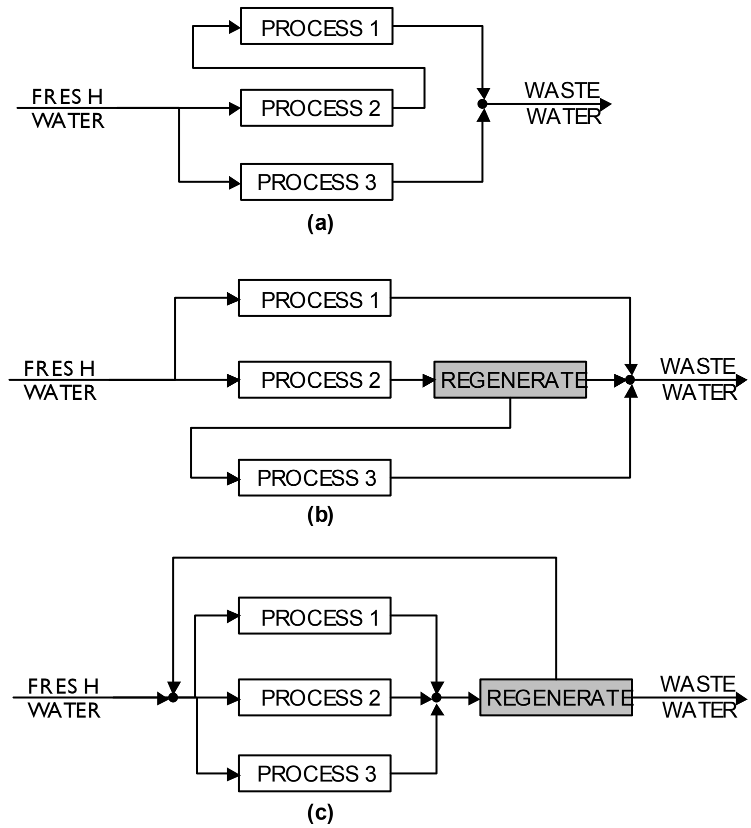

Figure 1.3
Water minimisation through (a) reuse, (b) regeneration reuse, and (c) regeneration recycling [6].

iii. *Regeneration reuse*. Wastewater can be regenerated by partial treatment to remove contaminants, which would otherwise prevent its reuse, and then reused in other operations (figure 1.3 (b)). When water is reused after regeneration it does not re-enter operations (or part operations) in which it has been previously used. Again, reuse after regeneration might require blending with wastewater from other operations and/or freshwater.

iv. *Regeneration recycling*. Wastewater can be regenerated to remove contaminants that have built up and then the water recycled. In this case water can re-enter operations in which it has been previously used (figure 1.3 (c)). Note that here recycling is possible not just around an individual operation but also around the entire system.

It is important to distinguish between these cases; in some situations recycling between operations might be allowed. In other cases it might not be allowed because of the build-up of contaminants not removed in the regeneration process.

1.6 Process Integration

Smith [12] described process integration of a process as being a two-stage activity. First, individual process steps are selected. Second, these individual steps are interconnected to form a complete process structure.

1.6.1 Conceptual Design Techniques

An entire process may be decomposed into subsets of interdependent functional groups. This hierarchical design approach [13] proposes to start with some critical piece of equipment of the flowsheet, usually the reactor. The flowsheet is developed from the inside out from the core operation (figure 1.4).

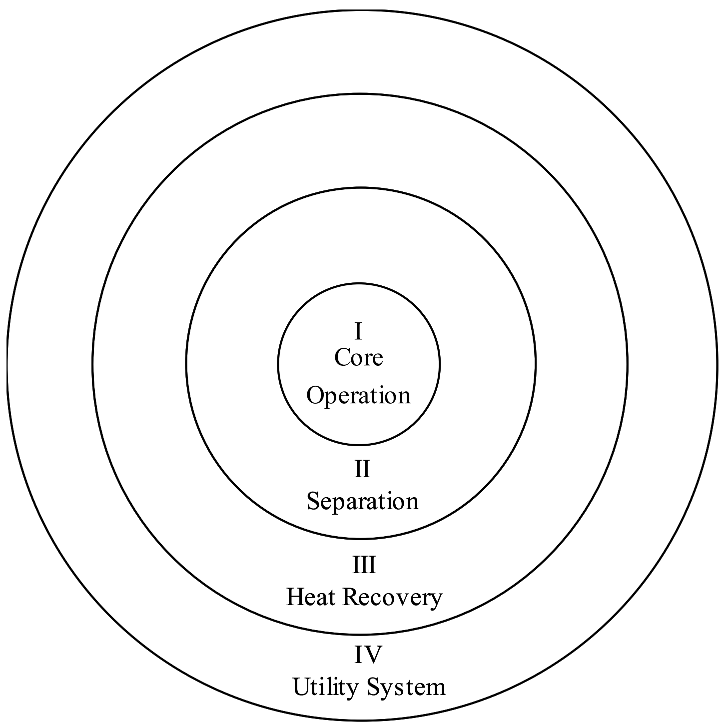

Figure 1.4
The onion diagram. Core operations (I), usually a formation process. Separation processes (II) such as distillation or ion exchange form the next layer. The heat exchanger network or Heat Recovery (III) is followed by the Utility System (IV), which consists of cooling towers, boilers for steam production etc.

At the heart of almost every chemical process lies a reaction or formation process, which produces the desired product, usually in an impure form. In order to purify this product, a second separation stage is required. The method of separation is dependent on the nature of the product from the formation stage. For example: organic mixtures may require distillation to separate the heavy and light products; dissolved aqueous species may be recovered by ion exchange; etc. Product streams may be in their final form after separation or may require some further processing steps. The material and energy balances are determined when the first two layers are fixed, which allows for the design of the heat recovery system. The design of this stage is dependent on the heat demands and supplies of the first two stages. In the final stage, the utility systems are designated to cater for the surplus demands of the inner stages. For example: steam, fired heaters or electrical heaters typically supply thermal energy, or alternatively excess heat is removed by ambient cooling (by air or water) or by refrigeration.

1.6.2 Pinch Analysis

Pinch analysis is a process integration tool, which was first developed for the design of heat recovery systems during the late 1970's [12]. Using the analogies between heat and mass-transfer, a similar approach was developed for the design of mass-exchange systems [14]. This work formed the basis for the design of water-using systems, the design objective being to minimise water consumption by maximising the reuse of water, using a graphical technique [11], which was termed Water Pinch Analysis [15]. However the technique was difficult (although possible) to extend to accommodate the practical constraints and characteristics of water-using systems, such as multiple contaminants, flowrate constraints, piping costs, etc. [12]. The added desire to introduce cost optimisation required that the problem be formulated using mathematical programming techniques.

The interpretation of industrial water reuse, regeneration and recycling using graphical and mathematical programming techniques forms the basis of the discussion in the Literature Review in Chapter 2.

1.7 The Application of Water Pinch Analysis in Industry

1.7.1 Previous Work

Water pinch analysis has been successfully applied in various industrial sectors. An indication of the wastewater reductions achieved are summarised in table 1.2, below.

TABLE 1.2
Examples of wastewater savings achieved using water pinch analysis [16]

Company	Process / Industry	Country	Wastewater Reduction, %
Cerestar	Corn processing	UK	25
Gulf Oil	Oil refining	UK	30
Monsanto	Agro-chemicals	UK	40
Parenco	Paper mill	Netherlands	20
Unilever	Polymers (batch)	UK	60
US Air Force	Military Base	USA	40

In South Africa, the technique has not previously been applied in the biochemical industry.

1.7.2 The Application of Water Pinch Analysis at AECI Bioproducts

AECI Bioproducts (Bioproducts) is part of an industrial complex located at Umbogintwini, approximately 26 km south of Durban, Kwazulu-Natal. This system was selected for an investigation of this nature as it is one of the major users of freshwater on the complex and hence discharges a related quantity of wastewater, amounting to approximately 400 ML per annum. Bioproducts is a manufacturer of l-lysine, which is an animal feed additive.

1.7.2.1 Project Aims

The aims of this project are as follows:

i. Apply water pinch analysis at Bioproducts, which consists of determining:
   - the set of contaminants that effectively limit water reuse within the system;
   - operating and fixed costs associated with operating the water-using network and necessary retrofit strategies;
   - a network configuration that satisfies the external constraints imposed upon the system at minimum cost;
   - operational improvements to the system in terms of retrofitting of treatment and regeneration operations, and additional piping requirements.

ii. Determine the elements of the water-using network that are the greatest barrier to further saving and improvement, and in so doing, suggest possible improvements that would aid in the implementation of similar projects in the future.

1.8 References

1. Reisner, M., *Unleash the Rivers*, in *TIME*. 2000. p. 66-73.

2. Uys, M., *A Structural Analysis of the Water Allocation Mechanism of the Water Act 54 of 1956 in the Light of the Requirments of Competing Water User Sectors.* 1996.

3. World Resources Institute, *South Africa at a Glance*, 2000, The World Bank/Agriculture and Natural Resources Dept. p. 4.

4. Clancy, L., *SA Plans its Water Security Beyond 2020*, in *Engineering News*. 1999.

5. Department of Water Affairs and Forestry, *Water Conservation Strategy for the Industry, Mining and Power Generation User Sector*, . 2000.

6. Smith, R., *Wastewater Minimisation*, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor. 1995, McGraw-Hill: New York. p. 93-107.

7. Mitchell-Fox, D., *Legal Aspects of Pollution Prevention*, in *Waste Minimisation Throug Process Design*, A.P. Rossiter, Editor. 1995, McGraw-Hill: New York. p. 17-28.

8. H.S. Peavy, D.R. Rowe, G. Tchobanoglous, *Environmental Engineering*. 1985, New York: McGraw-Hill.

9. Oliver, J.J., *Pollution Prevention or Pollution Control*, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor. 1995, McGraw-Hill: New York. p. 3-15.

10. Alva-Argaez, A., *Integrated Design of Water Systems*, in *Process Integration*. 1999, Manchester Institute of Science and Technology: Manchester.

11. Y.P. Wang, R. Smith, *Wastewater Minimisation.* Chemical Engineering Science, 1994. **49**: p. 981-1006.

12. Smith, R. *State of the Art in Process Integration*. in *PRES'99: 2nd Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction.* 1999.

13. Douglas, J.M., *A Hierarchical Decision Procedure for Process Synthesis.* AIChE, 1985. **31**(3): p. 353-362.

14. El-Halwagi, M.M., *Introduction to Numerical Optimization Approaches to Pollution Prevention*, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor. 1995, McGraw-Hill: New York. p. 199-207.

15. F.W. Buehner, A.P. Rossiter, *Minimize Waste by Managing Process Design*, in *Chemtech*. 1996. p. 64-72.

16. R.A Tainsh, A.R. Rudman. *Practical Techniques and Methods to Develop an Efficient Water Management Strategy*. in *IQPC conference: "Water Recycling and Effluent Reuse", 26 - 27 April*. 1999.

CHAPTER 2: Literature Review. Optimal Water Use Systems

2.1 Introduction

2.1.1 Mass Exchange Networks (MENs)

El-Halwagi and Manousiouthakis [1] first introduced the concept of MEN synthesis. They proposed a thermodynamically oriented procedure to identify thermodynamic bottlenecks, or pinch points. The pinch point limits the extent of mass-exchange between rich and lean process streams. A graphical targeting method, analogous to the method used by Linnhoff and Hindmarsh [2], was used to target for the minimum flow of mass separating agents (MSAs) required to remove mass from the rich streams. In order to accomplish the target, no mass should be transferred across the pinch. The minimum flow of MSA corresponds to a minimum requirement for the number of mass exchange units. Hallale and Fraser [3, 4] extended the technique proposed by El-Halwagi *et al*, to determine minimum total capital cost for MENs, which does not necessarily correspond to the minimum number of units determined by El-Halwagi.

2.1.2 Water Pinch Analysis

Water pinch analysis is MEN synthesis technology applied to the special case of water-using networks. Wang and Smith [5-7] adapted the MEN synthesis methodology of El-Halwagi *et al* to deal with simple industrial water-using operations. With reuse, recycle and regeneration of process water, minimum flowrate targets for freshwater demand could be identified, while removing the required amount of mass from the system. The graphical solution technique targets water flowrate and does not address costs directly. Instead it is assumed that costs are directly proportional to water flowrate.

2.1.3 Optimal Water Allocation

The concept of minimising industrial freshwater consumption is not a new one. Takama [8] addressed the problem of optimal industrial water allocation, by using a superstructure approach. A mathematical programming technique eliminates streams from a superset of all possible inter-process connections, to determine an optimal allocation strategy.

2.1.4 Mathematical Programming

Mathematical programming techniques have been used to solve the problem of optimal MEN synthesis [9]. Operating conditions are modelled by linear mass balance equations. Necessary linear and non-linear constraints are added to ensure that solutions are physically feasible. For example, concentration and flow constraints ensure that limiting operating conditions are satisfied, while maintaining a mass balance across the water-using operation. This facilitates the modelling of scenarios that have multiple contaminants and involve complex interactions between water-using operations. Operating cost factors may be specified, where necessary, as a function of water flowrate. In addition, by specifying a suitable annualisation term, capital costs for piping and installations may be included. The objective function is the sum of the cost equations. Determining the minimum value of the objective function, subject to the specified constraints, is a technique known as constrained optimisation. According to the nature of the constraints, a linear or non-linear program is specified. Commercially available optimisation software such as GAMS (General Algebraic Modelling System) utilises a combination of mathematical optimisation algorithms to determine minimum cost solutions. However, for non-linear models with integer constraints, optimality cannot be guaranteed.

This review looks at techniques for determining optimal designs of water-using networks in the processing industry.

2.2 Data

Numerous authors have proposed methodologies for obtaining the necessary data required for generating a representative model of a chemical system. In process integration projects, most of the time is required to obtain the desired data such as maximal inlet and outlet concentration [10].

2.2.1 Auditing Techniques and Requirements

Serageldin [11] proposed a hierarchical system for classifying operational sub-units of a processing plant in order to effectively track materials. This systematic method is designed to help companies identify sections of their process that are most problematic in terms of emissions.

Several publications address the management requirements for assisting in the completion of a plant-wide waste-audit [12, 13]. Specific requirements vary, but the consensus is for a top-down management commitment to the goals of the project. Crittenden *et al* [12] address some general techniques for reducing plant wide waste, which incorporate reuse, recycle and regeneration strategies. However, no publication has been identified, which specifically addresses the requirements for obtaining a representative set of data for completing a water pinch investigation.

2.2.2 Data Reconciliation

The goal of data reconciliation is to produce a consistent and representative set of data for a plant. Meyer et al [14] described a general method for data reconciliation applied to material balances for steady-state chemical processes. Sets of rules were proposed that facilitated the classification of measurements and mass balance equations. The purpose of doing so is to reduce the number of variables that require optimisation. The numerical method proposed determines the best fit of the variables, using redundant equations as constraints. Most data reconciliation techniques rely on a similar technique of fitting data by using a sum of least squares regression method.

2.2.3 Project Feasibility

Jodicke *et al* [10] presented a MINLP method for establishing the viability of potential projects with minimum data requirements. The model uses only information that is easily accessible, such as location of processes and holding tanks as well as the current water demand of each process. This effectively reduces the effort required to produce optimal solutions, which may be infeasible due to unforeseen circumstances that become clear only at the end of the project.

2.3 Modelling the Water-Using Network

In the discussion that follows, techniques that aim to integrate water-using networks have been broadly classified into two main groups:

i. Conceptual techniques.

ii. Mathematical programming techniques.

Conceptual techniques use graphical analysis tools to gain insight into the nature of the problem. In most instances, the elements of the overall system are addressed separately. For example, the water-using subsystem is designed first and the treatment network for the wastewater streams is determined as a second step. However, some authors use graphical insights to address the design of the overall system [3, 4, 15]. However, in the general case, conceptual techniques are limited, in that systems that have multiple contaminants and flowrate constraints are difficult to solve [16]. In addition, piping and discharge costs cannot be incorporated directly, as freshwater flowrate is targeted and not capital cost.

Mathematical programming techniques use optimisation algorithms to determine the design of water-using systems at a minimum cost of operation and installation (for the case of retrofit and new designs) [9]. Mathematical programming techniques can determine globally optimal solutions for the design of the water-using subsystem. However, neither the conceptual nor the mathematical programming approaches can guarantee globally optimal solutions for the design of the integrated system [17].

2.3.1 Elements of the Water-Using Network

Takama [8] addressed water use and treatment in a petroleum refinery. The industrial water-using model classified water use into four general systems (figure 2.1). Freshwater is required by operations that discharge wastewater, which is treated and discharged or regenerated for reuse and recycle.

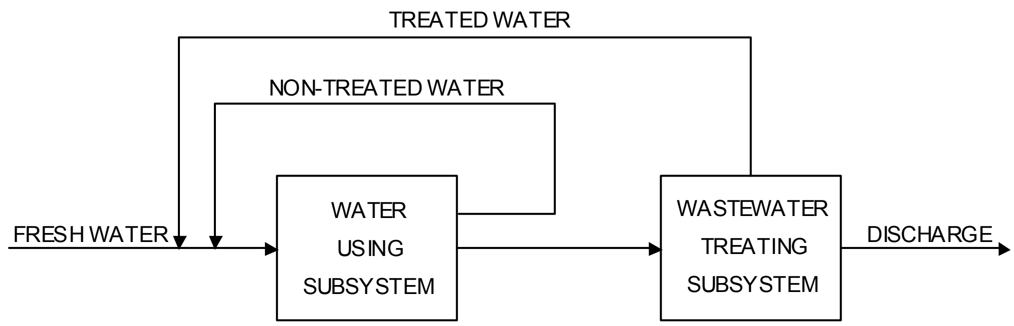

Figure 2.1
System for industrial water use and treatment

Hence, four basic related elements of an industrial water-using system may be specified. Alva-Argáez *et al* [18] characterised these elements as follows:

i. *Freshwater sources*, each with a maximum available flowrate, concentration of key pollutants and cost per unit used.

ii. Water and wastewater *treatment* plants, each with a maximum flow capacity, an efficiency for the removal of the key pollutants and possible water losses.

iii. *Water-using operations* each with a water flow demand and quality requirements.

iv. A *wastewater discharge point* where some environmental regulations must be met, in terms of maximum concentration of key contaminants, or maximum contaminant loads.

2.3.2 Mass Transfer and Flow Model

Wang and Smith [5] described *water-using operations* as operations that have a demand for water and generate wastewater when the water streams are exposed to process materials, such as a desalting operation for example. Utility wastewater is generated by the utility system, such as cooling tower blowdown. Treatment operations remove contaminants from wastewater streams for discharge to the environment or for reuse and recycle in the water-using subsystem.

Wang and Smith [6] proposed models for both the water-using operations and treatment operations that take into account inlet and outlet stream concentrations of the water stream. Mass transfer of contaminant is specified as a linear function of contaminant concentration (figure 2.2). Non-linear mass transfer relationships may be incorporated by breaking the operation up into stages and using linear segments for each stage .

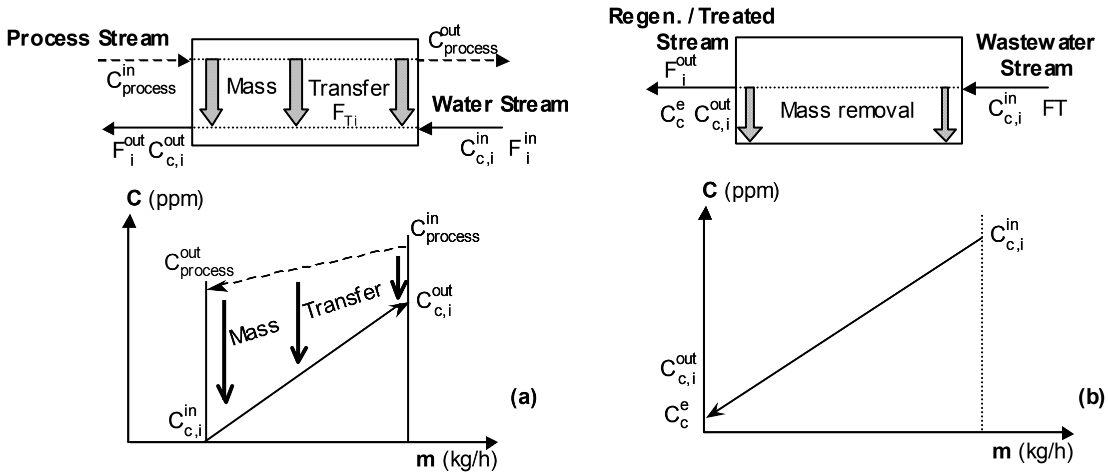

Figure 2.2
Fundamental model of water-using operation. Processes transfer contaminant from process stream to water stream (a). Regeneration or treatment operations remove contaminant from wastewater stream (b).

2.3.2.1 Water-Using Subsystem

The objective of the analysis is to determine the configuration of the water-using system. Process operating conditions, such as process stream flowrate, temperature and pressure are assumed fixed. Hence, the process stream in figure 2.2 (a) may be effectively discounted. The model for water-using operations within the water-using subsystem is reduced to an inlet water stream demand and a wastewater supply (figure 2.3, (a)). Contaminant addition is represented by a mass addition constant, Δm.

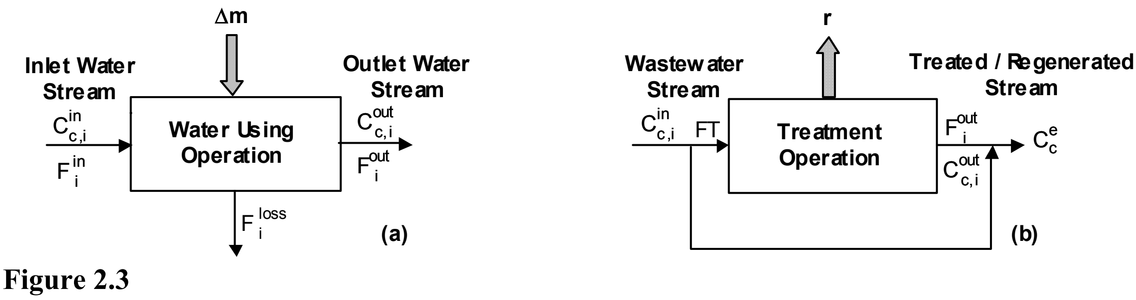

Figure 2.3
Mass transfer model for water-using operations (a) and treatment plants.

Unless specified as fixed, the flow demand for water-using operations is variable and depends on the rate of mass transfer from the process stream and the concentration of the inlet water stream.

Doyle and Smith [19] defined two types of mass-loading conditions for the water-using

operation may be fixed. The latter model exemplifies the practical situation of where contaminants have a limited solubility: in this case, they may be assumed to reach their maximum solubility, hence fixed outlet concentrations.

2.3.2.2 Treatment and Regeneration

Wang, and Kuo and Smith [6, 20] looked at the design of effluent treatment systems, as distinct from process wastewater reuse. The model for treatment operations takes a similar form to the model proposed by Wang and Smith for processes. A flow balance is maintained across the operation. Analogous to the mass-loading term, a removal ratio, *r* is specified for the performance of the unit. Alternatively, a constant outlet concentration may be specified. Treatment must reduce the outlet concentration to the specified environmental limit, C_c^e figure 2.2, (b).

Wang, and Kuo and Smith [5, 21] looked at incorporating regeneration into the design of the water-using subsystem. The model for operations that regenerate water streams is identical to the treatment model (although targeting and design methodologies are not ((section 2.4)). However, unlike treatment the aim of regeneration is to reduce the concentration of contaminants in a stream to a level where it is acceptable for reuse or recycle in the water-using subsystem. The performance of the regenerator is specified by a fixed removal ratio, *r* or a fixed outlet concentration, $C_{c,i}^{out}$ figure 2.3, (b). Although some treatment and regeneration operations are mass exchangers, i.e. a lean stream removes contaminant from the rich water stream; the general case is modelled as straightforward contaminant removal from the water stream.

2.3.3 Concentration and Flowrate Constraints

2.3.3.1 Concentration

Maximum inlet and outlet concentrations are established for the water-using streams entering and leaving a process. Wang and Smith [5] list a number of considerations for determining these limitations:

i. minimum mass transfer driving force (which may vary between different processes);

ii. maximum solubility;

iii. the need to avoid precipitation from solution;

iv. fouling of equipment;

v. corrosion limitations;

vi. minimum flowrate requirements to avoid settling of solid material; etc.

Most mathematical programming approaches [19], [18], [22], [23], [9] utilise linear inequality constraints to ensure the inlet concentration to water-using processes is below the physical maximum.

Contaminant concentration for specific pollutants or groups of pollutants must be below a predetermined limit before discharge to the environment. In addition to limiting the concentration of contaminants, it may be necessary to impose contaminant mass-flow constraints. This prevents dilution of effluent streams in order to achieve set environmental concentration limits. In the design of regional water distribution models Pingry and Shaftel, and Ocanas and Mays [24, 25] were amongst the first to propose a constraint on the mass-flowrate of contaminants to a discharge point, in a regional water distribution model.

2.3.3.2 Flowrate

Wang and Smith [7] described an approach to design water-using subsystems that have processes with flowrate constraints. In practice, many processes have a fixed flowrate requirement. Examples such as vessel cleaning, hosing operations, hydraulic transport, etc. tend to require a fixed flowrate regardless of the concentration of contaminant at the inlet. In addition, flow losses (F_i^{loss} figure 2.3, (a)) may need to be specified in order to model processes that have a fixed loss of water that cannot be reused. Examples are evaporation from cooling towers, or where water leaves with the product stream.

Mathematical programming models allow for linear flowrate inequality constraints to be specified, which limit flows to below a given maximum. Doyle and Smith [19] specified a linear flowrate constraint that constrains inlet flows to operations to below a maximum limiting value. This value corresponds to the flow demand when the mass transfer driving force is at a minimum. Alva-Argáez *et al* [23] presented inequality constraints that specify upper and lower limits for water demands for operations. Logic constraints may be included that limit the flowrate between operations. A binary variable tests for the existence of a connection between operations. This enables constraints to be applied to specific hypothetical inter-operational connections before optimisation. Logic constraints allow numerous practical considerations to be explored. In addition, a flow loss term is incorporated into the water user demand constraint. A negative loss term may be specified to model operations that have a gain in water.

2.4 Targeting for Minimum Water Flowrate

El-Halwagi and Manousiouthakis [1] were the first to use composite curves to address the general problem of mass-exchange between a set of rich process streams and a set of lean streams. This approach was adapted from the temperature-enthalpy curves used by Linnhoff and Hindmarsh [2] for heat exchanger networks.

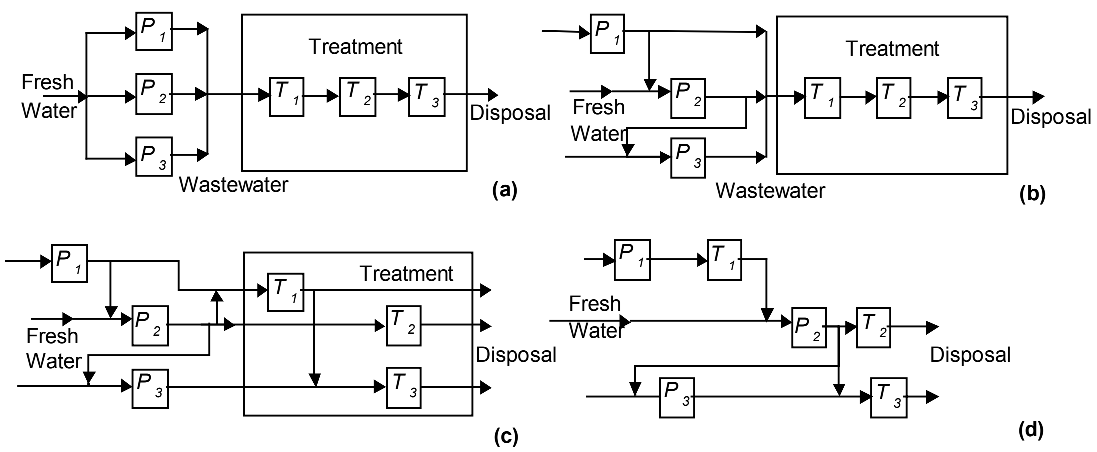

Figure 2.4
Network designs for conceptual solution techniques. Once-through water use and series treatment (a). Wastewater network design (b). Wastewater network design followed by treatment plant design (c). Total integration (d).

In his review of design procedures for water networks, Bagajewicz [17] illustrated the four strategies for industrial water consumption and reduction (figure 2.4). The conceptual methodologies that are summarised in the section 2.4.1, deliver solution strategies that correspond to those shown in figure 2.4, (b), (c) and (d). Conventional water usage is illustrated in figure 2.4, (a), where water is used on a once-through basis and treated in a series of treatment operations to remove contaminants, before discharge to the environment.

2.4.1 Mass Interval Composite Curves

Wang and Smith [5] addressed the minimisation of wastewater through partial or total reuse of process wastewater streams. A petroleum refinery was used as an example of how wastewater is generated. Initially, only one (pure) freshwater source was allowed, but the technique was extended to incorporate multiple sources at various qualities. A now well-known graphical technique to minimise wastewater was used. A limiting water profile for a process is defined by the linear relationship between its inlet and outlet concentration tolerance (figure 2.5). This line represents the boundary between infeasible and feasible operation in each water-using operation. Any water supply line operating at or below this limiting water profile will result in a feasible design. A limiting flowrate line may be defined (F^{lim}, figure 2.5) that has a gradient that corresponds to the maximum flowrate to the operation at maximum inlet and outlet concentrations. The freshwater line (*Fw*, figure 2.5) corresponds to the minimum bound of flow requirements for the operation. In this case, the driving force for mass exchange is at a maximum. This value is used as an upper limit to check the feasibility of optimal solutions.

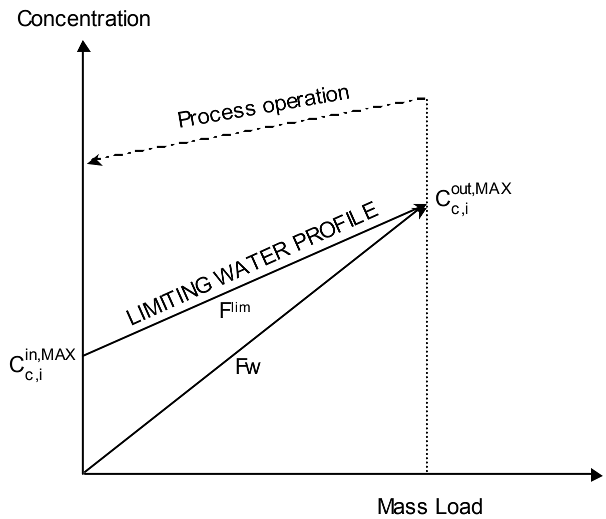

Figure 2.5
Limiting water profile for a water-using operation.

By plotting the limiting water profiles for all water-using processes within a system on a single set of axes, a composite curve may be generated for the system. The limiting inlet and outlet concentrations define concentration intervals. Within each concentration interval, the rate of change of mass load with change in concentration is assumed constant. This is demonstrated for four water-using processes in figure 2.6, (a). Combining operations within composition intervals generates the limiting composite curve (figure 2.6, (b)). The point at which the freshwater supply line touches the composite curve identifies the pinch point bottle neck: effective mass removal for the system cannot take place at a lower flowrate than the gradient represented by the freshwater supply line (a lower flowrate represents a steeper line).

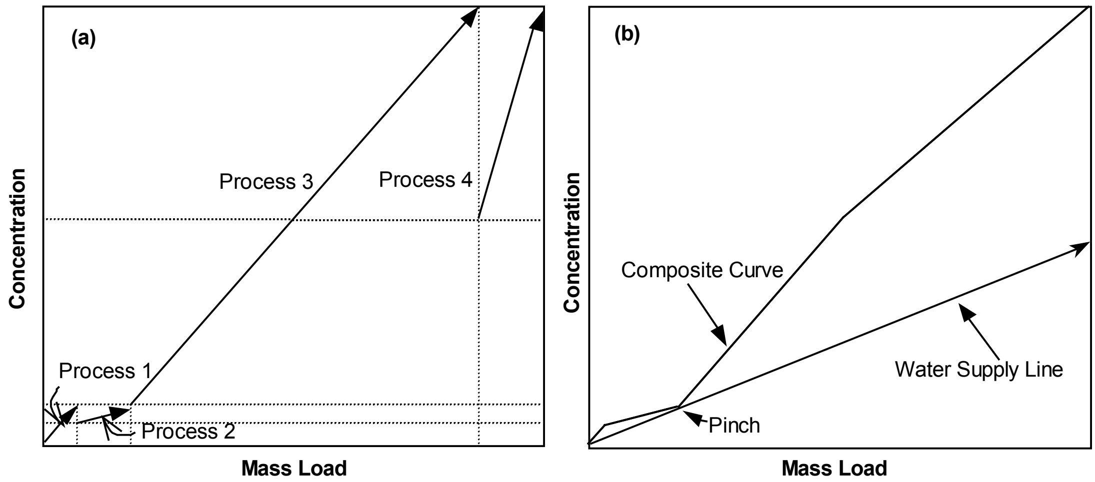

Figure 2.6
Composite curves for determining minimum freshwater requirements.

The authors proposed two techniques for constructing a network design from the composite plots, the 'maximum driving forces' and 'minimum number of water sources'. The minimum number of water sources method is discussed here. The design grid is constructed, as shown in figure 2.7, (b), from which the network can be obtained (figure 2.7, (c)).

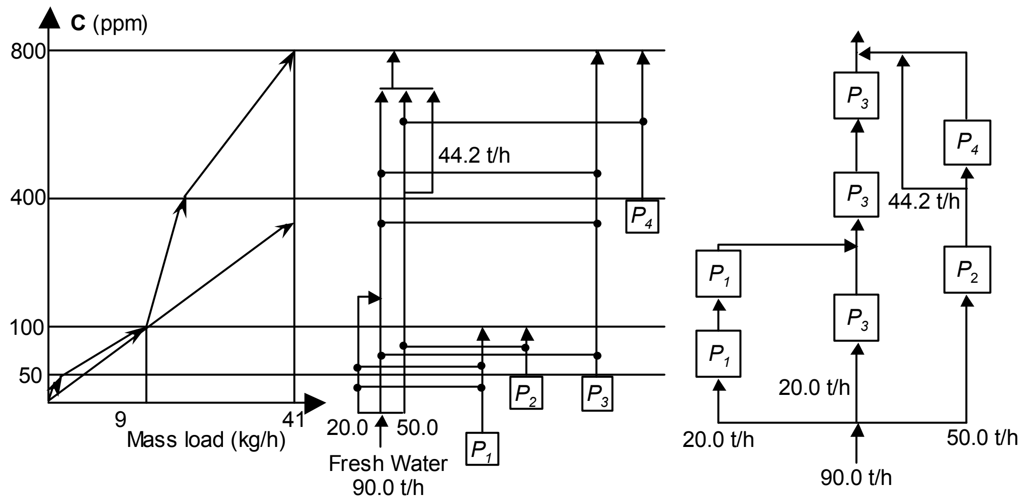

Figure 2.7
Single contaminant design grid procedure.

This design grid contains mixing in the middle of a process, which is not acceptable. To overcome this, a loop breaking technique is used, which eliminates bypassing and mixing. Figure 2.8 shows the loop and the result of the breaking procedure. Designs generated using this method result in water-using strategies like the example in figure 2.4 (b), where wastewater is minimised before treatment.

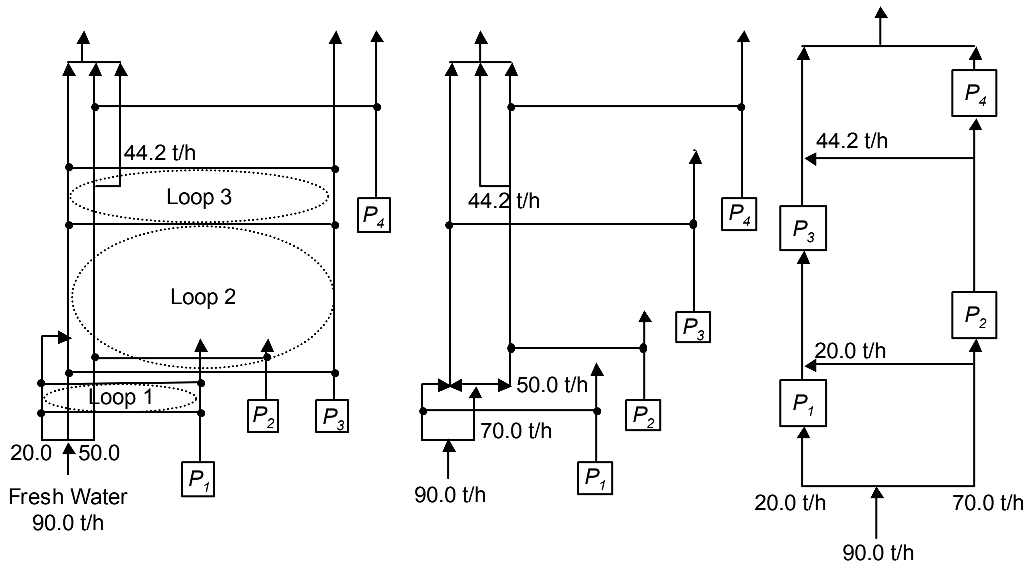

Figure 2.8
Loop breaking procedure.

The procedure was extended to deal with systems with multiple water sources [7]. The main assumption for multiple water sources is that purer sources are more expensive; hence, minimisation of the cleanest source will lead to minimum cost. This is accomplished at the expense of higher quality sources, which may be mixed with lower quality sources to form supplies at an intermediate quality (figure 2.9, (a)).

The same authors [7] presented a technique to limit inlet flows for operations that have fixed inlet flow requirements. Required flowrates to operations are maintained by incorporating

- local recycling around individual or groups of operations or,
- reuse of wastewater from individual operations.

Water is reused within an operation in ascending order of flowrate requirements. This satisfies the concentration constraint. For this method, the overall mass balance remains unchanged and the concentration restrictions are satisfied. Operations that have a water loss may be incorporated into the design by correcting the flow of the supply line (figure 2.9 (b)). Increasing the flowrate below the loss attains the freshwater target. The slope of the line above the loss gives the wastewater target.

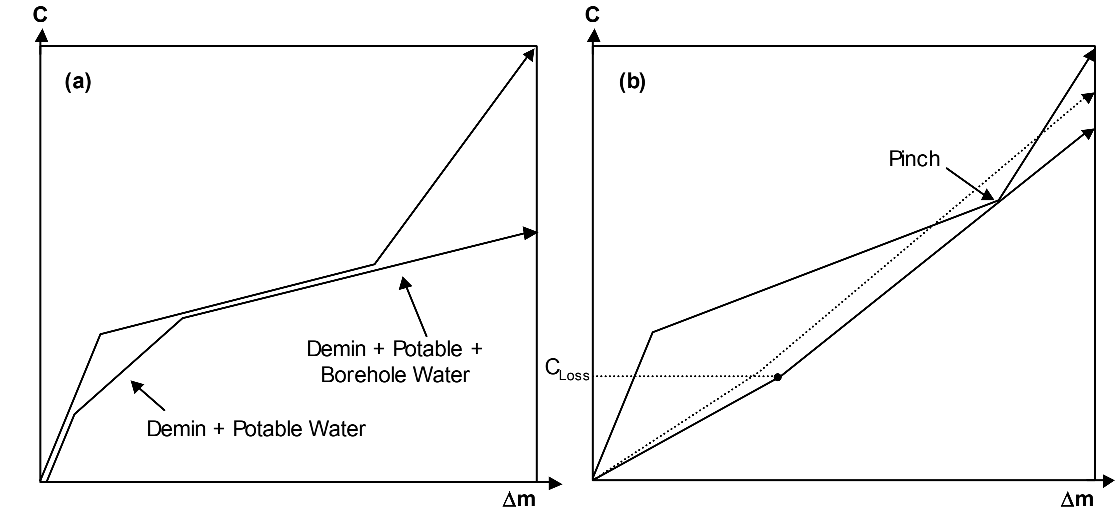

Figure 2.9
Incorporating multiple sources (a), and processes with a flow loss (b).

2.4.1.1 Effluent Treatment

A similar conceptual method was introduced by Wang and Smith [6] to deal with the design of effluent treatment systems. It was based on the assumption that the cost of treatment (capital and operating) is proportional to the flowrate treated. The problem was then to determine the minimum amount of effluent that must be treated in order to attain the environmental concentration limit (C_e, figure 2.10, (a) and (b)). An effluent composite is plotted of all the available wastewater streams (figure 2.10 (a)). A treatment line is matched against the effluent composite (figure 2.10 (b)) by rotating the treatment line around a fixed point *O*. This identifies the minimum flowrate of effluent that requires treatment. Because cost of treatment is assumed proportional to flowrate, minimising the effluent flowrate minimises treatment cost. For treatment operations that have a minimum operating cost, which does not correspond to the minimum flowrate, a feasible region is identified. This is bounded by the minimum flowrate (identified in figure 2.10 (b)) and the maximum flowrate, which is determined by the environmental limit.

The method was extended to deal with an inlet concentration limit for a treatment operation. The issue of multiple available treatment operations is also addressed for single contaminants. The sequence of treatment processes was determined by either inlet concentration constraints or economical factors. The first operation in the sequence has the greatest inlet concentration constraint. If concentration constraints do not apply, the cheapest operation is assigned to remove as much mass as possible. The treatment plant design was limited, as the structures that emerged from targeting were treatment operations operating in series, as in the example in figure 2.4 (b). Parallel configurations (figure 2.4 (c)), for example could not be considered. In addition, the results obtained were sub-optimal.

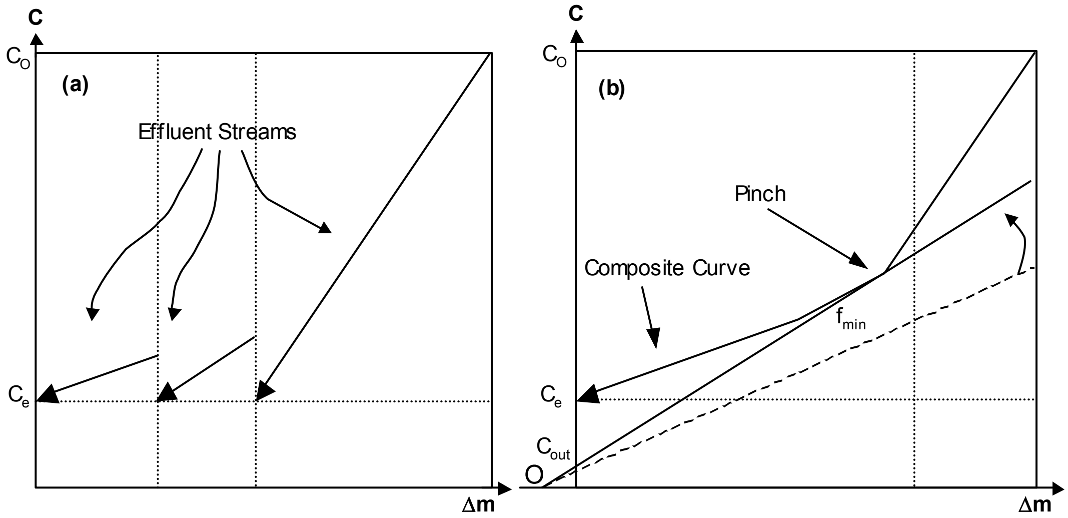

Figure 2.10
Effluent treatment flowrate targeting method.

Kuo and Smith [20] proposed an improved method for targeting minimum treatment flowrate. A rigorous thermodynamic analysis determines the exergy of the wastewater streams and predicts wastewater degradation due to mixing of streams of different qualities. This allowed for improved structural results such as parallel configurations, but remains an end-of-pipe treatment strategy, much like the example in figure 2.4 (c).

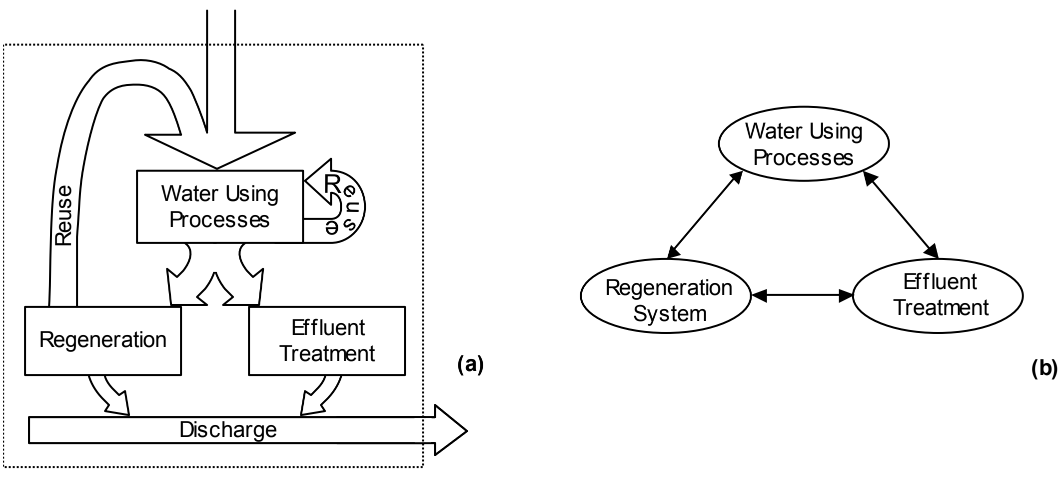

Figure 2.11
General industrial water flow scheme (a). Interactions between elements of the water system (b).

Kuo and Smith [15], classified industrial water use into three interacting subsystems: the water-using subsystem, the regeneration subsystem, and the effluent treatment subsystem (figure 2.11 (a)). These systems are interdependent (figure 2.11 (b)). For example, different wastewater system designs result in different effluent treatment strategies and costs.

2.4.1.2 Regeneration

Wang and Smith [5] addressed regeneration reuse and regeneration recycling for operations with single and multiple contaminant constraints. The basic requirement is that the freshwater supply must reach pinch concentration before regeneration. This will ensure that the minimum freshwater target is achieved.

Kuo and Smith [21] extended the method to address the interactions between wastewater minimisation and regeneration. A conceptual approach was used to solve the problem of finding the trade-off between optimal freshwater consumption and regeneration requirements. It was assumed here that regeneration costs are proportional to flowrate and regeneration removes a fixed amount (or percentage) of mass from the stream.

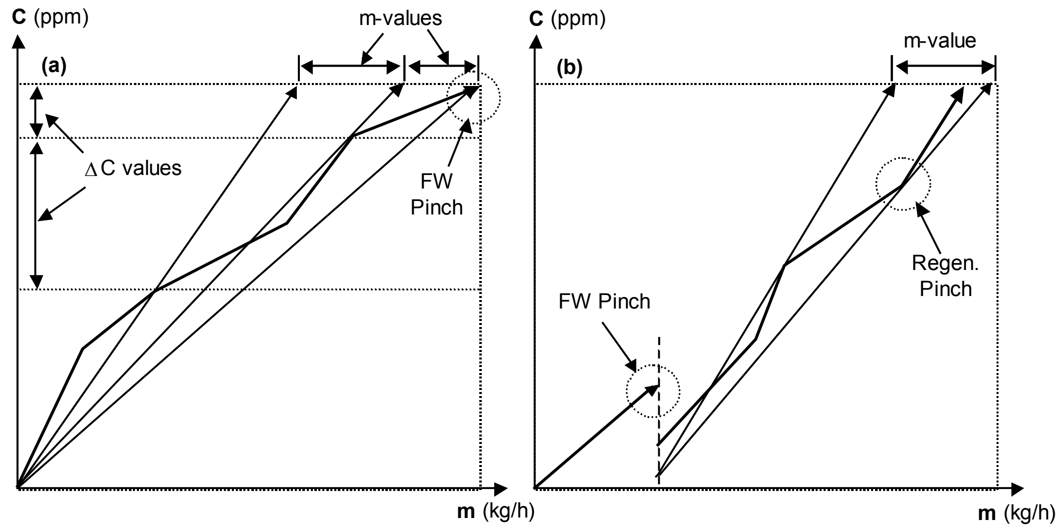

Figure 2.12
Procedure for simultaneously identifying freshwater targets and regeneration targets.

A dual mechanism was proposed to determine optimal regeneration reuse strategies. The first mechanism reduces freshwater demand by moving operations above the freshwater pinch. This defines two groups of operations: those that receive freshwater and those that can receive regenerated water. Operations that can receive regenerated water are identified by rotating the freshwater line anti-clockwise across the intervals defined by each process (figure 2.12, (a)). If the reduction in mass incurred (*m-values*, figure 2.12 (a)), is greater than the mass added by the process over the same interval (calculated by multiplying the flowrate to the process by the *ΔC values*, figure 2.12 (a)), the operation may be moved above the freshwater pinch. This is continued until no further operations may be moved and the freshwater and regeneration targets are defined. This results in two pinch points, the freshwater pinch and regeneration pinch, which are exploited in the second mechanism (figure 2.12 (b)). Here, regeneration and freshwater targets may be further reduced by rotating the regeneration line and moving operations in the regeneration group to the freshwater group. The methodology was extended to deal with regeneration recycles and process flowrate constraints. A targeting method for multiple contaminants was also discussed.

Kuo and Smith [15] proposed a methodology to deal with the interactions between the wastewater network design and effluent treatment designs, which was based on the observation that different wastewater network designs result in different effluent treatment plant designs. In addition, dilution of the wastewater, by increasing the flowrate target, reduces the number of effluent treatment processes required to attain the environmental limit. The problem is therefore to define the effluent treatment plant without the prior design of the wastewater network. A method for targeting for treatment flowrate from the process composite was illustrated that eliminates the need to design the wastewater network beforehand. Pockets defined by the concave regions of the wastewater composite curve are linked to create the effluent composite (figure 2.13). The treatment target may be established from this. The shaded region in figure 2.13 corresponds to the flexibility of operating conditions to accommodate changes in wastewater network design required to attain the treatment target.

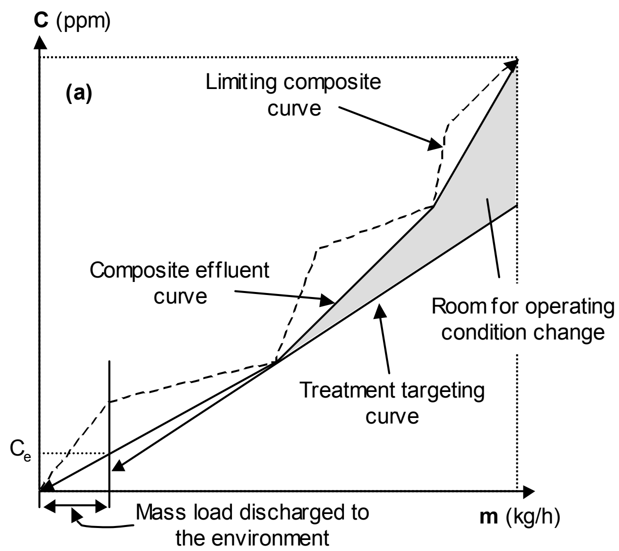

Figure 2.13
Generating a treatment curve from the wastewater composite curve.

The pockets of the limiting composite curve are divided into water mains. This establishes the amount of water that is discharged and the amount required for reuse. A design grid is drawn that connects the operations with the water mains. Mass balance simplifications are used to merge operations that cross water main intervals.

2.4.1.3 Geographical Constraints

Olesen and Polley [26] presented a simplified methodology for designing water-using networks handling single contaminants. A classification system was used to determine how water is assigned to operations that have inlets and outlets above and below the pinch point. The procedure was extended to address systems with water draw-offs and regeneration reuse.

The same authors [27] looked at geographical and piping constraints when addressing large water-using systems. The problem is subdivided into several geographical zones, each containing individual associated operations. Each zone has a unique pinch concentration and freshwater requirement. By finding the target for the overall problem, the potential for saving may be determined by linking zones and comparing the surplus water target for the overall problem with the combined targets for each zone. Explicit costs for piping are not taken into account and capital cost decisions based on geography are made by inspection. However, the technique of decomposing the problem can provide insights into addressing larger industrial problems with 50 or more water users.

2.4.2 Flow Interval Composite Curves

Buehner and Rossiter [28], proposed an alternative approach, which takes into account realistic operating scenarios. Inlet and outlet flows to processes are fixed. This allowed for the modelling of operations that have a demand for water that is not necessarily equal to the supply such as cooling towers, for example. By distinguishing inlet streams from outlet streams, processes with multiple inlets and outlets may be modelled as separate sources and sinks. As with the Wang and Smith method [5], process outlet concentrations may be linked to the inlet concentration via a linear mass-loading relationship.

A graphical approach to targeting for minimum freshwater consumption was developed. This graphical approach is part of a combination of graphical and mathematical programming techniques, which was trademarked WaterPinch. In this procedure, each relevant process or utility operation within the water-using subsystem is considered as having aqueous input and output streams. A single operation may have several input and output streams and each may be at different contaminant concentrations.

The input aqueous streams are plotted as a combined *demand composite* on a graph having *purity* on its vertical axis and aqueous stream flowrate as the horizontal axis (figure 2.14). In this context, purity may be defined as a negative concentration scale, starting at zero purity, which corresponds to water with no contamination, with increasing magnitudes on the negative axis corresponding to increasing contaminant concentrations. The composite defines the water demands, in terms of required input purities for the individual streams, for the overall plant. Similarly, the output water streams of all the operations can be plotted to form the *source composite* for the plant, defined in terms of the minimum output purities of the individual streams.

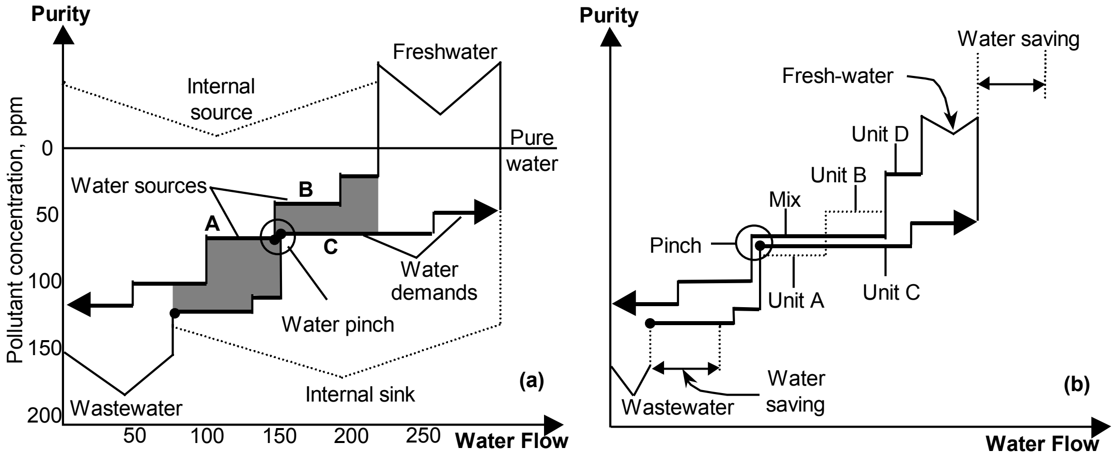

Figure 2.14
Composite curve of five water sources and four water sinks, showing design targets and minimum freshwater demand and wastewater production (a). Mixing of sources to produce an intermediate quality suitable for reuse, decreasing the amount of freshwater used and waste produced (b).

The example in figure 2.14 is for a plant with five process units (with four inlets and five outlets). The numbers on the vertical axis represent purity and increase downwards, with the highest purity water (at zero contaminant concentration) occupying the highest point on the vertical axis. The supply and demand composites are overlapped until they just avoid a crossover, and thus define the pinch point between the two composites. The overlap between the source and demand composite, shown by the shaded area, indicates the potential for water reuse. The available overlap is limited by the pinch point. Minimum freshwater demand and wastewater generation without mixing is also identified in figure 2.14 (a). The pinch point and the composite curves help to identify design improvements in an existing plant. No water from sources above the pinch point should satisfy demands for water below the pinch point. This would result in an increase in consumption beyond the target. Using freshwater to satisfy demands below the pinch, or sending water from sources above the pinch to waste treatment, will have the same effect. The representation guides the designer to identify modifications that can further improve targets for a plant. An example of this is shown in figure 2.14 (b). The water leaving Process Unit A is mixed with the water from Process Unit B, to generate a mixture at an intermediate concentration, shown as *Mix* in figure 2.14 (b). This mixture is suitable to satisfy part of the demand of Process Unit C, thus relieving the pinch-point bottleneck. This allows for further overlap of the source and demand composites, increasing the overall water recovery for the process.

2.4.3 Multiple Contaminants

The conceptual techniques presented above, are easily solved for cases where a single contaminant is present. Some situations may allow multiple contaminants to be lumped together as a single pseudo-contaminant [5]. Although the conceptual methodology may be extended to deal with problems involving multiple contaminants, they become difficult to apply to larger problems [16]. Optimality is not guaranteed in such cases. In addition, many realistic operating parameters and constraints, which are not directly related to flowrate, cannot be incorporated. Mathematical programming techniques (section 2.5) are needed to incorporate parameters and constraints that could not otherwise be included in conceptual models.

2.5 Mathematical Programming Techniques

2.5.1 Background

Mathematical programming, applied to optimisation [9], involves the task of identifying the value of an n-dimensional vector, *x*, that minimises (or maximises) a certain quantity called the objective function *f*(*x*) subject to *E* equality constraints and *m* inequality constraints, *h*(*x*) and *g*(*x*), respectively.

Mathematically, the general form of the problem may be stated as follows:

$$\min_x f(x)$$

Subject to:

$$h(x) = 0$$
$$g(x) \geq 0$$

where $x^T = [x_1, x_2, \ldots x_n]$, $h^T(x) = [h_1(x), h_2(x), \ldots h_E(x)]$, $g^T(x) = [g_1(x), g_2(x), \ldots g_m(x)]$ and T is the transpose vector. The objective of the optimisation algorithm may be to minimise the cost of the system or the amount of waste produced. Similarly, the purpose of the objective function may be to maximise the recovery of generated waste. The objective function is most frequently associated with some economic incentive, such as minimising the operating cost of a water-using system. Examples of equality constraints include material and energy balances and process modelling equations. Inequality constraints are frequently environmental (e.g. limiting concentrations of pollutants in effluent), technical (e.g. process inlet flowrate or contaminant level may not exceed a specified design limit) and thermodynamic (e.g. driving force for mass, heat or momentum transfer should be positive).

An optimisation problem in which the objective function, as well as all the constraints, are linear is called a *linear program* (LP); otherwise, it is referred to as a *non-linear program*

(NLP). Algorithms that contain continuous real variables (e.g. flowrate, pressure, temperature) as well as integer variables (e.g. 0, 1, 2…) is called a *mixed-integer program* (MIP). Depending on the linearity characteristics of the algorithm, MIPs can be further classified *into mixed-integer linear programs* (MILPs) and *mixed-integer non-linear programs* (MINLPs). A useful class of integer variables is the 0/1, or *binary* variables, which are most often used to model logical events and decisions. A 0/1 variable may be designated to assume the value of 1 when an event occurs (e.g. a unit operation is used) and 0 when that event does not occur.

Several commercially available computer programs have been developed. For linear problems (LPs and MILPs), a global optimum solution can be obtained. However, it is currently not possible to guarantee the global optimum of non-convex NLPs and MINLPs.

2.5.2 Regional Water Distribution and Reuse

Pingry and Shaftel [24] proposed a programming approach to integrated water management. They present a non-linear model, which takes into account both flow requirements and water quality. The model addresses the optimal design of water delivery systems, which does not consider recycling of water to the sources. The solution technique consisted of an iterative method in which a transhipment problem, with a non-linear objective function, was solved for a given set of quality parameters at each iteration; these quality parameters, consisting of the concentrations in the effluent from users and treatment plants were determined by a search technique. The model was applied to a hypothetical case to demonstrate its application.

Ocanas and Mays [25] proposed a similarly structured model for optimal reuse of wastewater on a regional basis. The objective was to determine the minimum cost solution to the problem of supplying water from different types and locations of sources to every user in the region, considering water reuse. The cost includes cost of water and wastewater treatment, and the transportation cost, including piping and pumping. Non-linear and linear constraints were specified and a non-linear objective function was solved using the large scale generalized reduced gradient method.

2.5.3 Industrial Water Distribution, Reuse and Treatment

Takama *et al* [8] addressed the problem of optimal industrial water allocation, by using mathematical programming to solve a refinery example. A superstructure (figure 2.15) of all water-using and treatment operations was set up and an optimisation was then carried out to reduce the system structure by removing irrelevant and uneconomical connections. The result is the structure, which represents the optimal water allocation strategy.

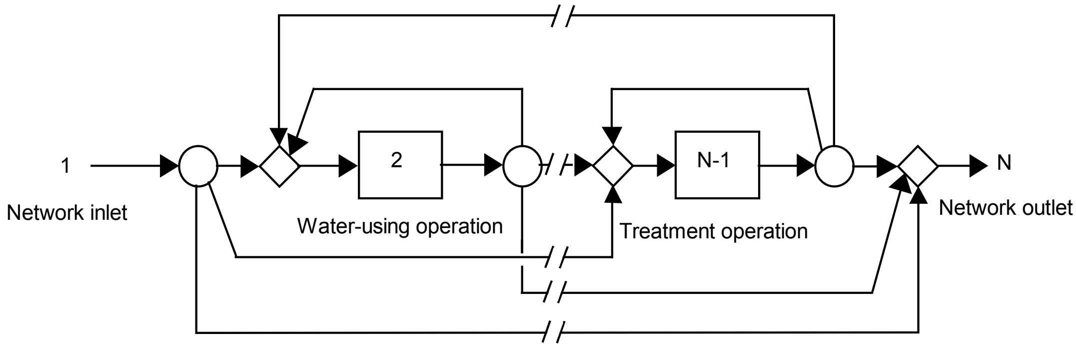

Figure 2.15
Superstructure of all possible inter-operational connections. Circles are splitter units, diamonds are mixer units, rectangles are water-using and treatment operations.

The superstructure consists of a total of N subsystems (nodes), which are the water-using and treatment operations, water sources and discharge points. The problem is stated as a dual optimisation problem. The first requirement is to optimise the allocation of water to the subsystems, i.e. determine the optimal structure. The second stage assumes a fixed structure, determined from the first stage, and optimises the design of the individual subsystems. The process is repeated with a new design parameter for each subsystem. In this paper, the authors only address the structural optimisation. Material balance relationships are specified to incorporate stream splitting and mixing. The objective function is defined as a function of return on investment, operating cost of the wastewater treatment system and freshwater costs. Linear mass loading and removal terms are specified for each subsystem. A solution method is presented that uses a penalty function to deal with constraint violations. The penalty function is added to the objective function. The minimisation of the objective function is carried out using the Complex method. An illustrative example is presented that looks at optimal water allocation in a petroleum refinery.

2.5.4 Wastewater Minimisation and Optimal Design of Treatment Plants

Doyle and Smith [19] proposed an automated method for synthesising water-using networks, which is an extension of the conceptual method of Wang and Smith [5]. Like the Takama [8] methodology, the solution procedure reduces a superstructure of inter-operational connections in determining the optimal network structure. A solution procedure is specified that uses a combination of linear and non-linear models to determine the minimum cost of water utilisation. The linear model assumes a fixed outlet water stream concentration, which allows the process mass load to vary. The solution to the linear model is used as an initialisation to a non-linear model that ensures a fixed Δm. The mass load is fixed by specifying a non-linear constraint. The variables are the inter-operational flowrates, the flowrates from freshwater sources and the outlet concentration from processes (for the NLP model). Flow variables are constrained to below a limiting flowrate, which corresponds to the flow demand of processes when the inlet concentration is at its maximum limit (see figure 2.5, F^{lim}). The approach allows for the inclusion of any number of freshwater sources at various purities, as required. Cost factors are included, allowing for a cost per unit flow used. A non-linear objective function is specified, which may be simplified to a linear function, if only the cost of freshwater is taken into account for the solution. The linear cost equation was used to determine the solution for the LP initialisation for the NLP model. Piping costs may be included in principle, but are not explicitly modelled.

Alva-Argaez *et al* [22] extended the work of Doyle and Smith [19] to include a more detailed objective function that explicitly takes into account contributing capital cost factors such as piping and additional treatment units. A linear mass balance constraint was specified, which prevented any violation of the mass balance across the treatment operation. A lower bound for contaminant removal was defined, for the case where water is used on a once through basis.

In presenting a methodology for the design of an industrial wastewater system, Alva-Argaez *et al* [18] proposed a linear cost correlation for pipe installations. The cross-sectional area of each pipe is calculated by assuming a flow velocity for each connection. With the material of construction known, the cost per unit length may be determined. Logic constraints were introduced which control the structure of the network with the use of binary (1,0) variables. Non-linear demand constraints, comparable to the fixed mass load constraint specified by Doyle and Smith [19], force the demand variables for each user to be satisfied. Combined with additional non-linear and linear water quality and flow constraints, the model becomes a MINLP optimisation problem.

In a later work, Alva-Argaez [23] proposed a two-step iterative decomposition procedure, for the MINLP model of the total water-using system. The solution methodology exploited insights into the nature of the optimal solution. In the first step, the outlet concentrations from water-using operations are fixed, which effectively linearises all non-linear constraints. The second step solves for the outlet concentration from processes using the flowrates determined in the first step, with objective being to minimise the excess capacity for mass transfer in each process. The optimal solution of this linear model results in an updated vector of exit concentrations for all operations and all contaminants, which can be used in successive iterations to generate corresponding flow variables. A non-linear cost function for stage-wise absorbers was proposed, based on the Kremser equation for number of stages. An iterative piece-wise linearisation methodology was proposed for this function, and was incorporated into the solution procedure. The solution terminates when the relative change in the objective value in the second step is within 1%.

Bagajewicz *et al* [29] provided a solution strategy for maximum reuse structures for wastewater minimisation. They used necessary conditions of optimality to determine global optimum for single contaminant systems. For optimal solutions:

i. All processes must be at maximum outlet concentration and,

ii. no process outlet concentration may be lower than the concentration of combined wastewater streams coming from its precursors.

Bilinear terms are eliminated by setting outlet concentrations to maximum. The number of variables can be reduced by using the second *monotonicity condition*. The methodology was extended to multi-component systems. For multi-component systems, the same conditions of optimality apply for one selected limiting component. A key component is specified for concentration monotonicity criteria, based on the process with largest freshwater flowrate. A maximum reuse rule is specified, which calculates the amount of wastewater that a process can receive from its precursors in such a way that the amount of freshwater consumed is minimised [17]. Using a branch and bound procedure, the maximum reuse for the network can be determined.

2.5.4.1 Heuristic Procedures

Based on insights into the nature of the problem, Liu [30] proposed a two-step heuristic solution procedure to determine optimal wastewater reuse strategies. The methodology does not guarantee optimality in all cases and some of the rules are incorrect [17]. However, the simple application allows for very rapid generation of solutions with little computational effort. The application of the methodology is demonstrated with the Wang and Smith [5] single and multiple contaminant examples

Galán and Grossmann [31] applied a heuristic search procedure for optimal design and synthesis of distributed wastewater treatment networks. The first step involves solving an NLP model with the objective function defined to minimise the total wastewater flowrate, using the upper bound of all variables as a starting point. The second step solves for the minimum flow for each unit using an LP relaxation of the NLP model. Then the NLP model is solved using, as initialisation points, the solution to the LP model. The third step involves solving the LP model with the objective function specified to minimise the total flow. As in the second step, this solution is used as an initialisation for the NLP problem. The NLP solution with the lowest objective function is selected as the optimum. The case of non-linear mass addition characteristics was addressed by solving a solvent extraction example.

2.6 Mathematical Programming Software

2.6.1 GAMS

The formulation and solution of major types of mathematical programming problems can be effectively performed with modelling systems such as GAMS (General Algebraic Modelling System) [32]. GAMS requires that the model be expressed in an algebraic form and interfaces with codes to solve the various types of problems. This modelling system can be run on most desktop PC computers, making its use and application widely available.

The solution of LP problems relies largely on the simplex algorithm. MILP methods rely largely on simplex LP-based branch and bound methods that consist of tree enumeration in which LP sub-problems are solved at each node, and eliminated based on bounding properties [33]. CPLEX and OSL are both popular codes for LP and MILP problems.

The solution of NLP problems relies on the reduced gradient method, for which the codes MINOS and CONOPT are popularly used. For convex problems, NLP methods can guarantee global optimality. When the problem is non-convex, the global optimum cannot be guaranteed.

2.6.2 WaterTarget

This program suite consists of two parts. The first, called WaterTracker, is a tool for the acquiring and analysis of plant data. The second part, WaterPinch, uses limiting data to generate optimal water reuse, regeneration and effluent treatment strategies [34]. WaterTarget interfaces with GAMS, which is used to solve the problems.

2.7 Optimisation and Water Reuse in the L-lysine Manufacturing Industry

2.7.1 Ion Exchange Modelling

Specific aspects of improving industrial l-lysine production have been addressed in the literature. In two separate papers, Kawakita *et al* [35, 36] addressed the modelling and optimisation of the cationic ion exchange process used for the extraction of l-lysine. A finite segment model was used to determine the breakthrough curves for the ternary cationic components. The model was validated experimentally by testing predicted pH values and the ratio of lysine to ammonium (the resin is in ammonium form before adsorption).

In the second paper, Kawakita *et al* used a simplified method to determine the optimal operating conditions of multicolumn adsorption of lysine from a lysine fermentation broth, where the columns move counter-current to a continuous lysine flow. Optimal operating conditions were calculated to maximise the amount of lysine adsorbed onto the first column, in a multicolumn adsorption process. The optimal arrangement, such as the number of resin columns in series for a given lysine fermentation broth, and the pH was determined. The optimal operating conditions determined by the model compared favourably with tested experimental values.

2.7.2 Process Wastewater Reuse

Finally, Hsiao and Glatz [37] looked at reuse of process effluent by testing the viability of recycling the fermentation broth effluent. The fermentation broth gives rise to a large volume of high COD effluent, which is rich in nutrients that may be reused as substrate. The viability of both a standardised medium and complex medium were investigated by measuring the concentration of l-lysine and the mass of cells in the fermentation broth after successive recycles. Recycling of broth effluent was hindered mainly by a loss in ion exchange column efficiency, which was reported to drop by approximately 17% for the recycle batch. The aim of the exercise was to minimise waste associated with l-lysine production.

2.8 References

1. M.M. El-Halwagi, V. Manousiouthakis, *Synthesis of Mass Exchange Networks.* AIChE, 1989. **35**(8): p. 1233-1244.

2. B. Linnhoff, E. Hindmarsh, *The Pinch Design Method of Heat Exchanger Networks.* Chem. Eng. Sci, 1983. **38**: p. 745.

3. N. Hallale, D.M. Fraser, *Capital Cost Targets for Mass Exchange Networks. Part 1: simple capital cost models.* Comp. Chem. Eng., 2000. **23**(2000): p. 1661 - 1679.

4. N. Hallale, D.M. Fraser, *Capital Cost Targets for Mass Exchange Networks. Part 2: detailed capital cost models.* Comp. Chem. Eng., 2000. **23**(2000): p. 1681-1699.

5. Y.P. Wang, R. Smith, *Wastewater Minimisation.* Chemical Engineering Science, 1994. **49**: p. 981-1006.

6. Y.P. Wang, R. Smith, *Design of Distributed Effluent Treatment Systems.* Chem. Eng. Sci., 1994. **49**(18): p. 3127-3145.

7. Y.P. Wang, R. Smith, *Wastewater Minimsation with Flowrate Constraints.* IChemE, 1995. **73, Part A**(November 1995): p. 889 - 904.

8. N. Takama, T. Kuriyama, K. Shiroko, T. Umeda, *Optimal Water Allocation in a Petroleum Refinery.* Computers and Chemical Engineering, 1980. **4**: p. 251-258.

9. El-Halwagi, M.M., *Introduction to Numerical Optimization Approaches to Pollution Prevention*, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor. 1995, McGraw-Hill: New York. p. 199-207.

10. G. Jodicke, U. Fischer, K. Hungerbuhler, *Wastewater Reuse: A New Approach to Screen for Designs with Minimal Total Costs.* Comp. Chem. Eng, 2000. **25**(2001): p. 203 - 215.

11. Serageldin, M.A., *Standardized Accounting for a Formal Environmental Auditing and Management System*, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor. 1995, McGraw-Hill: New York. p. 289 - 303.

12. B.D. Crittenden, *Waste Minimisation Guide*, , S.T. Kolaczkowski, Editor. 1992, The Institution of Chemical Engineers: Rugby, Warwickshire.

13. OWMC, *Industrial Waste Audit and Reduction Manual*, 1993, Ontario Waste Management Corporation: Canada.

14. M. Meyer, B. Koehret, M. Enjalbert, *Data Reconciliation on Multicomponent Network Processes.* Comp. Chem. Eng, 1993. **17**(8): p. 807-817.

15. W.J. Kuo, R. Smith, *Designing for the Interactions between Water-use and Effluent Treatment.* Trans IChem, 1998. **76, Part A** (March 1998) p. 287-301.

16. Smith, R. *State of the Art in Process Integration*. in *PRES'99: 2nd Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction.* 1999.

17. Bagajewicz, M.J., *A Review of Recent Design Procedures for Water Networks in Refineries and Process Plants.* Computers and Chemical Engineering, 2000. **24**(2000): p. 2093 - 2113.

18. A. Alva-Argaez, A.C. Kokossis, R. Smith. *Process Integration Technology for Wastewater Treatment Systems*. in *AIChE Annual General Meeting*. 1998. Miami Beach, Florida: AIChE.

19. S.J. Doyle, R. Smith, *Targeting water reuse with multiple contaminants.* Trans IChemE, 1997. **75**: p. 181-189.

20. W.J. Kuo, R. Smith, *Effluent Treatment System Design.* Chem. Eng. Sci., 1997. **52**(23): p. 4273-4290.

21. W.J. Kuo, R. Smith, *Design of Water-using Systems Involving Regeneration.* IChemE, 1998. **76, Part B** (May 1998): p. 94-114.

22. A. Alva-Argaez, A.C. Kokossis, R. Smith, *Wastewater minimisation of industrial systems using an integrated approach.* Comp. Chem. Eng, 1998. **22**(Supplement): p. S741-S744.

23. Alva-Argaez, A., *Integrated Design of Water Systems*, in *Process Integration*. 1999, Manchester Institute of Science and Technology: Manchester.

24. D.E. Pingry, T.L. Shaftel, *Integrated Water Management With Reuse: A Programming Approach.* Water Resources Research, 1979. **15**(1): p. 8-14.

25. G. Ocanas, L.W. Mays, *A Model for Water Reuse Planning.* Water Resources Research, 1981. **17**(1): p. 25-32.

26. S.G. Olesen, G.T. Polley, *A Simple Methodology for the Design of Water Networks Handling Single Contaminants.* Trans IChemE, 1997. **75, Part A**(May 1997): p. 420-437.

27. S.G. Olesen, G.T. Polley, *Dealing with Plant Geography and Piping Constraints in Water Network Design.* IChemE, 1996. **74, Part B**(November): p. 273-276.

28. F.W. Buehner, A.P. Rossiter, *Minimize Waste by Managing Process Design*, in *Chemtech*. 1996. p. 64-72.

29. M.J. Bagajewicz, M. Rivas, M. Savelski, *A New Approach to the Design of Water Utilisation Systems with Multiple Contaminants in Process Plants*. in *AIChE National Meeting*. 1999. Dallas: Electronic Source.

30. Liu, Z.-Y. *Wastewater Minimisation Using a Heuristic Procedure*. in *AIChE 1999 Spring Meeting*. 1999: AIChE.

31. B. Galan, I.E. Grossmann., *Optimization Strategies for the Design and Synthesis of Distributed Wastewater Treatment Networks.* Comp. Chem. Eng., 1999. **Supplement**(1999): p. S161-S164.

32. A. Brooke, D. Kendrick, A. Meeraus, R. Raman, *GAMS - A User's Guide*. 1998, Washington DC, USA: GAMS Development Corporation. 262.

33. I.E. Grossmann, J.A. Caballero, H. Yeomans, *Advances in Mathematical Programming for Automated Design, Integration and Operation of Chemical Processes.* 1999.

34. Linnhoff-March, *WaterTarget*, 1999, Linnhoff March Ltd.

35. T. Kawakita, Y. Ito, C. Sano, T. Ogura, M. Saeki, *Breakthrough Curve of Lysine on a Column of a Strong Cation-Exchange Resin of the Ammonium Form.* Separation Science and Technology, 1991. **26**(5): p. 619-635.

36. T. Kawakita, T. Matsuishi, Y. Koga, *Optimisation of Lysine Adsorption Process Using Strong Cation-exchange Resin.* Sep. Sci. and Technology, 1991. **26**(6): p. 869-883.

37. T. Hsiao, C.E. Glatz, *Water Reuse in the L-Lysine Fermentation Process.* Biotechnology and Bioengineering, 1996. **49**(3): p. 341-347.

CHAPTER 3: Investigation at AECI Bioproducts

3.1 Introduction

AECI Bioproducts is a manufacturer of feed grade l-lysine. This plant is part of an industrial complex located at Umbogintwini, approximately 26 km south of Durban, Kwazulu-Natal. Commissioned in 1995, AECI Bioproducts is a modern facility and has sophisticated quality and environmental standards. Freshwater is withdrawn from the Umbogintwini River and is pre-treated before use. The l-lysine is produced by batch fermentation and is extracted from the fermentation broth by ion exchange. Two effluent sources arise from the manufacturing process: a concentrated broth effluent and general process effluent, which are handled separately. Process effluent arises mainly from the following sources:

- the utility system;
- tank and unit operation cleaning;
- pump seals;
- storm water runoff and
- contaminated process condensate.

Process effluent is discharged via a sea pipeline and stringent environmental regulations limit the concentration of pollutants expelled in this manner. What remains after lysine extraction is broth effluent, which is removed from the site and handled by a local sewage works. In accordance with an agreement with the DWAF, neither broth effluent nor failed fermentation batches were to be discharged via the sea pipeline.

Umbogintwini Operating Services (UOS) is an effluent and water treatment facility that exists at the industrial complex. Umbogintwini river water is treated to an acceptable level of concentration by UOS for use in the plants at the complex. Some industries utilise the UOS effluent treatment facilities, however the Bioproducts process effluent is of a suitable quality for direct discharge via the sea pipeline; no additional treatment is required. Barring pH correction of the broth effluent, no onsite effluent treatment takes place. The degree of integration in the system is high; clean process condensate is reused in several operations. However, systematic methods for water cost reduction have not been implemented at any stage during the design or retrofit.

Although the plant uses approximately 400 ML of water per annum – relatively low for an industrial system – the system represents one of the major water users and associated effluent producers at the industrial complex. For this reason, AECI Bioproducts was selected as a suitable candidate for a water pinch investigation.

3.2 Process Overview

The manufacture of l-lysine is a semi-batch process: fermentation is a batch process, whereas the extraction, purification and granulation of the lysine product are carried out continuously.

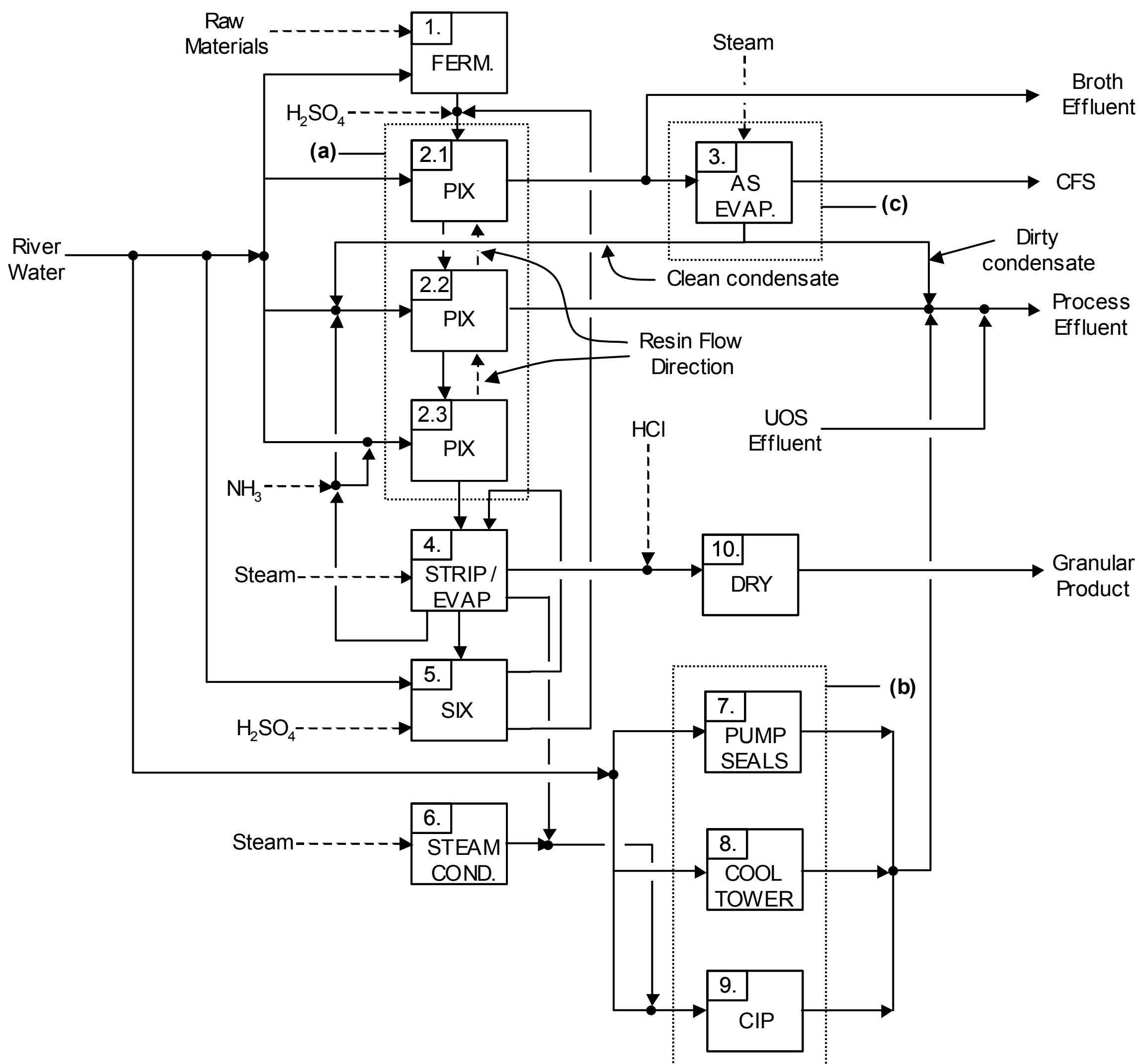

Figure 3.1
Flowsheet outlining water and raw material distribution, and process streams in the manufacture of l-lysine at Bioproducts.

The diagram in figure 3.1 provides a simplification of the manufacturing process. Aqueous and process streams are emphasised as solid black lines. The dashed lines represent raw material feeds and resin flow for the primary ion exchange process. Minor streams and processing details have been omitted from this diagram in order to preserve clarity. A more detailed diagram, which was used to complete the mass balance, is included in Appendix E.

3.2.1 Process Water

UOS provides treated water, which is drawn from the Umbogintwini River. The UOS water is stored in the Process Water Tank and is fed from here for use in all operations on the plant, except the cooling tower, which draws water directly from UOS without prior storage. The offices and development laboratories use Umgeni water. The most significant contaminant present in the UOS water supply is chloride ions, which present corrosion problems if allowed to accumulate.

3.2.2 Effluent Dilution from UOS

The treatment facility operated by UOS discharges treated effluent from other systems at the complex via the sea pipeline. AECI Bioproducts does not use the effluent treatment facility as the general process effluent from the plant is of a suitable quality for discharge directly to the sea after dilution with the effluent from the UOS effluent treatment facility.

3.2.3 Raw Materials

The raw materials are stored in a tank farm outside of the central processing area. For the fermentation process, the primary raw material is high-test molasses (HTM), which forms the main carbon source for the bacteria. The HTM is made up of glucose, fructose, and sucrose and contains a small amount of impurities, the most significant component of which is ash. Additional raw materials required as nutrients for fermentation include corn steep liquor (CSL), which is a protein source, along with the amino acids methionine and threonine, citric acid, phosphoric acid, ammonium sulphate (AS), vitamins, and minerals such as $FeSO_4$, $MnSO_4$ and $MgSO_4$.

Other raw materials include antifoam, which is required to prevent excessive froth generation during fermentation; ammonia, which is used for both pH correction during fermentation and regeneration of the primary ion exchange resin; and sodium hydroxide, which is used for pH correction of the broth effluent.

3.2.4 *Fermentation*

The *Corynebacterium glutamicum* bacterium produces the l-lysine, during the three-stage fermentation process. In the first stage, the population of bacteria cells is grown to a mass of 2g under sterile laboratory conditions. This is transferred to an $18m^3$ pre-fermenter, where the biomass increases to approximately 250kg, after 30-40 hours. The pre-fermenter feeds the main fermentation stage. Four $200m^3$ tanks are operated cyclically, each fermentation batch lasting 3-5 days. Throughout the first 8-12 hours, the biomass increases to 4-5 tons. Changing the balance of substrate nutrients during the remainder of the period, causes the cell population to plateau, and the micro-organisms begin to over-produce lysine.

3.2.4.1 *Sterilisation*

Foreign microbes must not enter the fermentation process. The mutated lysine producing micro-organism cannot compete with foreign microbes, and the fermentation batch must be discarded if contamination of this nature occurs. For this reason, all nutrients and antifoam required for pre-fermentation and fermentation - apart from the vitamins - are diluted with process water and heat sterilised. The sterilised media is stored in sterile tanks before use as feed to the fermenters. The vitamins are filter sterilised and are introduced directly into the fermenters.

The bacteria metabolise aerobically, and filter-sterilised air is used to supply the required oxygen. Gaseous NH_3 may be added with the air for pH correction. Refrigerated water is circulated through coils in the fermenters for temperature control. The fermenters are agitated continuously throughout the fermentation process to homogenise the broth.

Fermentation is complete when lysine production stops and the population of living cells begin to decrease. The mixture of cells and lysine solution, called fermentation broth, is transferred from the main fermenters into drop-tanks. A fraction of the fermentation broth is withdrawn from the drop-tanks and ultra-filtered to remove the biomass, which is recycled back to the drop-tanks. The lysine-rich permeate is fed to the lysine evaporator, where it is concentrated to a 28% lysine solution. This liquid-lysine product is sold locally as a spray-on animal feed additive. The remainder of the fermentation broth is acidified with sulphuric acid, which is added to the drop-tanks forming lysine sulphate. The liquid hold-up in the drop tanks and the cyclic batch fermentation production of lysine-rich broth is sufficient to continuously supply the primary ion exchange process with acidified broth at a flowrate of 10-13 t/h.

Lysine production may be summarised by the following chemical equation:

$$glucose + fructose + O_2 + (NH_4)_2SO_4 + NH_3 \rightarrow Lys_2SO_4 + CO_2 + byproducts$$

3.2.5 Primary Ion Exchange

The primary ion exchange (PIX) process (figure 3.1 (a)) consists of 30 cells of cationic ion exchange resin, arranged in a 20-stage revolving carousel (several of the stages consist of double-cell pairs). Because the resin beds are moving, the resin can be considered to flow in the direction of bed rotation. The function of the PIX process is to separate the lysine from the acidified fermentation broth. The process may be broadly classified into three main phases of operation: the adsorption phase, backwash phase and the strip phase.

3.2.5.1 Adsorption Phase

The acidified broth is fed from the drop-tanks to the PIX process. The fermentation broth is introduced to the adsorption zone and is fed counter-current to the resin flow. Because the fermentation broth is acidified with H_2SO_4, the lysine exists in both the +1 and +2 ionised states. In this charged state, the lysine ion has an affinity for the resin, molecules in the +2 state having a greater affinity than ions in the +1 state. The resin is in the ammonia form before the adsorption phase, i.e. NH_4^+ molecules are attached to the active sites in the resin. During adsorption, the charged lysine molecules from the fermentation broth are adsorbed by the resin, displacing ammonia into solution, forming AS. Lysine adsorption may be characterised by the following chemical reactions:

$$2R \cdot NH_4 + Lys^{2+} \xrightarrow{K_{ads,1}} R_2 \cdot Lys + 2NH_4^+$$
$$R \cdot NH_4 + Lys^{+} \xrightarrow{K_{ads,2}} R \cdot Lys + NH_4^+$$

Other charged species present in the broth compete with the lysine for adsorption sites. Small quantities of amino acids, such as valine, alanine and threonine, are present in the broth. Trace potassium ions have a high affinity for the resin and are adsorbed with the lysine. However, the major contaminant is ash, which is present in the HTM raw material. Concentrations greater than 3% can effectively reduce the lysine adsorption to zero, as charged ash particles block the active resin sites.

After adsorption, the AS-rich effluent that remains – the broth effluent – forms the major single source of effluent, in terms of cost of disposal, from the entire lysine producing process. Sulphuric acid from the secondary ion exchange (SIX) process (process 5, figure 3.1) is recycled to the adsorption zone of the PIX process. This recycle stream contains the metallic cation contaminants removed from the lysine solution in the SIX process. These cations are discharged with the broth effluent. The broth effluent is 60% solids sludge, high in free and saline ammonia, biomass and nutrients. At the time of the investigation, Bioproducts was prohibited by effluent exemption to release this biomass-rich effluent to the sea. The effluent was transported off-site to the Durban Southern Wastewater Treatment Works (SWW).

3.2.5.2 Backwash Phase

The loaded resin is rinsed to remove any product entrained on and between the resin beads. The beds are subsequently backwashed to remove loosely bound amino acid contaminants. The backwash effluent stream is fed directly to the sea pipeline. Dilute ammonia solution is used to displace the amino acids, which are adsorbed onto the resin with the lysine, but are more labile as they are in the +1 ionised state. These contaminants must be removed as they affect the purity of the final product.

3.2.5.3 Strip Phase

The lysine is displaced from the resin during the strip phase, by feeding a 4M ammonia solution, counter-current to the resin flow, after which the resin is in the ammonia form. The cells are rinsed with pure water (which is fed to the ammonia stripper) and purged with compressed air before re-entering the adsorption zone.

3.2.6 Ammonia Stripper and Lysine Evaporator Train

The ammonia and lysine-rich solution from the strip phase is fed to the ammonia stripper in order to remove the ammonia from solution. The stripped ammonia is recycled back to the PIX process. From the ammonia stripper, the lysine solution is concentrated in the third stage of a 3-stage evaporation process. From the evaporation third stage, the lysine solution is fed to the SIX process (see section 3.2.7) for further purification. The pure lysine solution from the SIX process is further concentrated in the first and second stages of the evaporation process.

3.2.7 Secondary Ion Exchange

The lysine solution is further purified in the SIX process. During lysine adsorption, metallic cations are adsorbed, with the lysine, by the resin. The most significant metallic contaminant is potassium. Positively charged metallic contaminants are removed by adsorption. As the feed is not acidified, lysine is not adsorbed, as it exists in a neutral state. The resin is regenerated with diluted H_2SO_4, which is recycled to the adsorption phase of the PIX process for feed acidification. Pure water is used to rinse the cells after regeneration (the rinse water is recycled to the PIX adsorption zone) and the cells are purged with compressed air, before re-entering the adsorption zone. The compressed air purge stream is reused in the PIX backwash.

3.2.8 Ammonium Sulphate Evaporator

About a third of the broth effluent is fed to the single-effect AS evaporator (figure 3.1 (c)), where it is concentrated to form an 80% solids AS-rich solution, which – when there is a demand – is sold as a cattle-feed supplement (CFS). The condensate from the AS evaporator is occasionally contaminated by contact with the process stream (the broth effluent in this case), due to overflow into the shell-side of the evaporator during boiling. Contaminated process condensate contains saline ammonia and suspended solids. Condensate with a suspended solids concentration of less than 1000ppm is used as part of the PIX backwash feed. However, if the suspended solids concentration rises above 1000ppm, reuse is prevented (by turbidity control). In this case, feed to the PIX backwash is prevented and the AS condensate tank is allowed to overflow and drain into the wash-down sump. The contents of the wash-down sump are discharged via the sea pipeline.

3.2.9 Steam Condensate

Pure condensate arises from the three-stage evaporation train. In addition, utility operations, such as steam heaters and pipe lagging, produce condensate. These have been grouped together as one operation in the diagram in figure 3.1. The condensate from these miscellaneous operations and utilities are combined with the pure condensate from the evaporation train, and reused as part of the feed to other operations.

3.2.10 Granulation and Bagging

The concentrated product from the first and second stages of the evaporator train is acidified with HCl. This stabilises the dried product. After acidification, the concentrated lysine is dried and granulated.

3.2.11 Cleaning and Cooling Utilities and Pump Seal Water

The auxiliary processes (figure 3.1 (b)) use UOS water either from the process water tank or directly, as is the case for the cooling tower. The clean in place system uses condensate, made up with process water. All of these water-using operations discharge their effluent via the sea pipeline.

3.2.11.1 Clean In Place System

Clean in place (CIP) is an automatic tank cleaning system. The water for the feed is comprised of condensate made up with process water when required. Sodium hydroxide is added as a cleaning agent. The CIP medium is pumped from a central storage facility and used where necessary.

3.2.11.2 Pump Seals

Two basic pumping systems were considered for this investigation. The tank farm pumps transfer material from the tank farm to the central processing facility. The process pumps transport liquids within the processing facility. The pump seal water is collected in the tank wash-down sumps for the tank farm pumps, and in the plant wash-down sumps for the process pumps.

3.2.11.3 Cooling Tower

The cooling tower draws makeup water directly from UOS, without prior storage. The blowdown rate is determined by the chloride concentration

3.3 Current and Potential Water Reuse and Recycle Opportunities

In general, reuse of effluent from the downstream processes in the fermentation process, is limited by the need to maintain a sterile medium for fermentation. Free and Saline Ammonia (FSA) and Suspended Solids (SS) are both monitored and limited in the effluent discharged to the sea. Chlorides pose a problem for operations sensitive to corrosion, such as stainless steel vessels and heat exchangers. Apart from pH correction, the effluent discharged to the sea is not treated on-site or at UOS.

3.3.1 PIX: Broth Effluent

At 16R/t, the PIX broth effluent has the highest per ton cost of disposal associated with its flow. It is high in SS, which is mainly in the form of biomass, as well as FSA, which is comprised mainly of AS, as the broth effluent is acidified with sulphuric acid. The concentrated nature of this effluent source compromises its viability for reuse in most operations. Recycling of broth effluent to the fermentation process would result in a recovery of both water and nutrients such as AS required as a substrate for cell metabolism. Hsiao *et al* [1] investigated pilot-scale broth effluent recycle with both a controlled fermentation medium and a complex fermentation medium.

However, this has not been considered at Bioproducts as a broth effluent recycle would lead to accumulation of charged ash particles (that arise from the HTM), which would reduce the PIX adsorption efficiency. Removal of ash from the HTM, which is the focus of current research at Bioproducts, may result in this becoming a viable endeavour.

3.3.2 PIX: Backwash Effluent

The main contaminant present in the backwash effluent is trace amino acids that are adsorbed with the l-lysine and are removed during backwash. A dilute ammonium solution is used as feed to the backwash stage of the PIX process. The NH_4^+ ions displace loosely bound mono-valent amino acids, such as valine and alanine, the predominant species being valine. The presence of free ammonia restricts reuse or recycle of this stream to the PIX strip and PIX backwash phase, however the amino acid contaminant prohibits this. Current studies focus on the extraction of valine from this source. Reuse and recycle of this source may then become feasible.

3.3.3 Condensate

As process steam is imported, pure condensate is not recycled to the boiler; hence it is a viable pure source. Current water saving practices see this source being used as part of the feed to the CIP process, as well as comprising a small fraction of the feed to the SIX rinse and PIX strip phase. Pure condensate is collected in the condensate tank, which is supplied with a makeup water feed, activated by a level controller.

The AS evaporator condensate is a viable source if it is pure. However, sporadic cross-contamination from the process stream can be an obstacle to reuse of this source. This was investigated by considering three models; the first two vary the contaminant level in the AS evaporator condensate, and the third looks at the case where condensate reuse is prevented (section 3.6).

3.3.4 PIX: Adsorption and Strip Phase

The PIX adsorption phase is sensitive to species, which compete with lysine, and requires a relatively pure feed stream. Micro-scale particles suspended in solution can become charged in the acidified medium and block active adsorption sites. Regeneration is required before any reuse of other wastewater streams. Similarly, the PIX strip phase requires pure water as feed to limit the contaminant concentration in the liquid lysine solution. As both these operations require pure water, the scope for reuse of contaminated process effluent is limited.

3.3.5 Pump Seals

Pump seal water may be reused, but the current design prevents this: pump seal water drains into an exposed sump beneath the pumps and from there, to the wash-down sumps. In both cases, considerable contamination results from exposure to the environment. A lack of qualitative data for the individual pump seal effluents restricted further investigation into this area.

3.3.6 Clean In Place

The overall quality of the CIP effluent after use in tank washing is poor. Cleaning chemicals such as sodium hydroxide limit the extent of reuse of CIP effluent in other operations. Reuse of cleaning water within the CIP system is an option, if sodium hydroxide levels are recharged and individual tank-cleaning concentration requirements are identified. However, the flowrate of water within the CIP system is too low, relative to the requirements of the total system, to warrant an investigation of this nature.

3.3.7 Cooling Tower

Cooling Tower blowdown is high in fungicidal and anti-corrosion chemicals, which limits its reuse. However, in petroleum refineries, cooling tower blowdown is frequently used as seal water for pumps [2]. Feed to the cooling tower must be as pure as possible in order to reduce the blowdown rate.

3.4 Model Constraints and Parameters

The following section summarises the types of constraints and model parameters, which are available in the literature, that can be specified using the Linnhoff-March software, WaterPinch [3]. The application of these constraints and parameters is discussed comprehensively in Appendix D, which addresses a case study of the system at Bioproducts using the Linnhoff-March software suite, WaterTarget. Section D.1.4.2 outlines the mass and flow balance relationships for water-using operations. Environmental and discharge constraints are discussed in section D.1.4.3. Constraints, which affect the connectivity of the water-using network, are discussed in section D.1.4.5.

3.4.1 Mathematical Programming Model

The following sets can be defined for the water-users [2] in the water-using system:

i. I = {i | i is an operation involved with the water-using system}, i = 1,2, …, N_{OP}.

ii. I_{OP} = {i | i is a water user in the water-using subsystem}, i = 1,2, …, N_{WU}.

iii. I_{TR} = {i | i is a water treatment operation}, i = N_{WU} + 1,2,…, N_{OP}.

iv. $I_{OP} \cup I_{TR} = I$.

where N_{OP} is the number of water-using operations and N_{WU} is the number of water-users in the water-using subsystem.

3.4.2 Model Constraints

3.4.2.1 Mass Balance

A general form of the linear equations used by Wang and Smith [4], [5] to describe contaminant mass addition and removal may be used to describe mass transfer for water-using operations:

$$C_{c,i}^{out} = C_{c,i}^{in} \cdot A + B \tag{3.1}$$

$C_{c,i}^{in}$ and $C_{c,i}^{out}$ are the inlet and outlet concentration for operation *i* and contaminant *c*. The terms *A* and *B* are constants that describe the way in which contaminant mass is added or removed.

3.4.2.2 Contaminant Concentration and Mass Flowrate

The inlet concentration to nodes can be constrained to be less than a predetermined maximum, $C_{c,i}^{in,MAX}$ [4]:

$$C_{c,i}^{in} \le C_{c,i}^{in,MAX} \tag{3.2}$$

Similarly, the mass flowrate of contaminants can be constrained at the inlet to nodes [6]:

$$M_{c,i}^{in} \le C_{c,i}^{in,MAX} \cdot F_{Ti} \tag{3.3}$$

where $M_{c,i}^{in}$ is the contaminant mass flowrate entering the node and F_{Ti} is the flowrate through the node, which takes into account flow losses. For environmental concentration limits, $C_{c,i}^{in,MAX}$ in equation 3.2 and 3.3 is replaced by the environmental concentration limit, $C_{c,i}^{e}$.

3.4.2.3 Water Availability

The amount of water withdrawn from a water source j can be prevented from exceeding a maximum limit, Win_j^U [6]:

$$\sum_i Fw_{j,i} \le Win_j^U \tag{3.4}$$

The WaterPinch software allows a lower bound to be specified, if necessary, which may be expressed as follows:

$$Win_j^L \le \sum_i Fw_{j,i} \le Win_j^U \tag{3.5}$$

where the lower limit for freshwater withdrawal is Win_j^L and $Fw_{j,i}$ is the freshwater mass-flowrate from source j to water-using operation i. If there is no specified lower bound, then $Win_j^L = 0$.

3.4.2.4 User Demand Constraints

The constraints related to the minimum and maximum water requirements for every water-using operation $i \in I_{TR}$ may specified as follows [6]:

$$F_i^L \le \sum_j Fw_{j,i} + \sum_{i'} F_{IPi',i} \le F_i^U \tag{3.6}$$

where $F_{IP\,i',i}$ is the flowrate from operation i' to operation i, and F_i^L and F_i^U are the minimum and maximum flow requirements, respectively. Note that Alva-Argáez *et al* include a flow loss parameter in the user demand constraints. This has been omitted in equation 3.6, as it may not be explicitly specified using the WaterPinch software, as water users in the water-using subsystem ($i \in I_{OP}$) have a fixed water demand and supply, (i.e. the loss term is implicit in the difference between the inlet and outlet flowrate) which are denoted, in subsequent sections, as F_i^{in} and F_i^{out}, respectively.

3.4.3 Objective Function

The objective is to determine the minimum cost solution to the problem of supplying water to every user in the system considering water reuse, regeneration, recycling, and effluent treatment [6], and subject to the specified constraints. The costs include the water and wastewater treatment costs and piping costs. Linear equations are used to describe the costs of the water-using network.

3.4.3.1 Freshwater

The total cost of freshwater supplies may be expressed as [6]:

$$\sum_j \sum_i \alpha_j Fw_{j,i} \tag{3.7}$$

where α_j is the cost of freshwater source j per unit mass. WaterPinch allows for a modified form of the freshwater cost equation, which includes fixed charges associated with freshwater use; hence equation 3.7 may be expressed as:

$$c_{Fw} = \sum_j \sum_i \alpha_j Fw_{j,i} + \beta_j \tag{3.8}$$

where the term β_j represents any fixed costs associated with the use of freshwater source j.

3.4.3.2 Piping

The piping costs are calculated as a function of water volume flowing in a pipe as follows. A flow velocity, $V_{j,i}$, is assumed for the system (typically between 1 and 2 m/s [6]) and with this information the cross-sectional area, $A_{CS\ j,i}$, and hence the diameter, may be calculated for each pipe [6]:

$$Fw_{j,i} = A_{CS\ j,i} \cdot V_{j,i} \tag{3.9}$$

for connections between freshwater sources j and operations i. The cost of new piping connections may be expressed as a function of the diameter, $D_{j,i}$, length of pipe, $L_{j,i}$, and an exponent, n, which accounts for the material of construction

$$C_{p\ j,i} = X \cdot D_{j,i}^{n} \cdot L_{j,i} \tag{3.10}$$

for new connections between freshwater sources j and operations i. The cost of piping and associated fittings is taken into account by the constant term, X [7]. Similar sets of constraints can be generated for the remaining new connections of the network. The total cost of new piping connections for the entire water-using system will be denoted as $c_{pipe.}$ The non-linear expression for the piping cost is linearised for each iteration of the optimisation algorithm [3].

3.4.3.3 Water Treatment and Discharge

The water and wastewater treatment operations and discharge costs can be accounted for using a similar form as the freshwater costs [6], with an additional constant term, b_i that takes into account fixed costs associated with the use of a treatment plant i (where $i \in I_{TR}$), or discharge point. The treatment cost equation may be expressed as:

$$c_{TR} = \sum_{i \in I_{TR}} a_i FT_i + b_i \tag{3.11}$$

The term FT_i represents the mass-flowrate to treatment plant i and a_i is the associated cost of treatment per unit mass.

3.4.3.4 Connectivity

Additional fixed and flow dependent costs, c_{IP}, can be associated with connections between individual operations. These are discussed with reference to a case study in Appendix D, section D.1.4.5.

3.4.3.5 Objective Function

The objective function is the minimisation of the sum of the freshwater costs, piping costs, treatment and / or discharge costs, and connectivity costs, i.e.

$$\min C_{TOT} = c_{Fw} + c_{pipe} + c_{TR} + c_{IP} \tag{3.12}$$

where C_{TOT} is the total cost of the water-using network per unit time. The WaterPinch software determines the structure of the water-using network, as well as the operating flows and concentrations of contaminants.

3.4.4 Sensitivity Analysis

The limiting concentration or concentration constraint of the water-using system is determined using a feature of the WaterPinch software called the *sensitivity analysis*. This determines the sensitivity of the objective cost to small changes in contaminant concentration constraints at inlets to operations, and contaminant concentration levels at the outlets from operations. The software reports initial values, which were tested by relaxing the inlet constraints over a range of concentration levels (section 3.7).

3.5 Water-Using System Model

3.5.1 Key Contaminants

Three contaminants were selected: free and saline ammonia (FSA), suspended solids (SS) and chlorides (Cl). Some contaminants were limiting, but were included in the analysis. The reason for this is discussed with reference to the case study in Appendix D, section D.2.1.

3.5.1.1 Free and Saline Ammonia.

Dissolved ammonium species, predominantly $(NH_3)_2SO_4$ and $NH_{3(aq)}$ (depending on the pH) are collectively classified as FSA. The concentration of this contaminant must be below 300ppm in the discharge to the sea. The following operations add or remove FSA to and from the water-using system:

- *Fermentation tanks*. AS is added during tank cleaning, which is manifested in the outlet from the CIP system, i.e. tank cleaning adds FSA to the system.
- *PIX adsorption*. Free ammonia is added, when ammonia is displaced from the resin by the adsorbed species.
- *The PIX backwash*. Adds free ammonia, which is discharged via the sea pipeline.

3.5.1.2 Suspended Solids

This is a broad-spectrum contaminant, which is limited to below 400ppm in the discharge to the sea. This concentration constraint is based on aesthetics since a brown coloured plume is visible in the region of the outlet of the sea pipeline at high SS concentrations. The following operations add or remove SS to the water-using system:

- *Fermentation*. The broth effluent is a high solids source comprised mainly of cellular residue, which is added during the fermentation process.
- *PIX backwash*. Cellular residue from the adsorption phase adds SS, to the backwash effluent.
- *Cooling tower*. Pick-up of atmospheric solids adds SS to the water system during evaporative cooling.
- *Tank cleaning*. General particle residue in tanks, such as cellular residue in the fermentation tanks, is added to the system during CIP.
- *Pump seals*. Although SS addition by the pump itself is marginal, SS pickup in the pump sumps is considerable due to exposure to the atmosphere.
- *UOS water supply*. The UOS water supply has a small quantity of SS, which is not removed during treatment.

3.5.1.3 Chloride

High chloride concentration causes corrosion problems in most operations. The cooling tower, and to a lesser extent, the pumps are especially sensitive to corrosion. Although this contaminant is not directly limited in effluent discharges to the sea, the conductivity must be below 2000mS/m. The cooling tower is the only operation that contributes to the chloride concentration in the system, by concentrating the UOS water makeup.

It was assumed that current operating concentration conditions at the inlet to each water-using operation was limiting. Three scenarios were investigated that look at potential for reducing cost by varying the concentration conditions of the AS condensate. In addition, the scope for reducing the cost associated with effluent discharge was investigated by relaxing the sea pipeline concentration constraint. Several operating scenarios were investigated, which explored the variability in the concentration of the AS evaporator condensate. In addition, the potential for relaxing environmental constraints was investigated. Several possible configurations for the water-using network were produced.

3.5.2 Elements of the Water-Using System and Model Assumptions

In order to carry out a water pinch analysis of a water-using system, only the elements that have a demand for water and a supply of associated wastewater need to be included. Hence, various process-related elements of the water-using system at Bioproducts can be omitted. This is demonstrated in figure 3.2, which interprets the simplified process representation in figure 3.1 as a water pinch supply and demand model. Most of the simplifications are straightforward: raw material, intermediate, and product streams that are required as part of the necessary processing stages (to produce the l-lysine product) are omitted, as they are a feature of the overall process and cannot change. Likewise, gaseous water streams such as process steam and cooling tower evaporation are not included in the model. Condensed process steam leaves the operations that require steam as condensate, which was included as a water supply. Additional miscellaneous simplifications were made, which are discussed in detail below.

3.5.2.1 PIX Strip

Two separate water sources were used to feed the PIX strip phase (figure 3.2 (d)): Condensate was used to dilute the ammonia solution; and freshwater at a different contaminant concentration was used to rinse the cells after stripping. For this reason, after omission of the process streams the PIX strip phase has been modelled as two water demands.

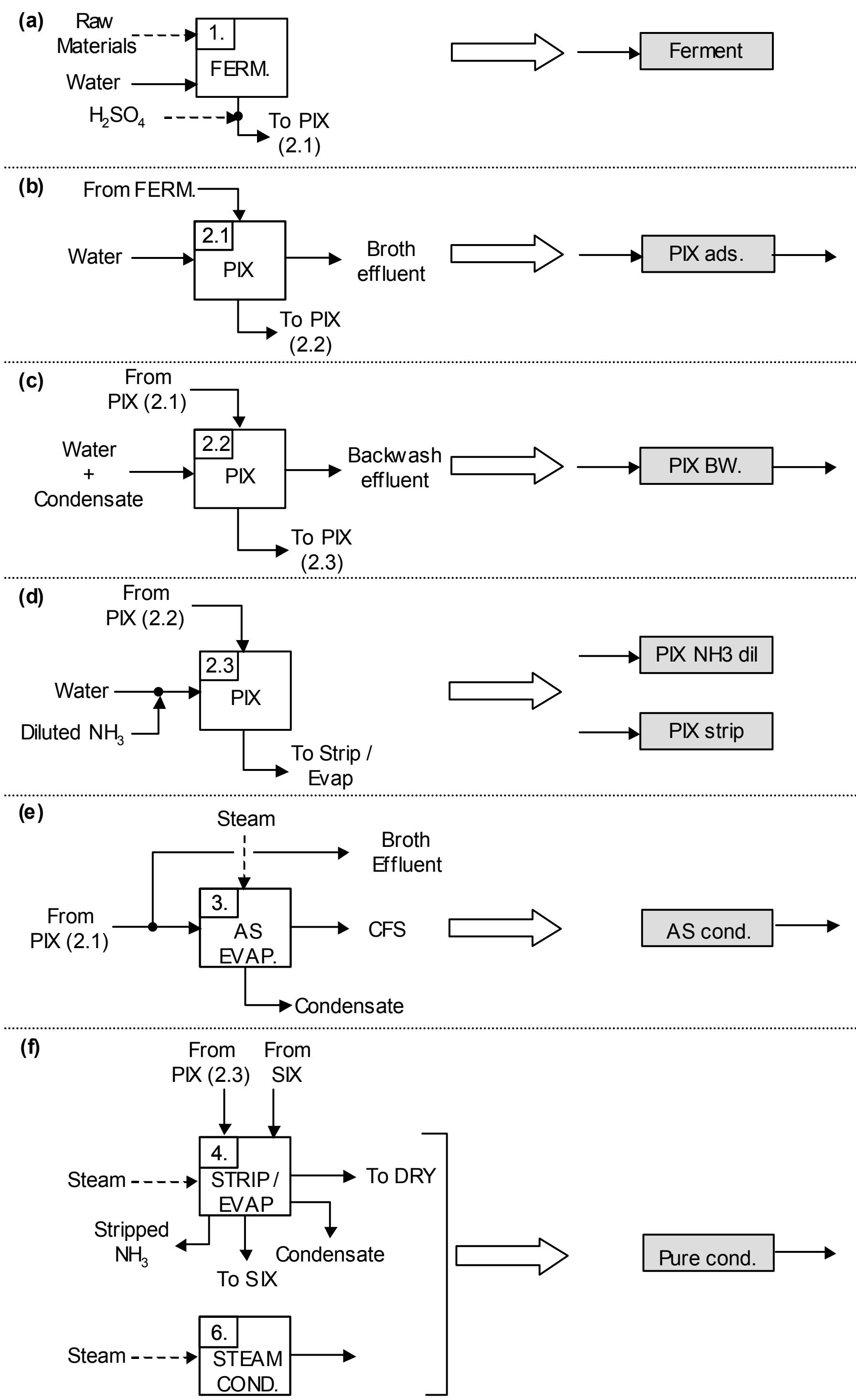

Figure 3.2
The set of water-using operations used for the pinch analysis model

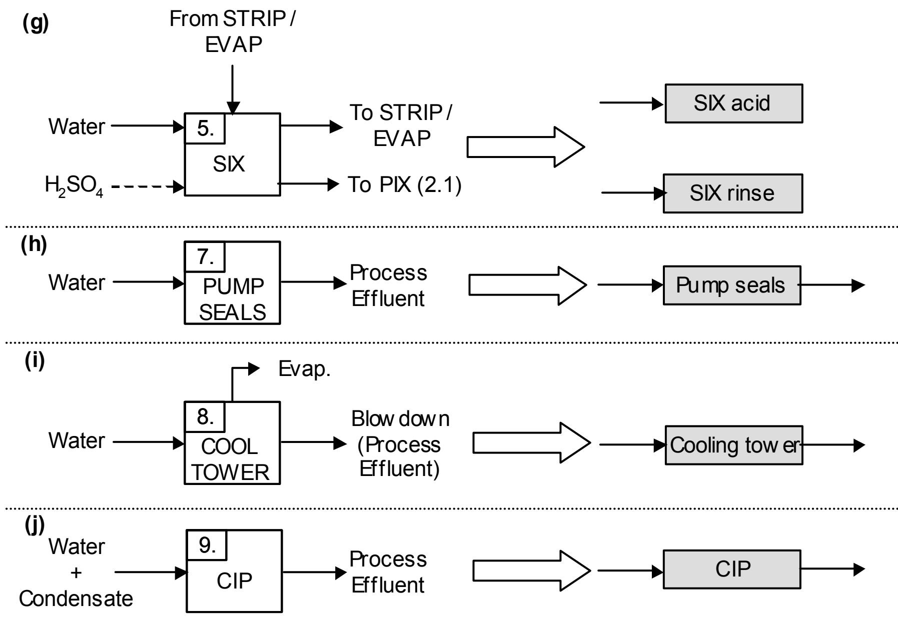

Figure 3.2 (cont.)
The set of water-using operations used for the pinch analysis model.

3.5.2.2 Evaporators and Condensate

In the analysis, all the pure condensate sources (figure 3.2 (f)) are treated as one source. This is reasonable, as they are of the same concentration, and are collected in the same tank (the condensate tank) on the plant.

3.5.2.3 SIX

As with the PIX strip phase, two water supplies at different contaminant concentration levels were used in the SIX operation (figure 3.2 (g)). Freshwater was used to dilute the sulphuric acid feed; and condensate was used to rinse the operation after each purification stage. For this reason, after omission of the process streams, the SIX operation is modelled as two water demands. In the case of the SIX-rinse outlet, only a fraction is available for reuse, as most is fed back into the adsorption cycle to recover residual l-lysine. This is a dilute stream that has a negligible effect on the configuration of the network and for this reason has been excluded from the analysis.

3.5.2.4 Clean In Place

The volumetric and concentration requirements for each individual tank cleaning are dependent on the tank dimensions and mass of contaminants present. It has been assumed that the concentration requirements for each individual tank are the same as for the collective tanks on the plant. This allows the CIP system (figure 3.2 (j)) to be treated as a single water-using operation, with a single demand and effluent supply. This is a valid simplification as, at a flowrate of approximately 6.38t/h, the demand from the CIP system is small compared to the demand of the entire system.

3.5.2.5 Pump Seals

As with the CIP system, the pump seals were treated as a single water-using operation, with a total demand of 6.50t/h .

3.5.3 Water Users

From figure 3.2, the water users considered in this study consist of:

- AS condensate;
- Fermentation;
- Cooling tower;
- Pump seals;
- PIX adsorption;
- PIX backwash;
- SIX acid dilution;
- PIX strip water;
- CIP;
- SIX rinse;
- Steam condensate (pure condensate producers grouped together);

The UOS dilution is included as a water source:

- UOS dilution.

One freshwater source was available from the UOS water pre-treatment facility. Two discharge points were available: the sea pipeline and the SWW. The sea pipeline was constrained to environmental limits, however, for the purpose of this investigation, the SWW did not impose any limiting constraints. A worst-case scenario was assumed, where the CFS product from the AS evaporator was not sold, but was combined with the broth effluent from the PIX adsorption stage.

The base-case water-using network configuration is available in figure 3.3. The flowrates that achieve this configuration are given in table 3.1.

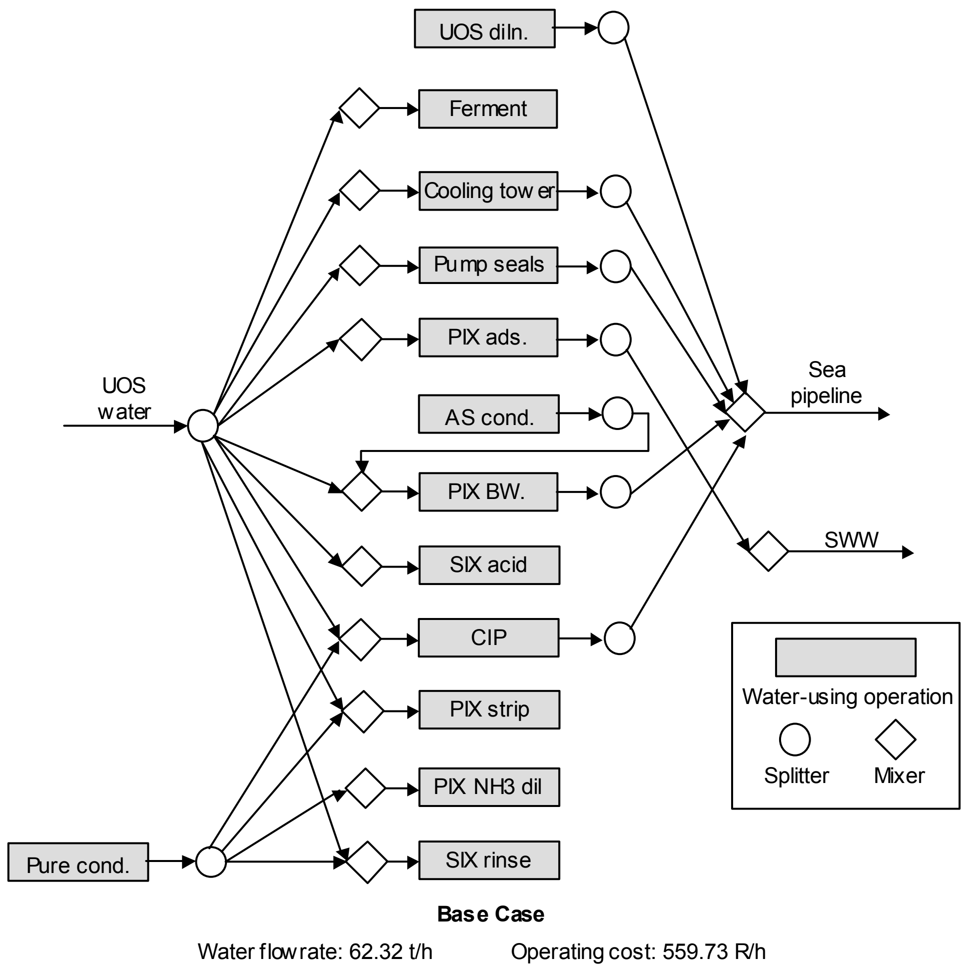

Figure 3.3
Base-case water-using subsystem configuration for the AECI Bioproducts system.

TABLE 3.1
Inter-operation flowrates for base-case configuration; flows in t/h.

From \ To	Ferment	CIP	Pump seals	Cooling tow er	PIX strip	PIX NH_3 dil.	PIX ads.	PIX b-w	SIX rinse	SIX acid	Sea pipeline	SWW
CIP											6.38	
Pump seals											6.50	
Cooling tow er											3.59	
Pure condensate		5.67			11.08	0.16			1.16			
UOS dilution											80.14	
PIX b-w											17.43	
PIX ads												24.97
AS cond.								6.40				
UOS w ater	3.99	0.71	6.50	29.76	1.35		14.44	4.05	0.14	1.38		

Existing flowrate (t/h)

No on-site treatment facilities exist; hence the problem becomes one of determining the configuration of the water-using subsystem. Three contaminants were included: FSA, SS and Cl. Equation 3.1 was used to relate the outlet conditions to the inlet concentration for each operation. The coefficients *A* and *B* are assumed constant for all operating scenarios investigated in section 3.6. The coefficient values for each operation that has a wastewater outlet are presented in table 3.2, below.

The contaminant concentration in the UOS freshwater source, pure condensate and UOS dilution were taken as constant, as were the flowrate from the pure condensate source and the UOS dilution. However, the freshwater flowrate was considered variable, (the upper and lower limits in equation 3.5 is unconstrained and zero respectively), as it is dependent on the configuration of the water-using system. Table 3.3 lists the flow and concentration characteristics of each of these sources.

TABLE 3.2
Mass loading relationships and flowrates for the water-using operations

Operation	Contaminant, *c*	*A* [-]	*B* [ppm]	F_i^{in} [t/h]	F_i^{out} [t/h]
Cooling Tower	SS	8.30	793.33	29.76	3.59
	FSA	8.30	0.00		
	Cl	8.31	0.00		
Pump Seals	SS	1.00	197.60	6.50	6.50
	FSA	1.00	0.00		
	Cl	1.00	0.00		
PIX adsorption	SS	0.00	350000	14.44	24.97
	FSA	0.00	35000		
	Cl	0.00	1000		
PIX backwash	SS	1.00	0.00	10.45	17.43
	FSA	0.60	240.05		
	Cl	1.00	0.00		
CIP	SS	1.00	7670.35	6.38	6.38
	FSA	1.00	0.00		
	Cl	1.00	0.00		

TABLE 3.3
Source flowrates and concentrations

Source	Flowrate [t/h]	Contaminant, c	C_c^{out} [ppm]
UOS freshwater	Variable	FSA	0.00
		SS	24.90
		Cl	80.63
Pure condensate	18.07	FSA	0.00
		SS	0.00
		Cl	0.00
UOS dilution	80.14	FSA	16.44
		SS	126.89
		Cl	80.63

The positions of the water-using operations are given in table 3.4. These were used to calculate the cost of new piping installations, if a new connection is identified.

TABLE 3.4
Approximate positions of the operations at AECI Bioproducts

Name	X position [m]	Y position [m]	Name	X position [m]	Y position [m]
Fermentation	20	35	Pump seals	0	5
PIX strip rinse	20	20	CIP	40	0
SIX acid dilution	30	15	PIX ads	20	20
SIX rinse	30	15	PIX b-w	20	20
PIX NH3 dil.	20	20	Cooling tower	5	90
UOS dilution	25	0	Sea outfall pipe	25	0
AS evap. condensate	40	25	SWW	30	10
Pure condensate	40	20	UOS water	0	10

New pipes were assumed to be constructed of stainless steel and a flow velocity of 1 m/s was assumed for the calculation of pipe diameter, for all connections. The cost coefficients used are given in table 3.5. The cost of using the SWW is based on the mass-flowrate of effluent (i.e. R/t of effluent). This contrasts with the sea pipeline: an annual license fee is charged by the water authorities for its use, which is can be translated to an hourly usage fee (i.e. R/h).

TABLE 3.5
Economic parameters

Freshwater cost, α_i	2.50 R/t
Discharge cost to SWW, a_i	16 R/t
Discharge to sea pipeline, b_i	4.41 R/h
Hourly cost per meter piping (based on 1" pipe diameter), X	4.78×10^{-3} R/(h·m)
Exponent for material of construction, n	0.9 (stainless steel)

Equation 3.11 was used to relate the hourly cost (in Rand) for piping and associated fixed costs for each new connection. For connections between freshwater sources j and water-using operations i:

$$C_{p\,j,i} = 4.78\times10^{-3}\cdot D_{j,i}^{0.9}\cdot L_{j,i} \qquad (3.13)$$

The length of piping, $L_{j,i}$ is calculated from the X,Y positions in table 3.4. Note that a similar set of equations can be generated for new piping costs for connections between water-using operations, treatment plants and discharge points. The total cost for new piping and associated fittings is the sum of the costs incurred for each new connection.

3.6 Water-Using System Model Analysis

The reuse potential of the AS evaporator condensate was investigated by presenting three scenarios, as follows

i. *Scenario A*. This scenario looks at the scope for reusing the AS condensate when the SS concentration is at a concentration of 1000ppm.

ii. *Scenario B.* The possibility of pure condensate is investigated in this scenario, where no contaminant is present.

iii. *Scenario C*. This scenario investigates the scope for saving when there is no reuse of AS condensate.

3.6.1 Scenario A

This scenario looks at the water-using system with the inlet constraints to the operations and discharge points set to the current operating concentration (table 3.9). A conservative approach to water reuse has been adopted, which is reflected in the table of prohibited inter-process flows (table 3.6). In this scenario, the AS condensate is at 1000ppm, which reflects a worst-case scenario for the concentration of this source (table 3.7) before reuse is prohibited on the plant (see section 3.2.8). The average conditions of the effluent discharged to the sea, taken for the month during which the study was made, violate the constraint for SS. Hence, the limit has been adjusted to reflect this (table 3.8).

TABLE 3.6
Matrix of existing capacities, and allowed and prohibited flows for Scenario A; flows in t/h.

From \ To	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH_3 dil.	PIX ads.	PIX b-w	SIX rinse	SIX acid	Sea pipeline	SWW
CIP	0		0	0	0	0	0	0	0	0	8.99	
Pump seals	0			0	0	0	0	0	0	0	8.99	
Cooling tower	0	0		0	0	0	0	0	0	0	5.22	
Pure condensate		20.44			20.44	20.44			20.44			
UOS dilution	0	0	0	0	0	0	0	0	0	0	95.84	0
PIX b-w	0	0	0	0	0	0	0		0	0	20.44	
PIX ads	0	0	0	0	0	0	0	0	0	0	0	28.30
AS cond.								8.99			8.99*	
UOS water	5.22	2.37	8.99	35.36	2.37	2.37	14.44	20.44	2.37	1.38		

[shaded box] Flow allowed
0 Flow prohibited

The general assumption was that effluent from operations where the concentration is unpredictable may not be reused as feed to sensitive operations (section 3.3), as additional unspecified contaminants may interfere with the normal operating conditions to produce an inferior product, or a failed batch. For this reason, the PIX adsorption and fermentation operations may only use pure water or condensate (UOS water or condensate). Use of condensate has been allowed in all operations. Reuse of CIP and pump seal effluent is limited to local recycling; reuse of the pump seal effluent has been allowed in the CIP process. Cooling tower blowdown has been deemed suitable for reuse in the pump seals only. UOS effluent dilution is constrained to the sea outfall pipe and may not be used anywhere else. Discharge of the broth effluent is constrained to the SWW, for off-site treatment, in accordance with the DWAF effluent agreement. Note that this constraint was later relaxed to determine the sensitivity of the configuration to relaxation of the environmental constraint for the sea pipeline.

TABLE 3.7
Conditions for the AS evaporator (Scenario A)

Operation	F_{out} [t/h]	Contaminant, c	$C_{c,i}^{out}$ [ppm]
AS condensate	6.40	FSA	0.00
		SS	1000
		Cl	0.00

The FSA concentration was assumed to be zero (table 3.7) for this scenario; however small quantities of this contaminant may have been present, but the concentration was not measured. The chloride concentration was negligible in this source, and was assumed to be zero.

TABLE 3.8
Sea pipeline discharge constraints for Scenario A

Discharge point	Contaminant, c	$C_{c,i}^{in,MAX}$ [ppm]	$M_{c,i}^{in,MAX}$ [g/h]
Sea pipeline	FSA	300	-
	SS	-	74984.29
	Cl	Unconstrained	-

The SS in the sea pipeline was limited by a mass-load constraint, rather than a concentration constraint, in order to prevent dilution of the effluent with purer sources. This mass-load constraint represents a concentration of 665.52ppm in the sea pipeline, which violated the environmental constraint of 400ppm, but reflected the average discharge conditions during the period of the investigation.

In this scenario, current operating conditions determine the maximum inlet concentration constraints for each operation (equation 3.2). The maximum outlet concentration is calculated using equation 3.1, by setting:

$$C_{c,i}^{in} = C_{c,i}^{in,MAX} \tag{3.14}$$

The chloride concentration in the broth effluent from the PIX adsorption stage is assumed to be at the same level as the freshwater chloride concentration.

TABLE 3.9
Inlet and outlet flowrate and maximum inlet and outlet concentration constraints for Scenario A

Operation	F_i^{in} [t/h]	F_i^{out} [t/h]	Contaminant, c	$C_{c,i}^{in,MAX}$ [ppm]	$C_{c,i}^{out,MAX}$ [ppm]
Cooling Tower	29.76	3.59	FSA	0.00*	0.00*
			SS	24.90	1000.00
			Cl	80.63	670.04
Pump Seals	6.50	6.50	FSA	0.00*	0.00*
			SS	24.90	222.50
			Cl	80.63	80.63
PIX adsorption	14.44	24.97	FSA	3990.00	35000
			SS	24.90	350000
			Cl	80.63	80.63
PIX backwash	10.45	17.43	FSA	100.00	300.05
			SS	625.00	625.00
			Cl	80.63	80.63
SIX rinse	1.30	Negligible (Flow out < 0.02)	FSA	0.00*	N/A
			SS	24.90	
			Cl	80.63	
CIP	6.38	6.38	FSA	0.00*	0.00*
			SS	24.90	7720.15
			Cl	80.63	80.63
PIX NH_3 dilution	0.16	Process stream	FSA	0.00*	N/A
			SS	24.90	
			Cl	80.63	
SIX acid dilution	1.38	Process stream	FSA	0.00*	N/A
			SS	1.38	
			Cl	80.63	
Fermentation	3.99	Process stream	FSA	0.00*	N/A
			SS	24.90	
			Cl	80.63	
PIX strip rinse	12.43	Process stream	FSA	0.00*	N/A
			SS	24.90	
			Cl	80.63	

* Zero contaminant concentration levels were used to approximate negligible amounts of contaminant present in sources, which is reflected as an inlet constraint and outlet value when negligible contaminant loading takes place.

The WaterPinch software was used to carry out the optimisation subject to the specified constraints. The configuration of the resulting water-using system determined by the software is shown in figure 3.4.

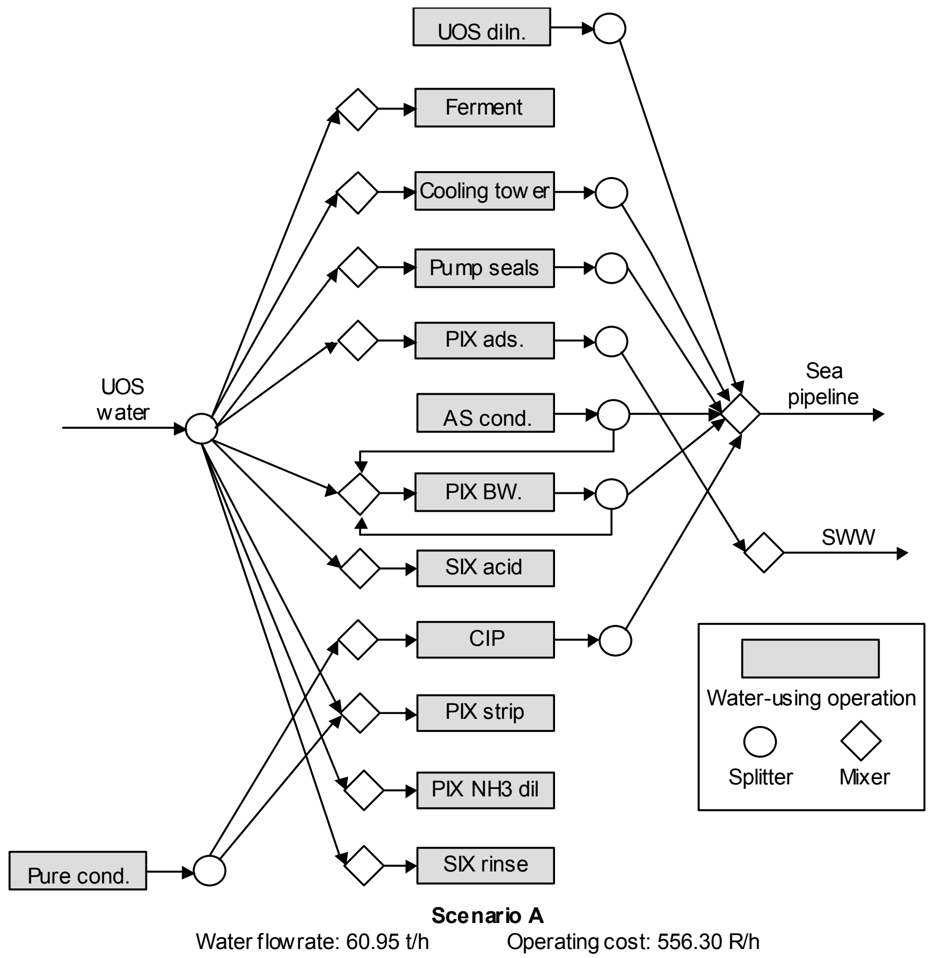

Figure 3.4
Configuration of the water-using network for Scenario A.

The flowrates for the above configuration are presented in table 3.10. The configuration does not differ substantially from the existing configuration (figure 3.3). The reuse of AS condensate is reduced, some of which is discharged to the sea pipeline. The major feature of this configuration is the recycle of the PIX backwash: about one fifth of the PIX backwash effluent is identified as suitable for recycle. This decreases the freshwater demand by 1.37t/h in this operation, leading to a decrease in the water-using system operating cost of 0.61% or R 29635 per annum (with 360 operating days). No extra piping capital costs are incurred as existing connections are utilised in this configuration and the flow capacities are not exceeded.

TABLE 3.10
Matrix of inter-operation flows for the configuration of the Scenario A water system; flows in t/h.

To / From	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH_3 dil.	PIX ads.	PIX b-w	SIX rinse	SIX acid	Sea pipeline	SWW
CIP											6.38	
Pump seals											6.50	
Cooling tower											3.59	
Pure condensate		6.38			11.53	0.16						
UOS dilution											80.14	
PIX b-w								3.48			16.43	
PIX ads												24.97
AS cond.								4.29			2.11	
UOS water	3.99		6.50	29.76	0.90		14.44	2.68	1.30	1.38		

Existing connection (shaded)

3.6.1.1 Initial Sensitivity Analysis

The limiting concentration constraint for this scenario was calculated using the WaterPinch *sensitivity analysis* feature, and was determined to be at the PIX backwash for FSA and SS and the sea pipeline for SS (figure 3.5 (a)). The potential for further relaxation of the SS constraint to the PIX backwash (as well as other constraints) is explored in section 3.7. Reducing the outlet concentration of SS from the AS evaporator provides the greatest potential for saving by regeneration of this stream.

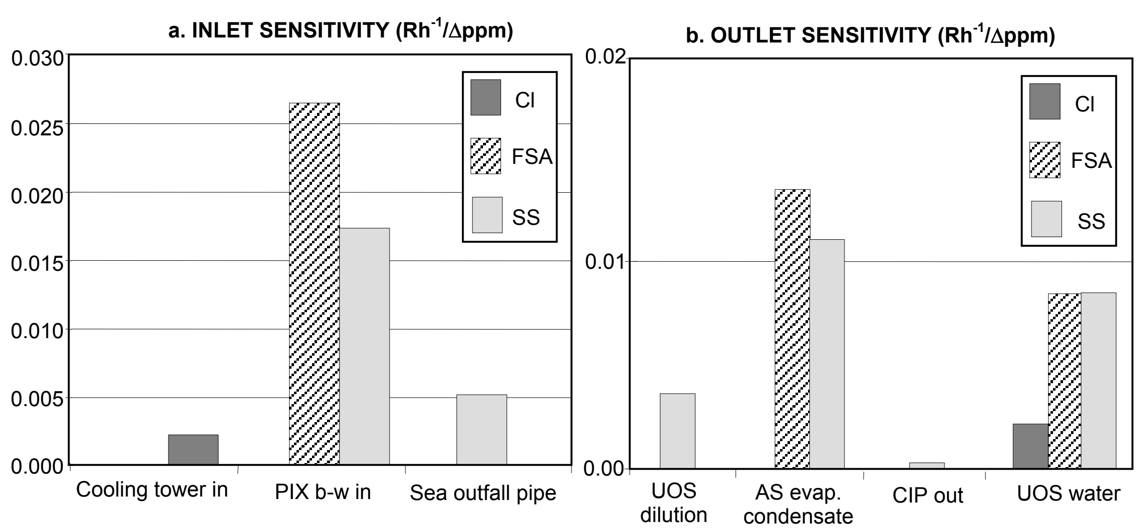

Figure 3.5
Inlet (a) and outlet (b) sensitivity values for Scenario A.

3.6.2 Scenario B

The system configuration was investigated for the case where the AS condensate is pure (table 3.11), i.e. no contamination of the condensate from the process stream occurs. Mass-loading characteristics (table 3.2) for the operations and inlet concentration constraints (table 3.9) remain the same as for Scenario A.

TABLE 3.11
Conditions for the AS evaporator (Scenario B)

Operation	F_{out} [t/h]	Contaminant, c	$C_{c,i}^{out}$ [ppm]
AS condensate	6.40	FSA	0.00
		SS	0.00
		Cl	0.00

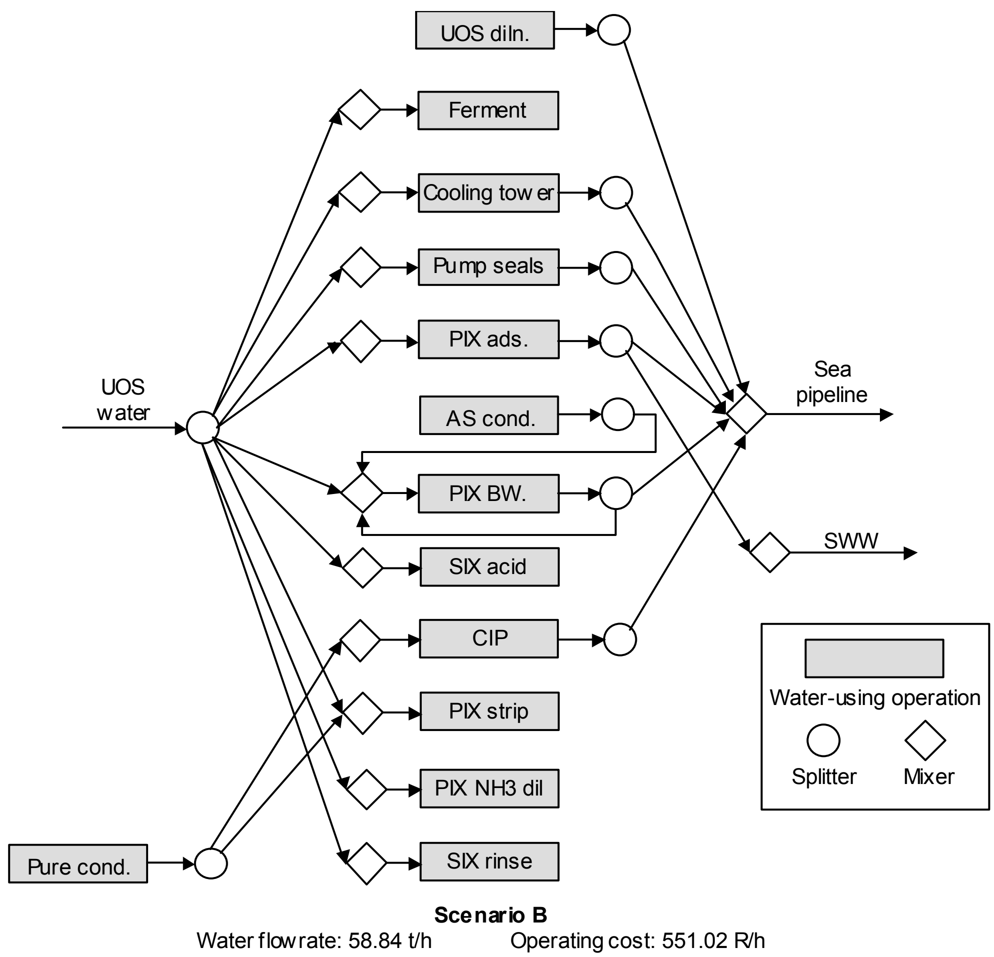

Figure 3.6
Scenario B: Configuration of the water-using system with pure AS evaporator condensate.

The network configuration generated by the WaterPinch software is presented in figure 3.6. The major feature of this configuration is the complete reuse of the AS condensate in the PIX backwash process. This reduces the freshwater demand to 58.84t/h, which is a total water-using system operating cost saving of 1.56% or R 75443 per annum.

The matrix of inter-operation flowrates is given in table E.7, Appendix E.

3.6.2.1 Initial Sensitivity Analysis

The limiting inlet constraint for this scenario was determined to be at the PIX backwash for FSA and the sea pipeline for SS (figure 3.7 (a)). The reported initial sensitivity of the objective cost to changing outlet concentrations is negligible for this scenario (figure 3.7 (b)).

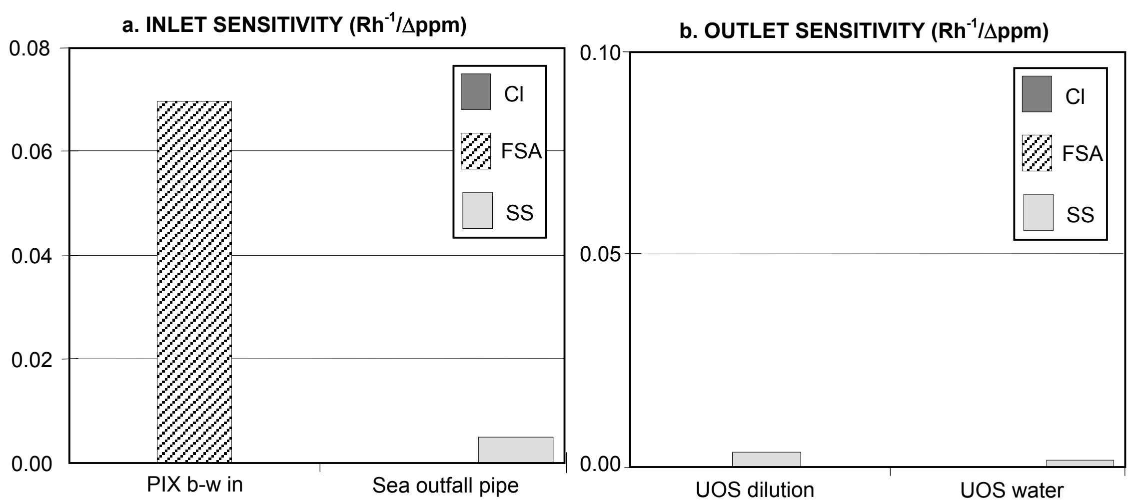

Figure 3.7
Inlet (a) and outlet (b) sensitivity values for Scenario B.

3.6.3 Scenario C

This scenario investigates the scope for saving when reuse of the AS condensate is prohibited, with the use of an additional constraint imposed upon the structure. Concentration constraints are identical to the settings for Scenario A (table 3.9). The structural constraints are similar (table 3.6), except that reuse of AS evaporator condensate is prohibited in all operations and may be discharged via the sea pipeline or to the SWW only. The configuration of the water-using network that satisfies these constraints is shown in figure 3.8 below.

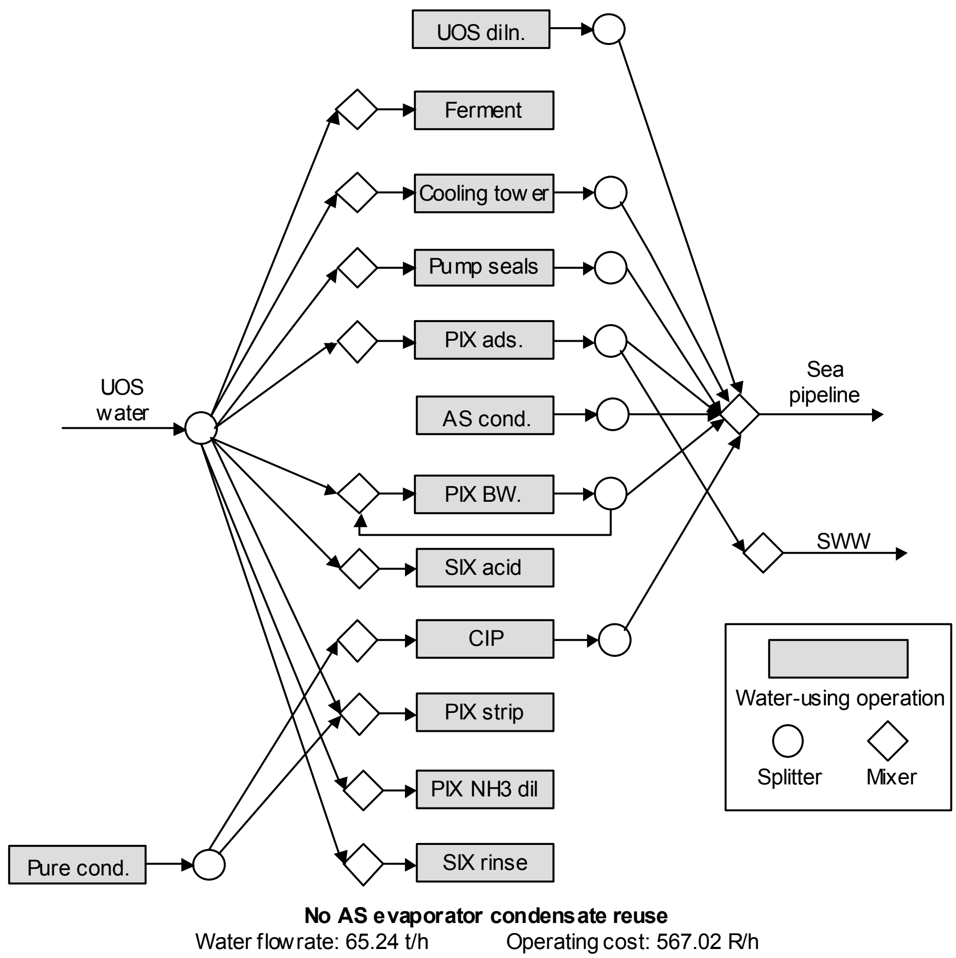

Figure 3.8
Scenario C: Configuration of the water-using system with the AS evaporator condensate reuse prohibited.

The configuration change of preventing the reuse of AS condensate results in an increase of freshwater supply to the PIX backwash, which in turn results in the increase in the water-using system operating cost, when compared with the base-case, to 567.02R/h.

3.6.3.1 Initial Sensitivity Analysis

The limiting inlet constraint for this scenario was determined to be identical to those reported for Scenario B. The reported initial sensitivity of the objective cost to changing outlet concentrations is negligible for this scenario, as for Scenario B. The sensitivity of the objective cost to the SS concentration in AS evaporator condensate is zero as a result of the structural constraint that limits its reuse elsewhere.

3.7 Model Sensitivity

The sensitivity of the solution was tested in order to determine the robustness of the network configuration, as well the scope for further saving when inlet constraints were relaxed or outlet conditions were changed. This was investigated by determining the response of the objective cost, flowrates, and contaminant concentrations to changing the following:

i. Freshwater cost parameter;

ii. PIX backwash SS inlet concentration constraint;

iii. Sea pipeline inlet mass-flowrate constraint for SS and FSA concentration constraint;

iv. AS evaporator outlet SS concentration level.

The concentration parameters that were investigated are the highest initial sensitivity values from Scenario A, reported in figure 3.5. The Scenario A model was used for part i., ii., and iii. of the investigation. The WaterPinch software was used to calculate the response of the objective function to changing the abovementioned cost, flowrate, and concentration conditions.

3.7.1 Freshwater

The sensitivity of the objective cost to changes in freshwater cost was explored first. In figure 3.9, a plot of the total objective cost (in R/h) as a function of the freshwater supply (in R/t), is presented.

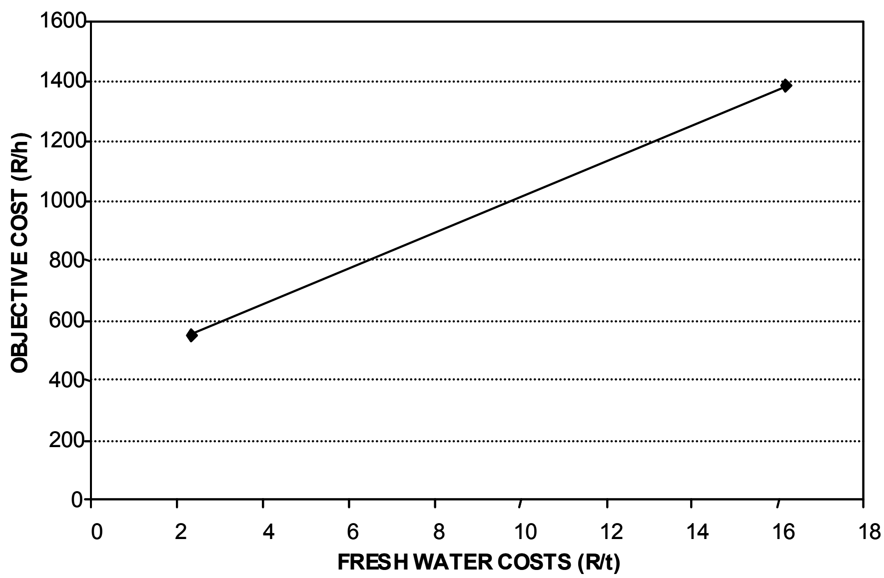

Figure 3.9
Sensitivity of the objective cost to freshwater costs.

From the plot it can be seen that there is a linear relationship between the cost of the freshwater and the total cost of the network. This implies that the structure of the network remains unchanged with a more expensive water source. This was investigated in figure 3.10, which describes freshwater flow demand as a function of its cost. It can be seen that the flow demand remained constant for increasing freshwater cost.

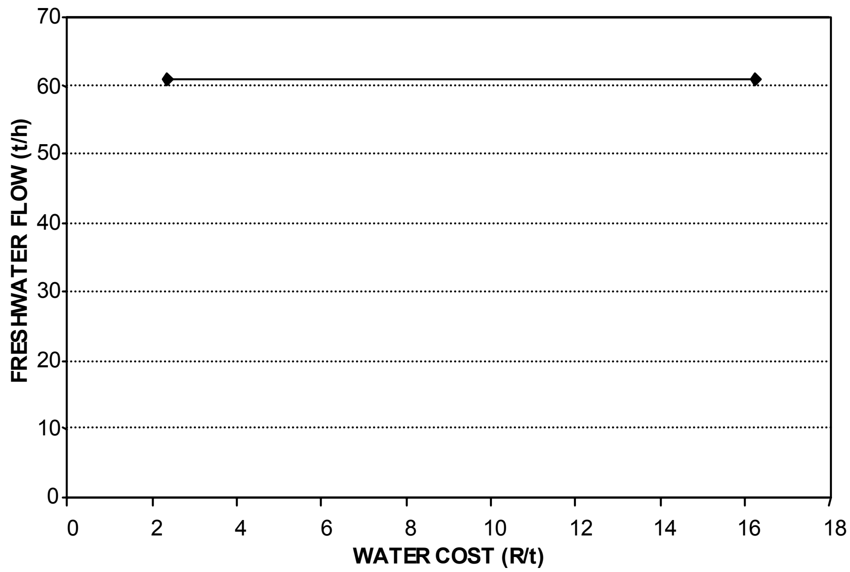

Figure 3.10
Sensitivity of the freshwater flowrate to freshwater costs.

3.7.2 Inlet Constraints

The sensitivity of the solution to changing the concentration constraint for the PIX backwash and sea pipeline were tested by relaxing the inlet constraint for SS, for the PIX backwash, and SS and FSA for the sea pipeline. The sensitivity of the objective cost to changing the inlet constraint for chlorides was found to be negligible for all operations.

3.7.2.1 PIX Backwash Sensitivity

In figure 3.11, a plot of the objective cost as a function of the change in the inlet SS concentration constraint to the PIX backwash operation, is presented. By relaxing the inlet constraint to the PIX backwash, the amount of AS condensate (at a SS concentration of 1000ppm) reused in this process may be increased, while simultaneously maintaining a backwash recycle flowrate of 3.48t/h. This resulted in an increase in the concentration of the effluent, as the SS mass flowrate in the sea pipeline increased with increasing rates of AS condensate reuse. This occurred at an inlet SS concentration constraint greater than 630ppm. Consequently, a fraction of the effluent from the CIP process must be diverted to the SWW, as the process effluent concentration reached the SS constraint in the sea pipeline at this point.

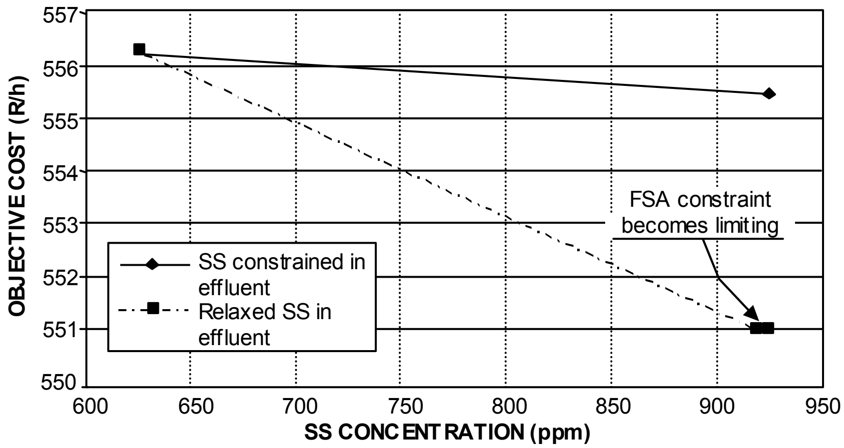

Figure 3.11
Sensitivity of the objective cost to relaxation of the inlet SS constraint to the PIX backwash.

The plot with the steeper negative gradient in figure 3.11 illustrates the effect of relaxing the SS constraint to the sea pipeline, which resulted in a greater potential saving as all process effluent (but not the broth effluent) may be discharged via this point. It can be seen that the objective cost decreases linearly with an increasing SS concentration constraint in the PIX backwash. At a SS concentration of 925ppm, FSA became limiting in the inlet to this process and further relaxation of the SS constraint beyond this point, did not result in a decrease in the objective cost. Note that at this stage, a structural constraint (table 3.6) prevented PIX adsorption effluent (broth effluent) from entering the sea pipeline.

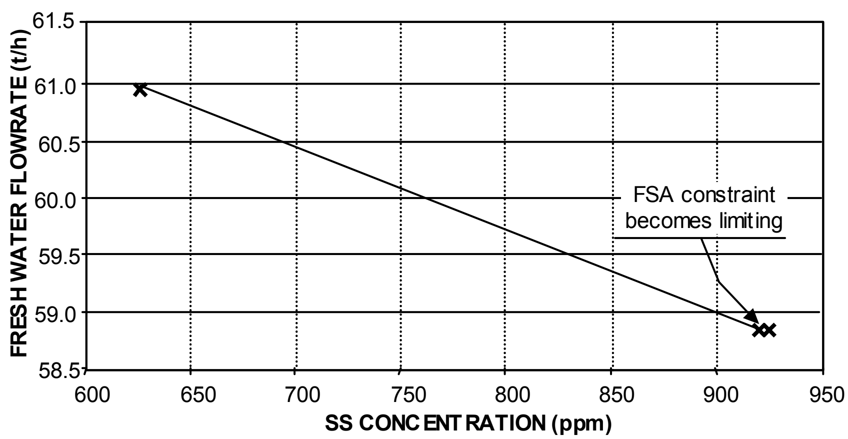

Figure 3.12
Overall freshwater flowrate as a function of SS inlet concentration constraint to the PIX backwash.

It may be inferred that there will be a linear decrease in overall freshwater flowrate with the relaxation of the SS concentration constraint to the PIX backwash. This is explored in figure 3.12, which describes freshwater flow demand as a function of the inlet SS concentration constraint. It can be seen that there is a linear decrease in overall freshwater demand until a SS concentration of 925ppm, where the FSA constraint became limiting.

3.7.2.2 Sea Pipeline Sensitivity

The sensitivity of the solution to changing the SS and FSA constraint in the sea pipeline was explored by relaxation of the SS mass-flow constraint, until the FSA concentration became limiting and thereafter, the sensitivity of the objective cost to changing the FSA concentration constraint was explored with SS unconstrained. The structural constraint preventing discharge of broth effluent was removed at this stage to allow for flow of this effluent source to this discharge point.

Figure 3.13 shows a linear decrease of the objective cost as a function of SS mass-flowrate in the sea pipeline. This trend continues until the FSA concentration constraint became limiting at 300ppm and the mass flowrate of suspended solids is approximately 360.6kg/h. Figure 3.14 shows a linear increase in FSA with relaxation of the SS mass flowrate.

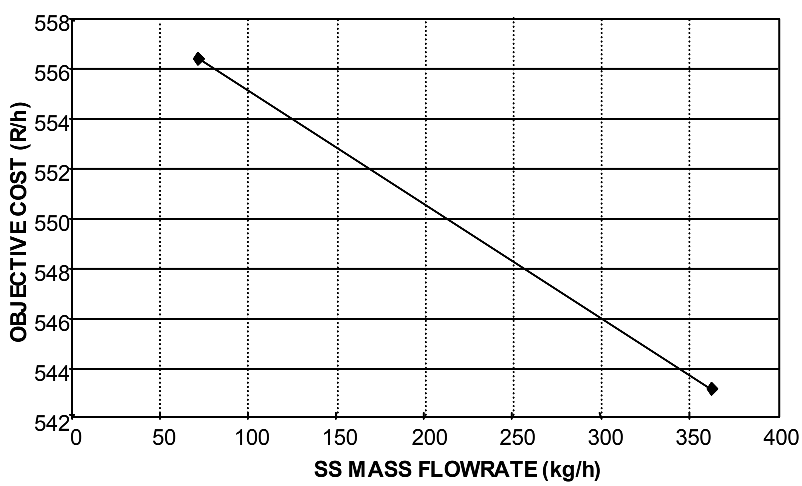

Figure 3.13
Objective cost sensitivity to SS concentration in the sea pipeline.

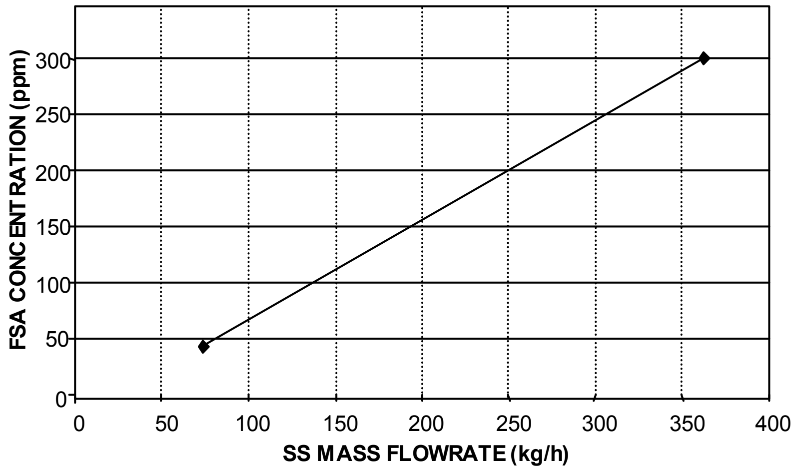

Figure 3.14
FSA concentration in the sea pipeline as a function SS mass-flowrate.

At the point at which FSA became limiting, at a FSA concentration of 300ppm, the FSA concentration constraint was relaxed to determine the sensitivity of the objective cost to FSA concentration. The objective cost was plotted as a function of FSA concentration in figure 3.15. Initially, in can be seen that the objective cost decreases linearly with an increasing FSA concentration constraint. However, after a concentration of 5000ppm was reached in the sea pipeline, the rate of cost decrease increases slightly. The reason for this became clear when the SS mass flowrate was plotted as a function of FSA concentration in figure 3.16. After a concentration of 5000ppm was reached, the SS mass flowrate increased at a higher rate than the FSA. Thus the volume discharged to the sea pipeline increased at this FSA concentration constraint in order to accommodate a higher flow of broth effluent and the flowrate of freshwater increased in order to dilute the effluent.

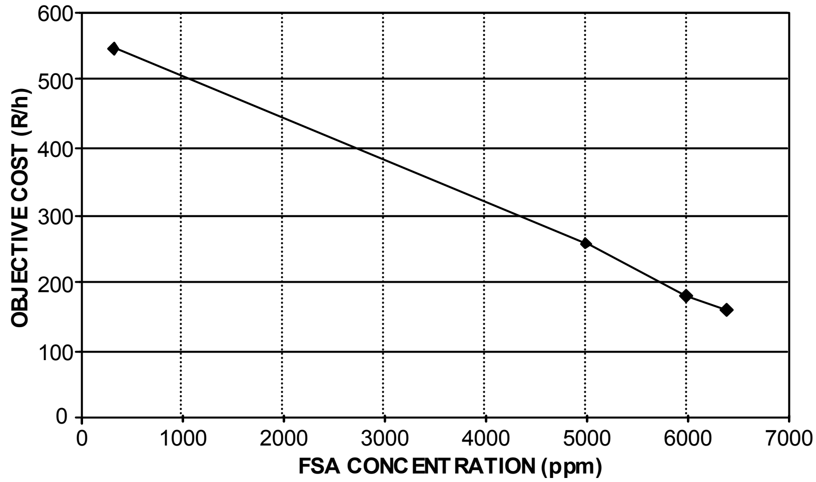

Figure 3.15
Objective cost sensitivity to FSA concentration in the sea pipeline.

The sensitivity of the configuration to increasing the FSA concentration constraint in the sea pipeline was explored in figure 3.17, which shows the plot of sea pipeline effluent flowrate and freshwater flowrate as a function of FSA concentration. The flowrate of effluent discharged to the sea pipeline increased above the rate predicted by a linear relationship. The freshwater flowrate increased from 60.95t/h to 67.26t/h in order to produce a more dilute effluent. This flowrate was maintained until the concentration of FSA in the sea pipeline rose above 6000ppm. At this point the freshwater flowrate dropped to 62.32t/h.

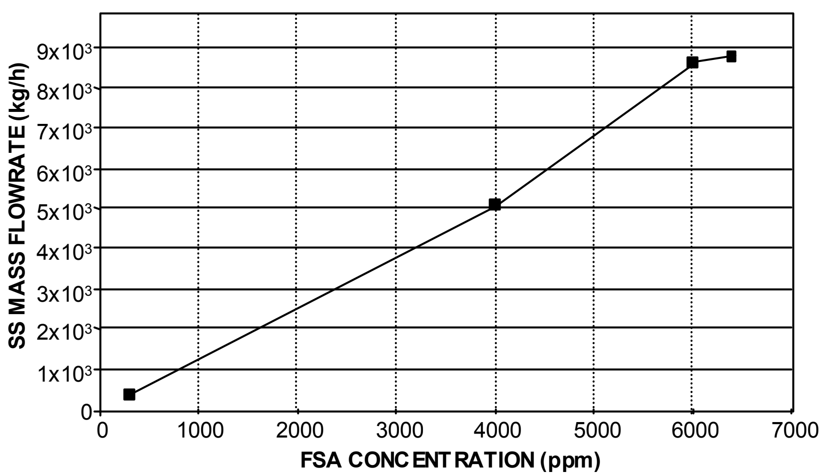

Figure 3.16
SS mass-flowrate as a function of the FSA constraint in the sea pipeline.

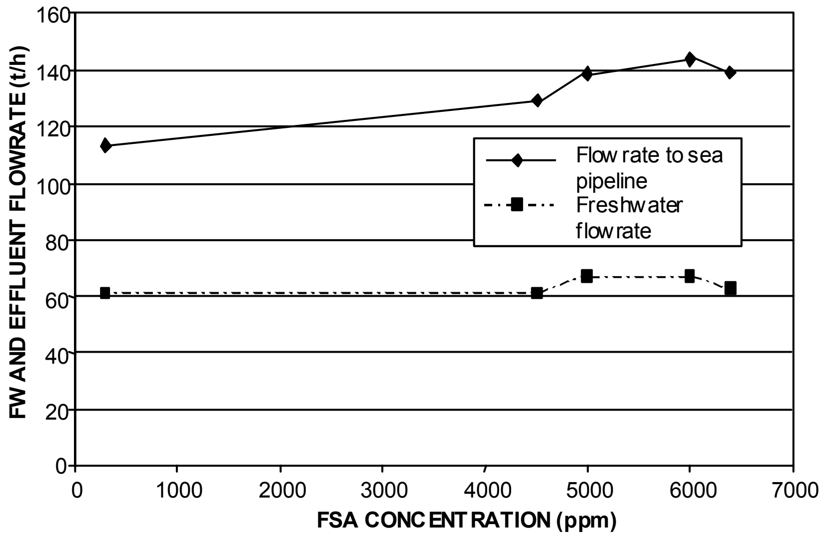

Figure 3.17
Sensitivity of the design to FSA concentration in the sea pipeline (in terms of freshwater and effluent flowrate).

The configuration of the water-using system with the FSA concentration constraint set to 5000ppm in the sea pipeline and SS unconstrained is shown in figure 3.18. The matrix of flows that satisfy this configuration is given in table E.9, Appendix E.

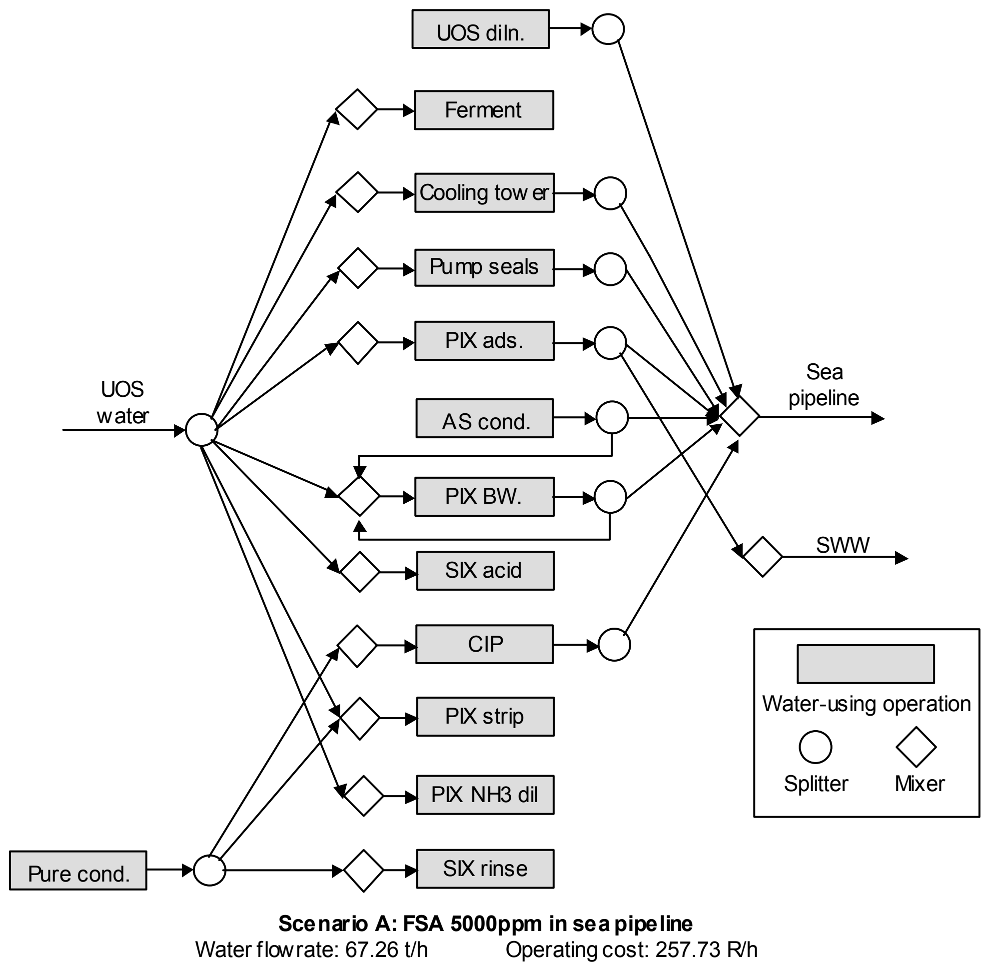

Figure 3.18
Scenario A: Configuration of the water-using system with the FSA concentration constraint in the sea pipeline relaxed to 5000ppm and SS unconstrained.

The significant configuration change identified in this case is the discharge of broth effluent to the sea pipeline. The increase in freshwater demand is due to flowrate changes in the following areas:

i. *PIX backwash*. A decrease in both the AS condensate reuse from 4.29t/h to 0.46t/h and backwash recycle from 3.48t/h to 1.00t/h resulted in an increase of 6.31t/h in the freshwater feed to this operation.

ii. *PIX NH3 dilution*. Use of 0.16t/h freshwater in the PIX NH3 dilution operation in place of condensate.

3.7.3 AS Condensate Sensitivity

The sensitivity of the configuration and the objective cost to the SS concentration in the AS evaporator condensate was investigated by determining the objective cost and reuse flowrate (in the PIX backwash) subject to increasing AS evaporator condensate SS concentration.

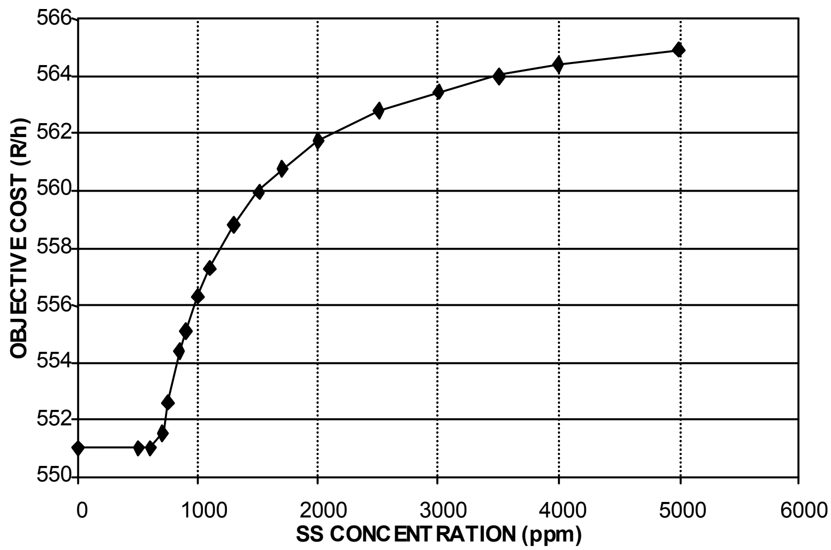

Figure 3.19
Sensitivity of the objective cost to AS evaporator condensate SS concentration.

In figure 3.19, the objective cost is initially constant at 551.02R/h as the AS evaporator condensate is completely reused in the PIX backwash process. At a concentration of approximately 700ppm, the objective cost increases sharply at first with reduced AS condensate reuse, but begins to level-off as the SS concentration increases above 1500ppm. The asymptotic magnitude of the objective cost with no AS reuse was identified as 567.02R/h. This represents the worst-case operating scenario for the AS evaporator, which was presented in Scenario C.

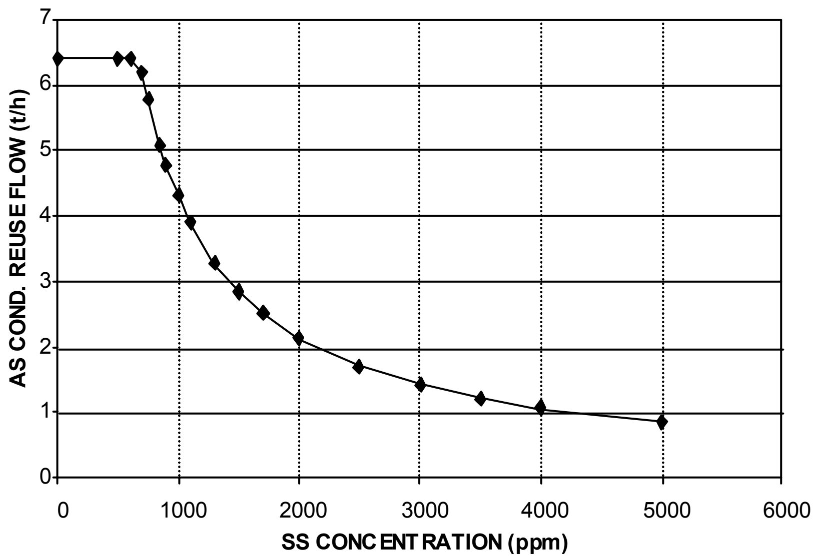

Figure 3.20
Sensitivity of reuse flowrate to AS evaporator condensate SS concentration.

The condensate reuse flowrate is plotted as a function of SS concentration in figure 3.20. At relatively low SS levels (below 2000ppm) this plot gives an indication of the scope for reuse of this source. Although not measured, at higher SS concentrations, a significant level of FSA contamination would be present.

3.8 References

1. T. Hsiao, C.E. Glatz, *Water Reuse in the L-Lysine Fermentation Process.* Biotechnology and Bioengineering, 1996. **49**(3): p. 341-347.

2. Alva-Argaez, A., *Integrated Design of Water Systems*, in *Process Integration*. 1999, Manchester Institute of Science and Technology: Manchester.

3. Linnhoff-March, *WaterTarget*, . 1999, Linnhoff March Ltd.

4. Y.P. Wang, R.Smith, *Wastewater Minimisation.* Chemical Engineering Science, 1994. **49**: p. 981-1006.

5. Y.P. Wang, R. Smith, *Design of Distributed Effluent Treatment Systems.* Chem. Eng. Sci., 1994. **49**(18): p. 3127-3145.

6. A. Alva-Argaez, A.C.Kokossis, R. Smith. *Process Integration Technology for Wastewater Treatment Systems*. in *AIChE Annual General Meeting*. 1998. Miami Beach, Florida: AIChE.

7. M.S. Peters, K.D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*. 4th ed. 1991, Singapore: McGraw-Hill.

Chapter 4: Discussion and Conclusion

4.1 Discussion

The scenarios investigated were compared with a base-case network design. Improvements to the base-case design are discussed below for each scenario. The implications of relaxation of the concentration constraints to the PIX backwash and the sea pipeline, as well as changes in the outlet SS concentration of the AS evaporator condensate, are discussed. Based on the results, suggestions have been made to improve operating conditions, which are in line with the aims of the investigation.

The configuration of the three scenarios is provided with the base-case design in figure 4.1 on page 4.3 for reference.

4.1.1 Scenario A

This scenario (see section 3.6.1, page 3.23) examined the case where the AS evaporator condensate at a SS concentration of 1000ppm, in which case reuse (to the PIX backwash inlet) is barely allowed. When compared with the base-case operating conditions, the improvements may be summarised as follows:

- An objective cost decrease of 3.43R/h or 0.61% was identified.
- This saving was incurred by a 1.37t/h reduction in freshwater flowrate (approximately 2.2% reduction) resulting from a recycle of water in the PIX backwash, with a recycle rate of 3.48t/h.

4.1.1.1 PIX Recycle

The solution for Scenario A identified the configuration change of the recycle of PIX backwash effluent back to the inlet (operation: PIX BW. figure 4.1, b). The AS condensate reuse in the PIX backwash was reduced; 4.29t/h was reused, as opposed to 6.40t/h in the base-case design, the remaining water demand being made-up by the combination of the PIX backwash recycle with freshwater. While this configuration change may seem counter-intuitive, using the total condensate source (at a concentration of 1000ppm) as feed to the PIX backwash prevents the backwash recycle, due to the comparatively high SS concentration in the condensate source. Consequently, more freshwater was used in the base-case model, which was required to dilute the AS condensate to meet the inlet concentration constraint for the PIX backwash operation. Amino acid contaminants, which are not considered in the model, will require removal in order to make it possible to recycle. The viability of this must be further investigated.

In addition, this design change may identify an improved operating practice, as the concentration and flowrate of the PIX backwash is more predictable than that of the AS evaporator condensate, thereby providing a reliable source for reuse or recycle.

4.1.2 Scenario B

This scenario (see section 3.6.2, page 3.29) examined the case where the AS evaporator condensate is pure, which reflects the best-case operating conditions for this unit operation. When compared with the base-case operating conditions, the improvements may be summarised as follows:

- An objective cost decrease of 8.71R/h or 1.56% was identified.
- The operating cost saving was incurred by a 3.48t/h reduction in freshwater flowrate (approximately 5.6% reduction) resulting from an increase in the degree of reuse / recycle of water in the following areas:
    a. PIX backwash recycle of 3.48t/h;
    b. Total AS evaporator condensate integration.

The cost reduction identified in this scenario, less the saving identified in Scenario A, reflects the upper limit for capital investment in process improvements – while sustaining an overall saving – that would lead to the AS evaporator condensate being of a suitable quality for total reuse. This amount is approximately 5.28R/h, or R 45619 per annum.

4.1.3 Scenario C

This scenario (see section 3.6.3, page 3.30) looked the case where there was no reuse of AS condensate (reuse was prevented by the inclusion of a structural constraint). This reflects a worst-case operating condition for the water-using network model, where the AS evaporator condensate is discharged directly to the sea pipeline (figure 4.1, d). An increase in cost of 1.30% was identified, when compared with the base-case operating conditions. However, when compared to operating conditions with no reuse of AS evaporator condensate, an improved network configuration was identified which lead to a saving of 1.54%. The improvement was made possible by the PIX backwash recycle, as in Scenario A and B.

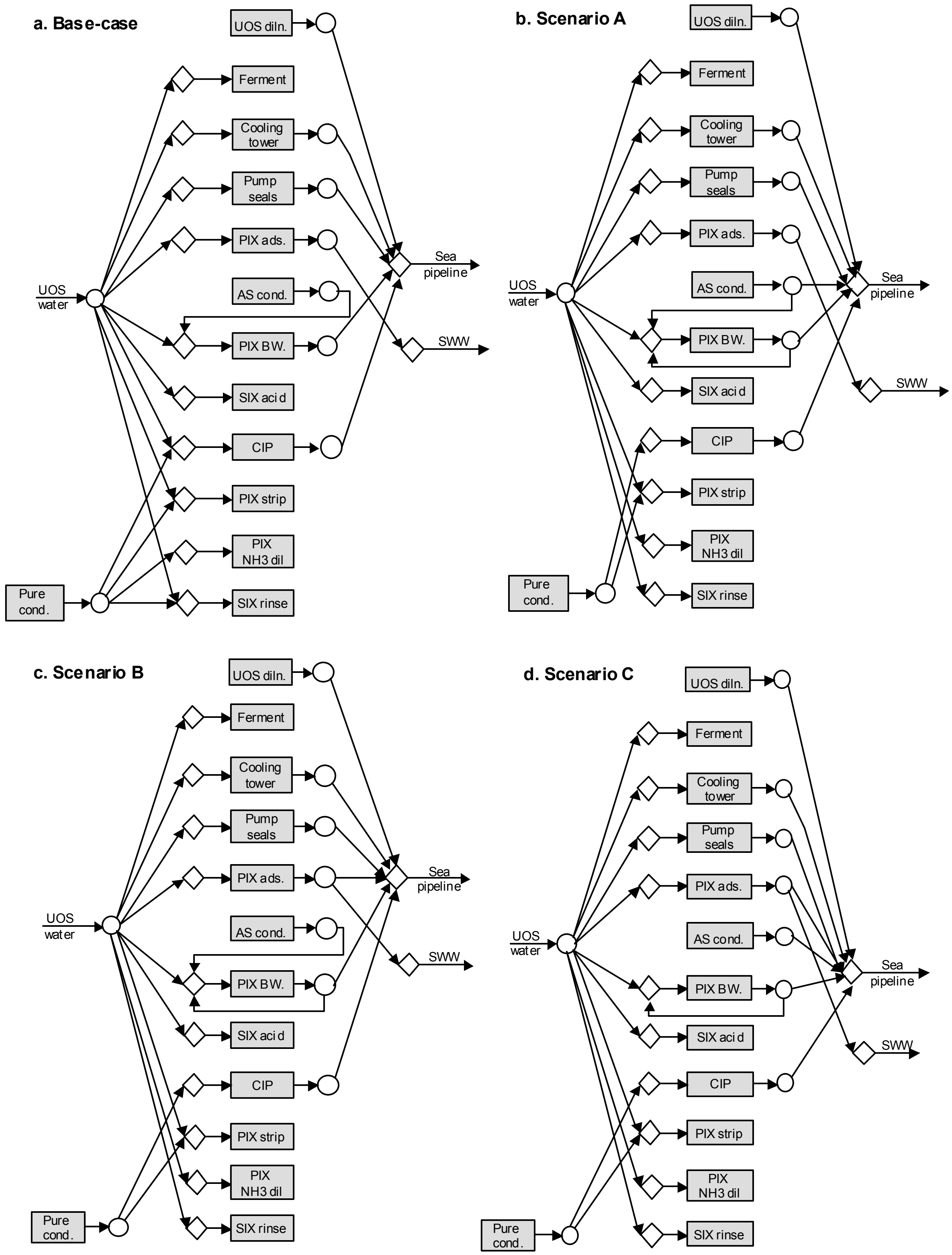

Figure 4.1
Water-using network configuration of the base-case with the three scenarios A, B, and C.

4.1.4 AS Evaporator Condensate Reuse

By testing the model under a range of AS evaporator condensate SS concentrations, the scope for reuse of this source was ascertained (section 3.7.3). As illustrated in figure 4.2 below, at concentrations below 700ppm, the AS condensate is of a suitable contaminant concentration for total reuse, without requiring freshwater dilution, hence the objective cost and freshwater flowrate are constant within this range. As the concentration increased, an inverse relationship between reuse flowrate and concentration was observed. The proportionality constant, *p*, was calculated by multiplying the flowrate values by the concentration values in this region. Above 2000ppm reuse has been prohibited due to the likely presence of FSA (this level has been assumed and would need to be further investigated). Hence the relationship between reuse flowrate and outlet concentration may be expressed as follows:

$$F_{AS\,cond,PIX\,bw} = \begin{cases} 6.40 & \text{if } C^{out}_{SS,AS\,cond} < 700\text{ppm} \\ p\cdot\left(C^{out}_{SS,AS\,cond}\right)^{-1} & \text{if } 700\text{ppm} \leq C^{out}_{SS,AS\,cond} < 2000\text{ppm} \\ 0 & \text{if } 2000\text{ppm} \leq C^{out}_{SS,AS\,cond} \end{cases} \qquad (4.1)$$

where p = 4284.00t/(h·ppm) ± 0.79% for outlet SS concentrations in the specified range. The deviation in *a* is a result of small fluctuations in the computation of the result, which is a characteristic of the software.

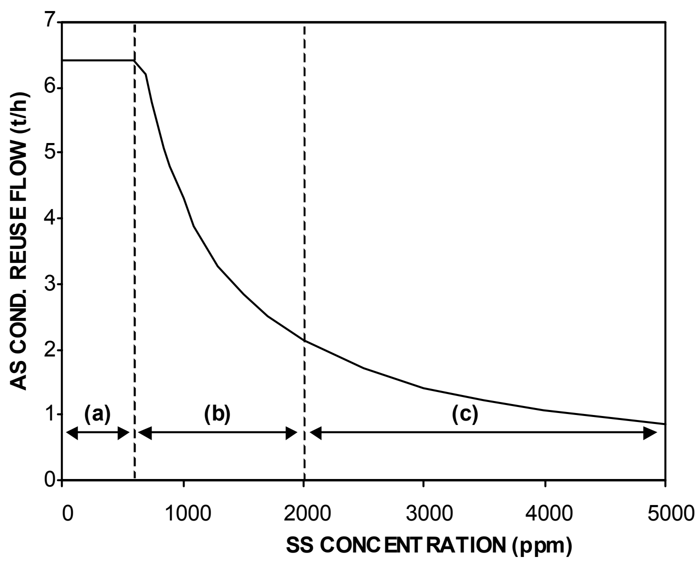

Figure 4.2
AS evaporator condensate reuse flowrate as a function of outlet concentration of SS. In the region $C^{out} < 700$ppm (a), complete reuse of the condensate is allowed. In the region 700ppm $\leq C^{out} < 2000$ppm (b) the reuse flowrate is governed by the inverse relationship of equation 4.1. For outlet concentrations greater than 2000ppm reuse is prevented due to the likely presence of FSA.

Equation 4.1 could be used as an improved control measure for the flowrate of the AS evaporator condensate to the PIX backwash. For the purposes of the investigation, the FSA concentration in the AS evaporator condensate was not measured. At the time of the investigation, the operating practice was to prevent all reuse of AS evaporator condensate at SS concentrations greater than 1000ppm.

4.1.5 Sea Pipeline Constraint

4.1.5.1 SS Mass-Flowrate Constraint

The potential for saving was investigated by relaxing the SS mass-flowrate constraint from its setting, at the time of the investigation, of 74.984×10^3g/h (which corresponds to a concentration of 665.52ppm) over a range. At the point at which the FSA concentration constraint became limiting (at a SS mass-flowrate of 360.42kg/h), the objective cost had decreased to 543.26R/h. This corresponds to a financial saving of 2.94% when compared with the base-case objective cost. No further freshwater savings were incurred (apart from those identified in Scenario A), as the additional financial saving was associated with a reduction in flowrate of broth effluent to the SWW.

4.1.5.2 FSA Constraint

At the point at which the FSA constraint became limiting, the SS constraint was removed and the FSA concentration constraint was relaxed over a range to determine the potential for further improvement. As before, a linear decrease in the objective cost was observed, until a FSA concentration constraint of approximately 4500ppm was reached. At this point the freshwater flowrate increased slightly to dilute the effluent and allow for an increase in the rate of discharge of broth effluent via the sea pipeline. This dilution was permitted in this case as the concentration constraint did not prevent an increase in effluent flowrate, as a result of dilution with freshwater. Although this occurred at a high concentration constraint it may be inferred from this result that concentration constraints can in some cases be counter-productive, i.e. operating conditions can be worsened instead of improved in attaining an economically efficient solution.

4.1.5.3 Unconstrained Sea Pipeline

The total potential for saving (i.e. when all the sea pipeline constraints are removed) was as follows:

- The objective cost decreased to 156.79R/h, which corresponds to a saving of 71.99%. This was mainly accomplished by discharge of all broth effluent via the sea pipeline, effectively making the SWW discharge point redundant.
- No further freshwater saving was identified (apart from those identified in Scenario A) with the removal of the sea pipeline constraints.

4.1.6 Overall Saving

The structure of the water-using network is robust for all outlet conditions of the AS evaporator condensate. As discussed above, the only alteration in the optimal configuration is the incorporation of the PIX backwash recycle. This remained at a flowrate of 3.48t/h for all scenarios investigated. However, varying the flowrate of the AS evaporator condensate to compensate for fluctuation in the level of impurities requires a process modification that will involve further capital investment.

The distribution of operating concentrations for the AS evaporator condensate is unknown, hence determining the average overall annual saving that would be accrued by implementing the discussed changes is indefinite. The saving identified in each scenario is illustrated by comparison with the base-case operating cost (figure 4.3).

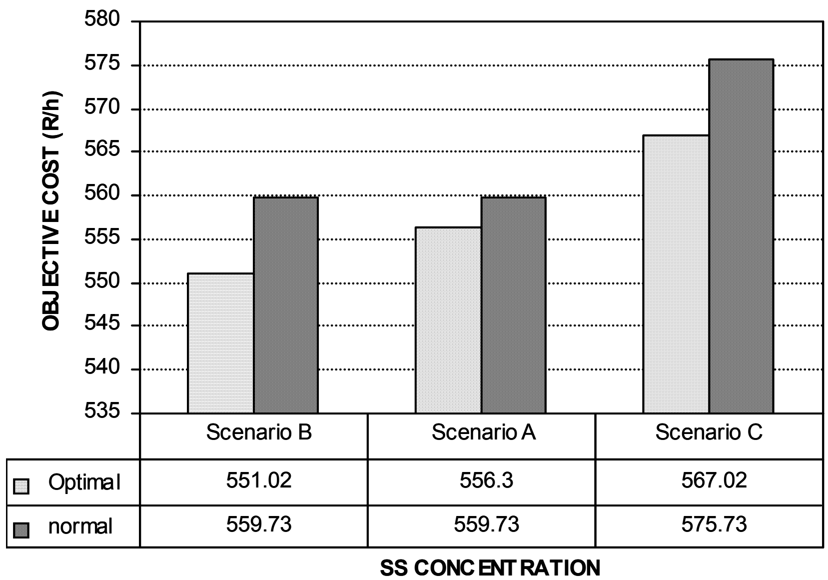

Figure 4.3
Comparison of the optimal design cost with the current water-using network operating cost.

Figure 4.3 shows that the optimal water-using network hourly operating cost lies between R 551.02 with complete integration of the AS evaporator condensate, and R 567.02 with no reuse. In terms of percentage saving, a minimum saving of 0.61% (Scenario A) and a maximum saving of 1.56% (Scenario B) is attainable, with no relaxation of the limiting concentration constraint. This saving corresponds to a minimum freshwater saving of 2.2% and a maximum saving of 5.6%.

4.1.7 Barriers to Saving

4.1.7.1 Obstacle to Process Integration

The Scenario A objective function was shown (in figure 3.5, section 3.6.1.1) to be most sensitive to changing the SS and FSA constraint at the inlet to the PIX backwash. Relaxation of the inlet constraint for SS resulted in an increase in reuse of contaminated AS evaporator condensate, thereby further reducing the overall freshwater demand. It was demonstrated (in figure 3.11) that a larger saving could be realized if the inlet SS constraint to the sea pipeline was relaxed, which allowed for all process effluent, with the exception of the broth effluent (a structural constraint prevented the broth effluent from entering the sea pipeline) to be discharged to this point. Hence, the analysis demonstrated that the SS concentration constraint at the sea pipeline was a barrier to economic saving, as well as improvement of operating conditions through increased process integration.

4.1.7.2 Broth Effluent Discharge Legislation

At the time of the investigation, legislation concerning the broth effluent prevented discharge of this effluent source via the sea pipeline. It was demonstrated that partial or complete relaxation of the sea pipeline constraint along with the removal of the structural constraint that forbids discharge of the broth effluent to the sea pipeline, resulted in the largest potential economic saving. The cost of discharging to the SWW amounts to 399.52R/h an amount which is 71.38% of the base-case water-using system operating cost, and between 97.87% (Scenario B operating conditions) and 99.15% (Scenario A operating conditions) of the total achievable saving. In order to effectively reduce overall water usage costs, this effluent source must be addressed. Some suggestions are as follows:

- Investigate feasibility of a broth effluent recycle as suggested by Hsiao *et al* [1]. This would require prior removal of the HTM ash contaminant.
- Implement a quantitative constraint for the sea pipeline that is in line with the impact of the broth effluent source, as opposed to the current practice of forbidding any discharge from this source via the sea pipeline. Discharging effluent at night, for example, may circumvent aesthetic issues, if dispersion in the sea is adequate.

4.1.8 Summary

From the investigation of the water-using system at Bioproducts, the improvements to the cost of operating the water-using network, and reductions in freshwater consumption, when compared to the base-case model, are summarised in table 4.1, below.

TABLE 4.1
Summary of economic and freshwater savings at Bioproducts.

Action	Cost saving		Freshwater saving	
	Amount / [R/h]	Percent / [%]	Amount / [t/h]	Percent / [%]
i. PIX backwash recycle.	3.41	0.61	1.37	2.20
ii. Discharge of Broth effluent to sea pipeline.	399.52	71.38	0.00	0.00
iii. AS condensate reuse (Scenario B).	5.26	0.94	2.11	3.39
Total	408.19	72.93	3.48	5.58

4.2 Conclusion

A robust optimal design was identified, with a recycle, which was consistent for all scenarios investigated. The limiting constraints that were an obstacle to further economical improvement were identified using the sensitivity analysis feature of the WaterPinch software and these initial values were investigated by relaxation of the limiting constraints. Further potential improvements to the water-using system were suggested based on the analysis. It was found that a small degree of saving could be obtained by process integration to the extent of a recycle of the PIX backwash and improved control measures governing the reuse of the AS condensate. The degree of reuse of the AS evaporator condensate was determined to be dependent on the concentration of the source and the nature of this dependency was determined over a range of concentrations. However, the major potential saving lay in the relaxation of the sea pipeline constraint and allowing for discharge of the broth effluent to this point.

4.2.1 Recent Developments

Recent developments at Bioproducts, implemented before the completion of this work, have seen a relaxation of the sea pipeline discharge constraint, permitted by the water authorities. This change was motivated, in part, by the results of this investigation, which highlighted the sea pipeline constraint, as well as the effluent exemption regarding the handling of the broth effluent, as being the major barriers to saving. This development is an affirmation of the capabilities of water pinch analysis as a means of negotiation between industrialists and water authorities to motivate – in this case – changes in environmental regulations and discharge permits, which have been identified as limiting further improvement.

4.2.2 Future Work

Water pinch analysis has proved to be an effective means of reducing costs associated with industrial water usage. Increasing pressure for industry to curb emissions will lead to the technique becoming an accepted means of designing water-using networks for both new installations and for retrofit projects, that are both economically efficient and environmentally compliant. This is in line with aims of the WDCS proposed by the DWAF, which is to "create financial incentives for dischargers to reduce waste and use water in a more optimal way" [2].

It has been demonstrated here that even in relatively simple networks with low capacity for additional saving, water pinch analysis can identify new options for improvement. However a considerable obstacle to the application of the technique remains to be the protracted data-gathering phase, where required flowrate and contaminant data is established. Old and inefficiently run installations that would potentially benefit the most from the technique rarely have, on-hand, sufficient data to carry out an analysis. Determining flowrate data is relatively uncomplicated when compared with determining concentration data, which often requires expensive and time-consuming laboratory analysis. Consequentially, the time taken to complete the data gathering exercise can render design results redundant, as operating practices may have changed during the data-gathering period.

Recent work [3] has concentrated on the aspect of determining the feasibility of implementing a water pinch investigation, with minimal data requirements. Future work in the application of the technique must strive to obtain results in a time-efficient manner.

Another obstacle to the application of the technique is the lack of quantitative data concerning the impact of industrial discharges on the environment. Environmental limits are often established by public opinion and aesthetics. Complementary research fields such as Life Cycle Analysis (LCA) will continue to play a vital role in determining the impact of industrial effluents and thereby provide quantitative constraint data for industrial discharges to the environment.

4.3 References

1. T. Hsiao, C.E. Glatz, *Water Reuse in the L-Lysine Fermentation Process.* Biotechnology and Bioengineering, 1996. **49**(3): p. 341-347.

2. Department of Water Affairs and Forestry, *Water Conservation Strategy for the Industry, Mining and Power Generation User Sector*, 2000.

3. G. Jodicke, U. Fischer, K. Hungerbuhler, *Wastewater Reuse: A New Approach to Screen for Designs with Minimal Total Costs.* Comp. Chem. Eng, 2000. **25**(2001): p. 203 - 215.

Appendix A: Nomenclature

A	Coefficient relating outlet concentration to inlet concentration [-].
a	Cost coefficient associated with flow through treatment plant [R/t].
A_{CS}	Cross sectional area of new pipe connection [m^2].
B	Additive term relating outlet concentration to inlet [-].
b	Fixed cost term associated with use of treatment plant [R/h].
C	Concentration [ppm].
c	Cost [R/h].
C_{TOT}	Total cost [R/h].
D	Pipe diameter [m].
F	Flowrate [t/h].
F^{lim}	Limiting flowrate [t/h]
F^{loss}	Flowrate loss [t/h].
FT	Flowrate to treatment plant [t/h].
F_{Ti}	Operation through flowrate [t/h].
Fw	Freshwater mass flowrate [t/h].
I	Operation involved with the water-using system.
I_{OP}	Water user in the water-using subsystem.
I_{TR}	Water treatment operation.
L	Pipe length [m].
M	Mass addition rate of contaminant [g/h].
n	Exponent pertaining to piping and associated fittings material of construction [-].
N_{OP}	Number of water-using operations.
N_{WU}	Number of water users in the water-using subsystem.
p	Proportionality constant relating AS condensate reuse flowrate to the inverse of the outlet concentration [t/(h·ppm)].
V	Stream flow velocity [m/s].
Win^L	Minimum withdrawal from freshwater source [t/h].
Win^U	Maximum withdrawal from freshwater source [t/h].
X	Pipe and associated fittings installation cost coefficient, per unit length of pipe [R/(m·h)].
X'	Once-off cost coefficient for piping and associated fittings per unit length of pipe [R/m].
$X_{monthly}$	Monthly cost coefficient for piping and associated fittings per unit length of pipe [R/(m·month)].

X_{pipe} Once-off cost coefficient for 1*”* piping per unit length of pipe [R/m].

Greek symbols

α Cost coefficient associated with freshwater extraction rate [R/t].

β Fixed cost term associated with use of a freshwater source [R/h].

Subscripts

i Water-using operation.

c Contaminant.

Fw Freshwater.

i′ Water-using operation ($i \neq i'$)

IP Inter-operation connection.

j freshwater source.

pipe Pipe.

process Process stream.

TR Treatment.

Superscripts

e Environmental limit.

in Inlet.

L Lower limit.

MAX Maximum.

out Outlet.

U Upper limit.

Appendix B: Sample Calculations

B.1 Data Conversions

B.1.1 Standard Deviation, Mean, and Confidence Interval

Using raw data for the flowrate freshwater to the PIX adsorption (JNC-14 to PIX in figure E.1), which has a population of $n = 162$, and significant outliers, the sample standard deviation, s_y was calculated using equation C.1 (Appendix C):

$$\sum y^2 = 3.719 \times 10^4$$

$$\left(\sum y\right)^2 = 5.475 \times 10^6$$

$$\therefore s_y = \sqrt{\frac{162 \times 3.719 \times 10^4 - 5.475 \times 10^6}{162 \times (162 - 1)}}$$

$$= 4.601 \, \text{m}^3/\text{h}$$

The mean for the same population was calculated using equation C.2:

$$\sum y = 2.340 \times 10^3$$

$$\therefore \bar{y} = \frac{2.340 \times 10^3}{162}$$

$$= 14.458 \, \text{m}^3/\text{h}$$

The confidence interval around the mean was calculated using equation C.3 and the uncertainty in the flowrate was determined to be:

$$14.46 \pm 1.96 \cdot \frac{4.601}{\sqrt{162}}$$

$$= 14.46 \pm 0.361 \text{m}^3/\text{h}$$

B.1.2 Flow Data

B.1.2.1 Mass Flowrate from Volumetric Flowrate

The volumetric flowrate was converted to a mass flowrate by multiplying the density by the volumetric flowrate. Except for the fermentation broth and the broth effluent, which both have a density of 2 t/m^3, the density of all streams have been assumed to be 1 t/m^3. The calculation is trivial and is not demonstrated.

B.2 Mass Loads

The mass load, *Δm*, for suspended solids in the cooling tower operation (data taken from table 3.2) was determined by mass balance, as follows:

For $F_{in} = 29.76$ t/h, $C_{SS}^{in} = 24.9$ppm, $F_{out} = 3.59$ t/h, $C_{SS}^{out} = 1000$ppm

$$\Delta m = F_{out} \cdot C_{SS}^{out} - F_{in} \cdot C_{SS}^{in}$$

$$\begin{aligned} \therefore \Delta m &= 3.59 \cdot 1000 - 29.76 \cdot 24.9 \\ &= 2848.98 \text{ g/h} \end{aligned}$$

Converting these values into the format of equation 3.1, we have:

$$A = \frac{F_{in}}{F_{out}}, B = \frac{\Delta m}{F_{out}}$$

$$\begin{aligned} \therefore A &= \frac{29.76}{3.59} = 8.29 \\ B &= \frac{2848.98}{3.59} = 793.59 \end{aligned}$$

B.3 Piping and Installation Costs

B.3.1 Hourly Cost

The cost for 1-inch 316 stainless steel piping is 64.00 R/m (price quote from Process Pipes Pty, Ltd.). The once-off cost of piping and fittings, *X'*, is determined using the fittings cost ratio, *F* [M.S. Peters, 1991 #41] as follows:

For $F = 1.4$, $X_{pipe} = 64.00$ R/m,

$$\begin{aligned} X' &= (1 + F) \cdot X_{pipe} \\ \therefore X' &= (1 + 1.4) \cdot 64 \\ &= 153.6 \text{R/m} \end{aligned}$$

With an assumed amortisation period of 5 years, and an interest rate of 13% per annum the monthly pipe and installation cost was calculated using the *Hewlett Packard 48GX* financial solver feature, (with N=60, I%YR=13, PV=153.60) and was determined to be:

$$X_{monthly} = 3.49 \text{ R/(month} \cdot \text{m)}$$

Hence, the hourly cost per meter of piping and associated fittings was calculated as follows:

For d_y = 365 days per annum, m_y = 12 months per annum, and h_d = 24 hours per day,

$$\begin{aligned} X &= \frac{X_{monthly} \cdot m_y}{d_y \cdot h_d} \\ &= \frac{3.49 \cdot 12}{365 \cdot 24} \\ \therefore X &= 4.78 \times 10^{-3}\ \mathrm{R/(h \cdot m)} \end{aligned}$$

B.3.2 Sea Pipeline Hourly Usage Cost

The annual permit cost for using the sea pipeline was R38631.60 at the time of the investigation. This was converted to an hourly cost as follows:

$$\begin{aligned} &= \frac{38631.60}{d_y \cdot h_d} \\ &= \frac{38631.60}{365 \cdot 24} \\ &= 4.41\mathrm{R/h} \end{aligned}$$

Appendix C: Statistical Analysis

C.1 Sample Points

For flowrate and purity parameters, numerous sample points were obtained for some of the streams. The maximum and minimum range for a given set of data points is determined by calculating the 95% confidence interval for the sample mean. The mean, maximum and minimum values for a stream specify the margin for relaxation of the sample points during data reconciliation.

The standard deviation is a measure of how widely values are dispersed from the average value (the mean). The standard deviation for a sample is estimated as follows:

$$s_y = \sqrt{\frac{n\sum y^2 - \left(\sum y\right)^2}{n(n-1)}} \qquad \text{(C.1)}$$

Where n is the number of sample points and y is the value. The sample mean is calculated as follows:

$$\bar{y} = \frac{\sum y}{n} \qquad \text{(C.2)}$$

If we assume a confidence interval of 95 percent, we need to calculate the corresponding area under the standard normal curve. This value is ± 1.96. The confidence interval is therefore:

$$\bar{y} \pm 1.96 \cdot \frac{s_y}{\sqrt{n}} \qquad \text{(C.3)}$$

Appendix D: Case Study

D.1 Introduction

D.1.1 Case Study

The following case study is intended as a stand-alone document, which outlines a water pinch investigation carried out using the Linnhoff-March software, WaterTarget. The system at AECI Bioproducts is used to illustrate the functionality of the software.

D.1.2 Outline of a Water Pinch Investigation

A water pinch investigation consists of several steps that are required to create a satisfactory design. These are as follows:

i. Determine the water-using network.

ii. Establish flowrate and concentration data (measured data) and mass balance data (model data) for sources, water-using operations and discharge points.

iii. Reconcile the data to establish a consistent mass balance for the water-using system so that inlet and outlet conditions for water-using operations are known.

iv. Simplify the network to exclude process streams that do not offer any scope for integration.

v. Determine the optimal design assuming current operating conditions are limiting.

vi. Establish sensitive operations close to the pinch that offer further scope for saving by relaxation of constraints or by regeneration of streams.

vii. Return to step (v) to determine the new design with the changed constraints and outlet conditions. Continue with step (vi) if any capacity remains for relaxation or regeneration.

viii. Check suitability of design e.g. by simulation.

ix. Implement design if feasible.

D.1.3 WaterTarget

The above steps may be interpreted using the Linnhoff-March software WaterTarget, which is comprised of two programs, WaterTracker, for data gathering and reconciliation, and WaterPinch for determining optimal water network designs and analysis of sensitive operations.

A water pinch investigation carried out using this software may be summarised by the flowchart in figure D.1, below. This flowchart serves as a summary of the WatertTarget computational steps carried out for the case study conducted at AECI Bioproducts.

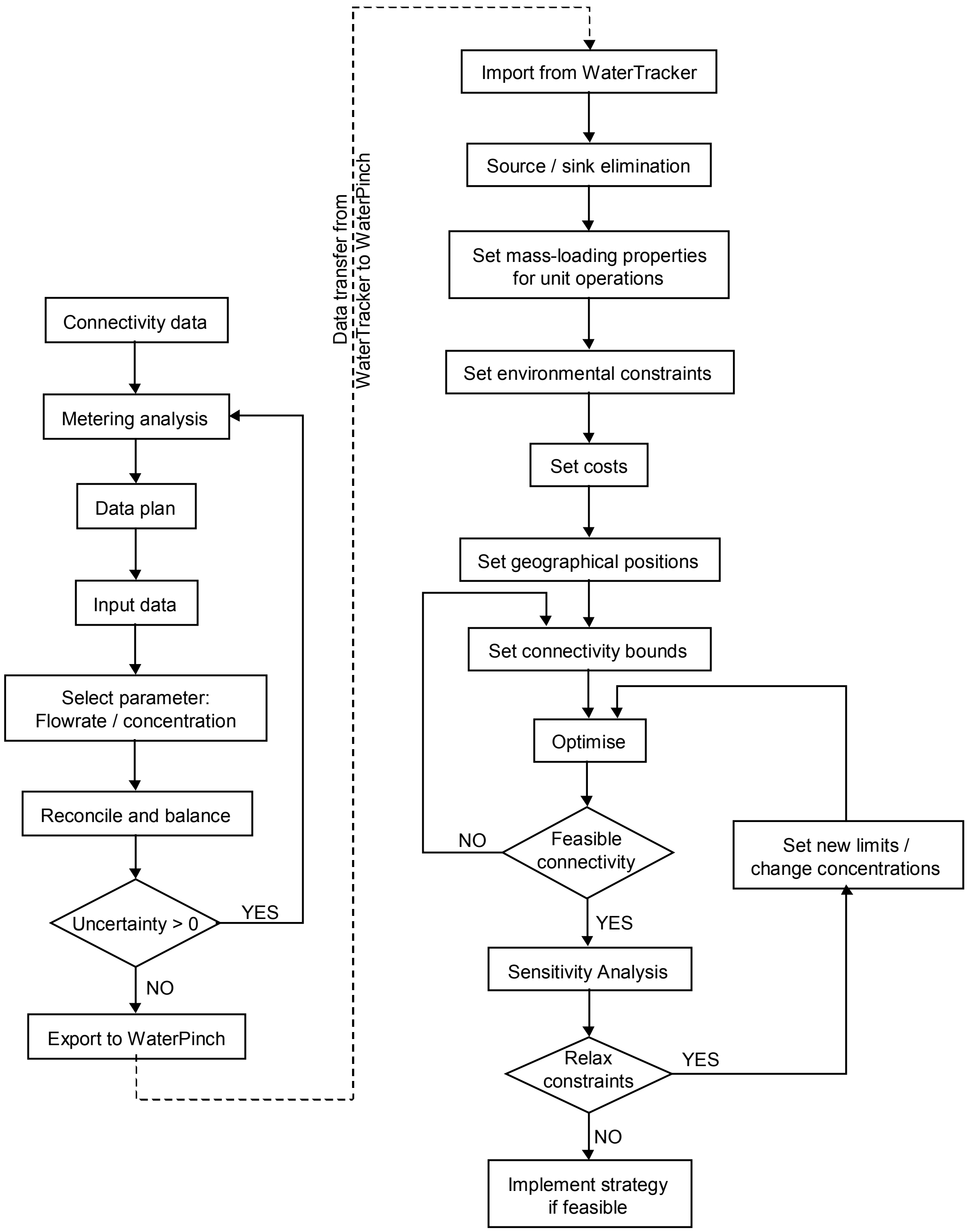

Figure D.1
Outline of a pinch investigation carried out using WaterTarget.

D.1.4 Elements of the Water-Using System

The water-using system (figure D.2 (a)) is comprised of various *nodes*, which may be classified as follows:

– Sources: inlets to the water-using system.

– Sinks: outlets from the water-using system.

– Operations: Unit operations that use water and affect the mass-flow of contaminant within the overall system. The water-using operations may be subdivided into two groups:

  (i) Water-using subsystem: typically operations that have fixed water demands and supplies. Operations within the water-using subsystem typically *add* contaminant mass to the system via mass-transfer from a *process stream* (figure D.2 (b)).

  (ii) Wastewater treating system: typically operations that treat or regenerate effluent arising from the water-using subsystem. Operations within the wastewater treating system typically *remove* contaminant mass from the overall system (figure D.2 (c)).

– Streams: Connections between nodes that represent material flow from one node to another.

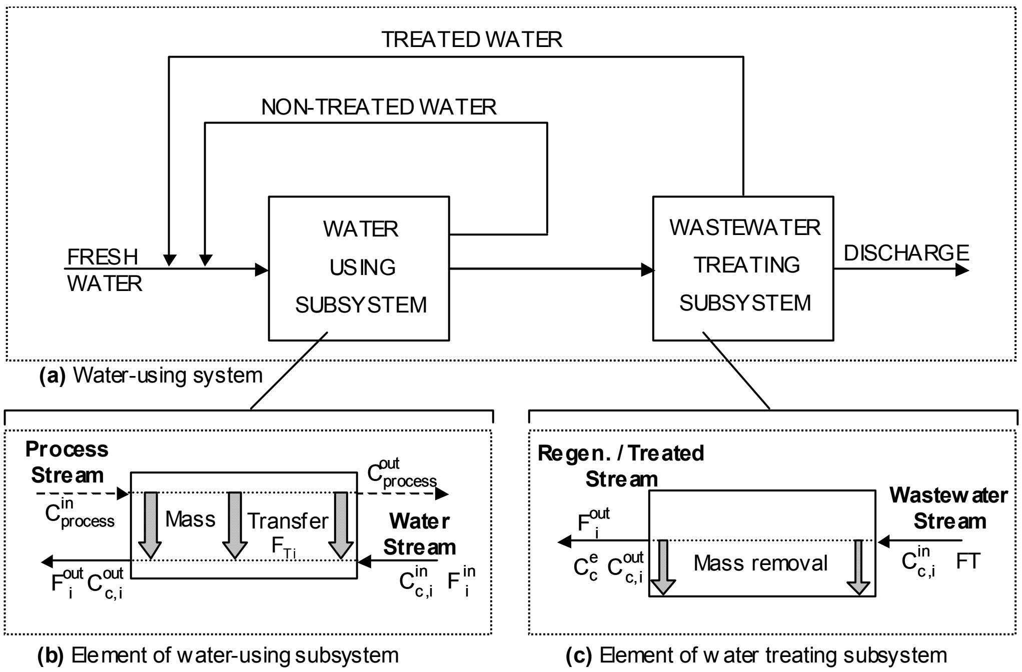

Figure D.2
A conceptual view of an industrial water-using system (a). Processes (b) and treatment / regeneration (c) unit operations. The dashed inlet and outlet line in (b) denotes the *process stream*.

Sources and sinks form the boundary of the water-using system, i.e. other water-using operations may exist outside of this boundary, but are not considered as part of the analysis.

D.1.5 WaterTracker

D.1.5.1 Types of Data

Measured flowrate and contaminant concentration data is termed *measurement information*. Besides measurement information, numerical *model information* may be used. The following information is designated as model information:

- split fractions,
- flowrate and concentration mass balance relationships,
- specification of contaminant gains and losses and
- hardware constraints, such as physical limits on flowrates, maximum allowed inlet concentrations, etc.

D.1.5.2 Metering Analysis

In WaterTracker, all numerical data is optional. One of the main functions of the software is to assist with choosing which data items to enter. Initially, a valid network structure may be analysed without any numerical data. The software guides the user towards a reliable water balance by suggesting the most strategic measurement information (stream flowrates and concentrations) required.

The software will not suggest entry of model information during metering analysis. It will, however, take all the model information into account when selecting the most strategic next piece of measurement information.

D.1.5.3 Data Entry and Reconciliation

For each stream, measurement information is entered and a range of uncertainty is specified in terms of a minimum and maximum value. When the range is not explicitly known, a default range of 2, 5 or 25% may be specified, depending on the users' confidence as to the accuracy of the measurement information.

Before data reconciliation, the software checks the data for conflicts. Data conflicts arise largely due to the following two reasons (these are characteristics of the software and not necessarily an aspect of Data Reconciliation theory):

(i) Measurement information contradicts model information. For example, a mass balance relationship linking an operation outlet parameter to an inlet parameter *should not* be simultaneously specified with a measured inlet and outlet parameter for the same operation.

(ii) A discontinuity exists between two successive or related measured parameters (such as the inlet an outlet of an operation), i.e. a continuous region cannot be identified within the ranges of related parameters. This type of clash is illustrated in figure D.3, below. Figure D.3 (a) illustrates the case where an overlap is identifiable between the maximum range of point 1 and the minimum range of point 2. However, a clash is reported when a discontinuity exists (figure D.3 (b)).

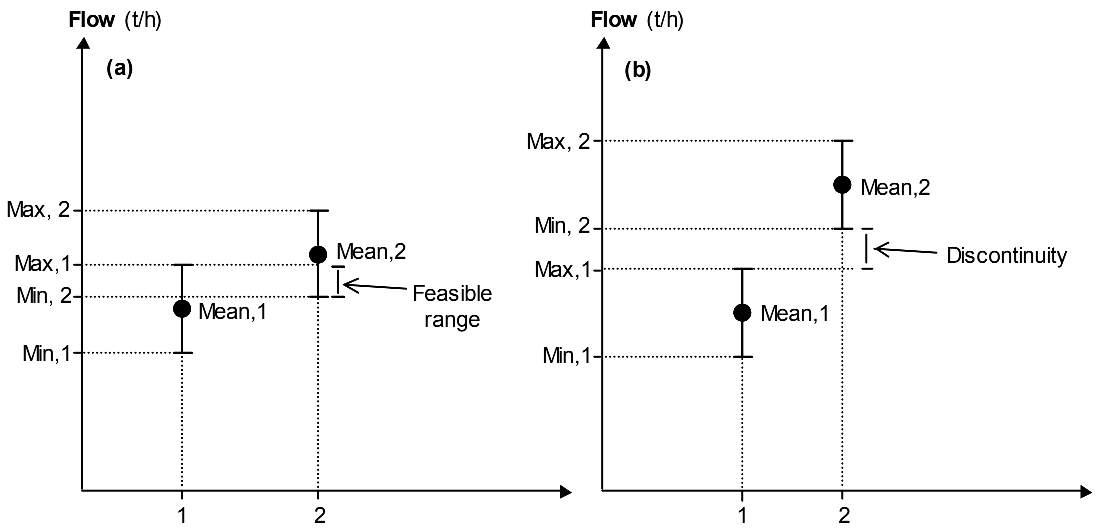

Figure D.3
Illustration of feasible (a) and infeasible (b) related measured information.

Data reconciliation determines the best fit of the measurement information within the specified range, while maintaining a balance across each node, subject to the specified model information.

D.1.6 WaterPinch

When a balanced model has been obtained, which is consistent with the specified uncertainties, i.e. inlet and outlet flowrates and contaminant concentrations have been specified or calculated for each node, the balanced data may be exported from WaterTracker to WaterPinch.

D.1.6.1 Inlet and Outlet Classification

In WaterTracker, some sources, sinks and associated operation inlets and outlets, may have been included to complete the balance, but are not required for the pinch analysis, as they are inherent to the system, and cannot change. As a first step these are eliminated to produce a set of nodes that have either a supply of water (a source) or a demand for water (a sink), or both (a unit operation). Nodes that have a fixed flowrate demand or supply are termed *process sinks* and *process sources*, respectively. Nodes that have a variable flowrate demand and supply are termed *utility sinks* and *utility sources*, respectively. Nodes that have both an inlet and an outlet are termed *unit operations*. Hence, a *process unit operation* will have fixed inlet and outlet flowrates (a flow balance is not necessarily maintained across a process unit operation). A maximum of five inlets and outlets may be specified for an individual process unit operation. *Utility unit operations* have a variable inlet flowrate, which may be split into a maximum of two dependent outlet flows (i.e. the flow balance is conserved across a utility unit operation). The inlet flowrate may be constrained between a minimum and maximum tolerance.

D.1.6.2 Contaminant Mass Addition and Removal

The concentration of contaminants present in unit operation outlet streams may be related to the inlet stream concentration by a linear mass-loading relationship. The general form of the relationship is as follows:

$$C_{c,i}^{out} = C_{c,i}^{in} \cdot A + B \qquad \text{(D.1)}$$

where, $C_{c,i}^{out}$ is the outlet concentration of contaminant *c* in operation *i*. $C_{c,i}^{in}$ is the inlet concentration. The terms *A* and *B* are constants that describe the way in which contaminant mass is added or removed. For process unit operations (figure D.4 (a)) the outlet concentration may be expressed in terms of a contaminant mass addition term, Δm_i, which is the difference between the outlet and inlet contaminant mass flowrate for operation *i*:

$$C_{c,i}^{out} = \frac{C_{c,i}^{in} \cdot F_i^{in} + \Delta m_i}{F_i^{out}} \qquad \text{(D.2)}$$

Utility unit operations typically remove contaminant mass (figure D.4 (b)). Outlet concentrations for utility unit operation *i*, may be related to the inlet concentration using a contaminant fractional removal term, r_i ($0 \le r_i < 1$):

$$C_{c,i}^{out} = C_{c,i}^{in} \cdot (1 - r_i) \qquad \text{(D.3)}$$

A utility unit operation may have a maximum of 2 outlets. The outlet flowrate may be expressed as a fraction of the inlet flow, as follows:

$$F_i^{out} = s_i \cdot F_i^{in} \qquad \text{(D.4)}$$

where s_i is the splitting fraction to outlet 1 ($0 < s_i < 1$).

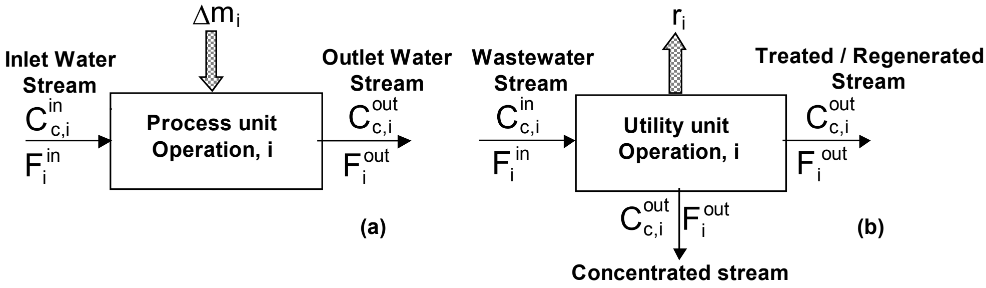

Figure D.4
Process (a) and utility (b) unit operation models.

If no concentration link is specified for process unit operations, the outlet concentrations are assumed to be constant and equal to the balanced value from WaterTracker. For utility unit operations, the default setting for the outlet(s) concentration is zero (inlets may be limited to conditions determined by the balance, or are unlimited).

D.1.6.3 Environmental and Discharge Constraints

The user enters environmental and discharge constraints, which apply to utility sinks. They are of the following form:

(i) Flowrate: constrained between a minimum and maximum or unconstrained.

(ii) Concentration: limited to a maximum value or unconstrained.

(iii) Contaminant mass flowrate: or *Flowrate* x *Concentration*, which is limited to a maximum value or is unconstrained.

Typically, environmental constraints are limited in terms of concentration (ii.). A contaminant mass flowrate restriction may be preferred if effluent dilution is a problem (concentration may be reduced by dilution, whereas contaminant mass flowrate cannot be reduced by dilution).

D.1.6.4 Costs

Two basic cost types may be specified: fixed hourly costs, or variable operating costs (or both in some cases). Fixed costs are one-off costs that are incurred when a decision is made that has a related fixed cost (e.g. the installation cost of connecting two operations). Fixed costs are converted to a time-dependent basis by means of a predetermined *annualisation factor*. Piping costs are a specific type of fixed cost, which are activated whenever a new connection is required between two operations (existing connections may be used up to the maximum flowrate tolerance). Piping costs per unit pipe length may be specified by the following equation:

$$c_{pipe} = K_i \cdot D_i^n \qquad (D.5)$$

The coefficient, K_i, is the purchase cost of a new pipe per unit length, for a given pipe diameter, and D_i is the inside diameter of the pipe. The exponent, n, accounts for the material of construction of the pipe (e.g. n = 0.6 for carbon steel and n = 0.9 for stainless steel). In order to incorporate piping costs, the geographical positions of the water-using operations must be known, in order to calculate the length of pipe required to make a new connection. In general, fixed costs are associated with integer constraints and can slow the optimisation process significantly.

Variable costs are dependent on water or contaminant mass flowrate (i.e. cost per unit flow). Typically freshwater sources, effluent sinks and utility unit operations have variable costs associated with the amount of water extracted, discharged and treated.

D.1.6.5 Bounds

Structural constraints and cost parameters, which are loosely termed *bounds* in the software, act on the optimisation algorithm to restrict, prevent or encourage connections between nodes. Strictly speaking, a bound is a constraint *or* an economic parameter that acts on, or is activated by, a single possible connection between a source and a sink. In this way, the configuration of the optimised network may be controlled to an extent. Seven types of bounds are available in the software and are summarised as follows:

(i) *Flow* =. Forces the total flow through the connection to be the specified value.

(ii) *Flow max*. Specifies an upper limit on the total flow through the connection.

(iii) *Flow min*. Specifies a lower limit on the total flow through the connection.

(iv) *Existing flow*. Indicates that there is an existing connection with an existing maximum flow of the specified value. In this case, the existing connection can be freely used up to its stated capacity. Any additional flow between the source and sink has to flow through a new connection, which will incur fixed piping costs.

(v) *Ztol*. The minimum flow required to justify a new connection. No new connection will be made unless the flow on the new connection is greater than the specified value.

(vi) *Variable Cost*. The flow-dependent cost of using a new connection

(vii) *Fixed Cost*. The fixed (capital) cost incurred for making a new a new connection.

Bounds set for *Variable cost, Fixed cost*, and *Ztol*, apply only to the flow through new connections. Bounds are specified in matrix format with the constraints or parameters relating source j to sink i, are entered in column j, row i.

D.1.6.6 Optimisation

Optimisation determines the design of the network that satisfies the specified constraints at the minimum overall cost. This minimum design cost, called the objective cost, is the time-dependent cost of operating the network. All fixed costs that are incurred, directly contribute to the objective cost. The product of variable costs and the flowrate to the associated node, results in a time-dependent operating cost, which contributes to the objective cost. All flowrates to nodes that contribute to the objective cost either as a fixed cost, variable cost, or both are summarised in the results summary.

D.1.6.7 Sensitivity Analysis

The WaterPinch *Sensitivity Analysis* feature identifies the sources and sinks, where changes to the water-using system yield the largest savings; these are the areas where future engineering effort should be concentrated. The sensitivity values report the change in operating cost for a small change in concentration, in a graphical format. The values are reported for both the inlet concentration constraints (inlet sensitivity) and the outlet concentration values (outlet sensitivity).

Inlet sensitivity indicates the amount that the objective cost is decreased when an inlet concentration constraint to a node is relaxed. Outlet sensitivity values report the amount of decreased cost when an outlet concentration is reduced. Outlet sensitivity values indicate streams that are appropriate for treatment, whereas inlet sensitivities indicate scope for further integration.

D.2 AECI Bioproducts Model

Elements or nodes of the water-using system may be represented, on WaterTracker, by using various basic model types. The water-using system at AECI Bioproducts is composed of the following elements:

– *Sources*:

  i. Umbogintwini river water (pre-treated by Umbogintwini Operating Systems (UOS)).

  ii. Effluent treatment plant (ETP) dilution. UOS effluent dilution.

  iii. Steam (feed for evaporators and heater). Predominantly used for evaporation and heating, and is required to balance with condensate.

  iv. Raw Materials (NH_3 solution for ion-exchange regeneration and fermentation feed).

– *Sinks*:

i. Sea Outfall pipeline. General process effluent is discharged via this sink.

ii. Southern Wastewater Works (SWW). This sink handles the concentrated Biomass effluent.

iii. Product. The concentrated lysine evaporator product, required to complete the mass balance around the lysine evaporator.

– *Water-using operations* (process operations):

i. AS (ammonium sulphate) evaporator and

ii. lysine evaporator;

iii. PIX (primary ion exchange) adsorption,

iv. PIX backwash and

v. PIX strip.

vi. SIX strip and

vii. SIX rinse;

viii. CIP (clean in place system);

ix. Cooling tower;

x. Pump seals;

xi. Plant wash-down sump and

xii. tank farm sump;

xiii. Fermentation.

– Tanks, which were included as *junctions*:

i. TB 3201: Backwash tank;

ii. TB 3206: Condensate tank;

iii. TB 3203: Ammonia solution makeup tank;

iv. Biomass tank: For fermentation broth effluent;

v. Effluent tank: For general process effluent.

vi. RMX-1: Ratio mixing of process steam with stripped lysine solution (from PIX adsorption phase).

Additional junctions were added to model mixing and splitting of streams, as follows:

vii. FW Distribution 1, 2;

viii. FW Distribution 2;

ix. PSW Distr.: Pump seal water distribution;

x. JNC-9, 11, 12, 13, 14.

The water-using network created using WaterTracker is illustrated in figure D.8.

D.2.1 Key Contaminants

Three contaminants were selected: free and saline ammonia (FSA), suspended solids (SS) and chlorides (Cl). Several other contaminants that do affect reuse in the water-using system were omitted from the investigation, as they only affect specific or localised areas of the model. Some examples are:

i. Amino acids: threonine, valine, alanine, methionine, etc. These are by-products of fermentation and affect the recycle of effluent from the PIX backwash operation. They were not included as they affect only the PIX backwash operation.

ii. Metallic cations: Ca^{++}, and K^{+}. Calcium reduces the affinity of the cationic resin in the PIX adsorption phase and is predominant in the fermentation broth and broth effluent. Potassium affects the purity of the product and is removed in the SIX operation, recycled back to the PIX adsorption zone (with H_2SO_4), and is discharged with the broth effluent. Calcium was ignored as the broth feed is a process stream and the broth effluent is not reused elsewhere. Potassium was not included as it was adsorbed (PIX adsorption), removed (SIX) and discharged (broth effluent) on a closed loop and did not affect any other area of the operation.

iii. Other contaminant groups: such as COD, BOD, and conductivity. These are collective classifications, which take into account a wide range of other contaminants (some of which were included in the analysis), such as SS, Cl and FSA. They were not included, as key contaminant concentrations must be independent of each other, to avoid double accounting errors.

iv. Sorbs, oils, and greases (SOGs): This was mainly present in the form of glycerol and occurred in small quantities in the broth effluent. Since the broth effluent was discharged to the SWW (the concentration of SOGs is limited in the sea pipeline discharge point), this contaminant group was not included.

D.2.1.1 Free and Saline Ammonia.

Dissolved ammonium species, predominantly $(NH_3)_2SO_4$ and $NH_{3(aq)}$ (depending on the pH) are collectively classified as FSA. At the time of the investigation, the concentration of this contaminant was limited to below 300ppm in the discharge to the sea. The following operations add or remove FSA to the water-using system:

- *Fermentation tanks*. AS is added during tank cleaning, which is manifested in the outlet from the CIP system, i.e. tank cleaning adds FSA to the system.
- *PIX adsorption*. Free ammonia is added, when ammonia is displaced from the resin by the adsorbed species.
- *PIX backwash*. Loads free ammonia, which is discharged via the sea pipeline.

D.2.1.2 Suspended Solids

This is a broad-spectrum contaminant, which, at the time of the investigation, was limited to below 400ppm in the discharge to the sea. The following operations add or remove SS to the water-using system:

- *Fermentation*. The broth effluent is a high solids source comprised mainly of cellular residue, which is added during the fermentation process.
- *PIX backwash*. Cellular residue from the adsorption phase adds SS, to the backwash effluent.
- *Cooling tower*. Pick-up of atmospheric solids adds SS to the water system during evaporative cooling.
- *Tank cleaning*. General particle residue in tanks, such as cellular residue in the fermentation tanks, is added to the system during CIP.
- *Pump seals*. Although SS addition by the pump itself is marginal, SS pickup in the pump sumps is considerable due to exposure to the atmosphere.
- *Freshwater supply*. The freshwater supply has a small quantity of SS, which is not removed during pre-treatment.

D.2.1.3 Chloride

Although recorded as chloride concentration, chloride is an indicator for associated cations, such as sodium and potassium. High chloride concentration causes corrosion problems in most operations. The cooling tower, and to a lesser extent, the pumps were especially sensitive to corrosion. Although this contaminant is not directly limited in effluent discharges to the sea, the conductivity must be below 2000mS/m. The cooling tower was the only operation that contributes to the chloride concentration in the system, by concentrating the UOS water makeup.

The measurement and model information, as well as calculated values for the AECI Bioproducts model are given in section D.5.2, table D.9 (flowrates). Contaminant information is given in table D.10, D.11 and D.12. For the flowrate parameters, mostly measured information has been specified.

D.3 Building a WaterPinch Model

D.3.1 Source and Sink Elimination (Inlet and Outlet Classification)

Source and sink elimination is demonstrated in figure D.5, below. It shows how the PIX strip operation, ammonium stripper and lysine evaporator are represented using WaterTarget and interpreted as a WaterPinch model.

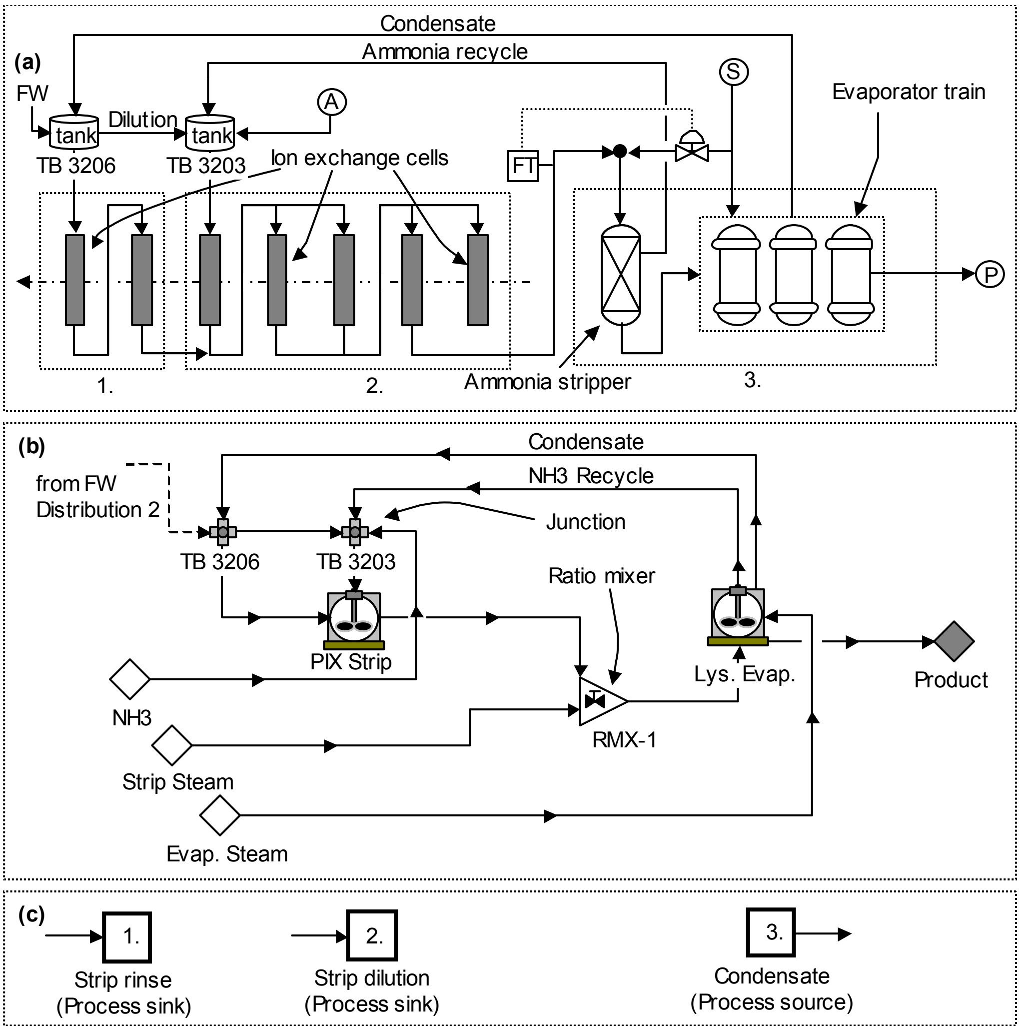

Figure D.5
Illustration of source / sink elimination. The PIX strip, ammonia stripper and evaporation sub-network (a), is represented using WaterTarget for the mass balance (b). The network is reduced (c), showing the streams (sources and sinks), which were relevant to the water pinch investigation.

In figure D.5 (a), rinse water was fed from the condensate tank (TB 3206) to the rinse stage of the PIX strip cycle. Dilution water was required to makeup the ammonia solution that was fed from the ammonia tank (TB 3203) to the PIX elution zone. Both these water demands (rinse and dilution) should be included in a water pinch analysis (operation 1 and 2, figure D.5 (c)). However, the ammonia feed (*A*) was excluded, as it is a raw material stream. Similarly, the PIX intermediate product streams flowing between each cell and to the evaporator train were excluded, as they are both process streams and cannot be re-routed. By applying the same technique to the ammonia stripper and the lysine evaporator train, the steam supply (*S*), stripped ammonia recycle (to TB 3203) and the concentrated product (*P*) were both excluded. Only the process condensate stream was included in the water pinch analysis (operation 3, figure D.5 (c)), as it is a fixed supply of water (process source), which may be used elsewhere. Hence, the lysine evaporator became a process source.

The level of simplification required to complete the mass balance (over the sub-network) using WaterTracker is shown in figure D.5 (b). The controller that regulates steam flow to the stripper was represented as a ratio mixer (RMX-1), which was used because the ratio control setting is a known data parameter. Tanks were represented as simple junctions. A single process was used to represent the PIX strip process, with multiple inlets representing the various feeds. The ammonia stripper and lysine evaporator may be similarly compounded into a single process. The simplification of the sub-network shown above, is not unique; the flowsheet in figure D.5 (a) may be represented in several different ways, using WaterTracker.

The classification of the WaterTracker streams, to create the WaterPinch model, for the entire system, is given in table D.13 (section D.5.3).

D.3.2 Processes and Utilities

After source and sink elimination, the remaining water-using nodes for the system at AECI Bioproducts are as follows:

- Freshwater: utility source;
- AS evaporator condensate: process source;
- Fermentation: process sink;
- Cooling tower: process unit operation;
- Pump seals: process unit operation;
- PIX adsorption: process unit operation;

- PIX backwash: process unit operation;
- SIX acid dilution: process sink;
- PIX strip water: process sink;
- CIP: process unit operation;
- SIX rinse: process sink;
- Steam condensate (pure condensate producers grouped together): process source;
- Effluent treatment plant feed from UOS (ETP dilution): process source;
- Sea outfall pipe: utility sink;
- Southern wastewater works (SWW): utility sink.

The initial constraints and outlet conditions (flowrate and concentration) of the process streams were defined by the inlet and outlet conditions determined by the mass balance. These parameters are listed in table D.1 (a) and (b), below. Later, after sensitivity analysis, sensitive streams that were candidates for constraint relaxation and regeneration were identified, and the initial constraints may be changed, if possible.

Unless specified by the user, inlets to utility operations are unconstrained. The user specifies relevant cost data (extraction, treatment and discharge). Utility source and sink data for the investigation at AECI Bioproducts is given in table D.2 (a) and (b), below.

TABLE D.1 (a)
Process sink constraints.

	Name	Flow	Max SS	Max FSA	Max Cl
		[t/h]	[ppm]	[ppm]	[ppm]
1	Fermentation	3.99	24.90	0.00	+INF
2	PIX strip rinse	12.43	24.90	0.00	+INF
3	SIX acid dilution	1.38	24.90	0.00	+INF
4	SIX rinse	1.30	24.90	0.00	+INF
5	Pump seals in	6.50	24.90	0.00	80.63
6	CIP in	6.38	24.90	0.00	+INF
7	PIX ads in	14.44	24.90	3990.00	+INF
8	PIX b-w in	10.45	625.00	100.00	+INF
9	Cooling tower in	29.76	24.90	0.00	80.63
10	PIX NH3 dil.	0.16	24.90	0.00	+INF

TABLE D.1 (b)
Process source conditions.

	Name	Flow	SS	FSA	Cl
		[t/h]	[ppm]	[ppm]	[ppm]
1	UOS dilution	80.14	126.89	16.44	80.63
2	AS evap condensate	6.40	1000.00	0.00	0.00
3	Pure condensate	18.07	0.00	0.00	0.00
4	Pump seals out	6.50	222.50*	0.00*	80.63*
5	CIP out	6.38	7695.25*	0.00*	0.00*
6	PIX ads out	24.97	350000	35000	1000
7	PIX b-w out	17.43	625.00*	300.05*	31.01*
8	Cooling tower out	3.59	1000.00*	0.00*	670.04*

The asterisk markings for the entries in table D.1 (b) indicate that the value is used as an initial estimate for optimisation (this applies to process unit operations only).

TABLE D.2 (a)
Utility source conditions and costs.

	Name	Flow min [t/h]	Flow max [t/h]	Variable Cost [R/t]	Fixed Cost [R/h]	Existing Capacity [t/h]	SS [ppm]	FSA [ppm]	Cl [ppm]
1	UOS water		+INF	2.50			24.90	0.00	80.63
2	dummy source		+INF	1000.00			0.00	0.00	0.00

TABLE D.2 (b)
Utility sink constraints and costs.

	Name	Flow min [t/h]	Flow max [t/h]	Variable Cost [R/t]	Fixed Cost [R/h]	Existing Capacity [t/h]	SS [ppm]	FSA [ppm]	Cl [ppm]
1	Sea outfall pipe		+INF		4.14		+INF	300.00	+INF
2	SWW		+INF	16.00			+INF	+INF	+INF
3	dummy sink		+INF	1000.00			+INF	+INF	+INF

In the tables above, *+INF* is used to indicate that the parameter is unconstrained. The fixed cost parameter for the sea outfall pipe is due to an annual license fee, which is paid for its use.

D.3.2.1 Dummy Utilities

Dummy source and dummy sinks (table D.2 (a) and (b)) are used to identify areas that are too tightly constrained as well as any structural (see *Bounds*, section D.3.5) errors that may be present. Dummy sources are expensive, *pure* sources; if an operation has a demand for a dummy source it usually implies that there is not enough freshwater available to satisfy the constraints of the operation. Dummy sinks are expensive, *unconstrained* sinks; analogous to dummy sources, if an operation discharges to a dummy sink it implies that the available sinks are too tightly constrained to handle the concentration of effluent from the operation concerned. The penalty for utilising a dummy utility is the high associated cost. The optimisation algorithm will only identify the need to utilise the utility if there are no other options available.

D.3.2.2 Base Case Water-Using System

Although not essential, it was useful at this point to define a base-case water-using system (figure D.9) for the purpose of comparison. Constraining all flows to the existing configuration using the bounds editor does this (i.e. new connections are prevented by setting the *flow* = constraint to zero).

D.3.3 Mass Loading Properties

The general equation D.1 was used to define the relationship between the outlet stream and the inlet stream for the operations where this link is definite. The mass loading parameters, *A* and *B*, are given in table D.3, below.

TABLE D.3
Mass loading relationships for the water-using operations.

	Operation	Contaminant	A [-]	B [ppm]
1	Cooling Tower	SS	8.30	793.33
		FSA	8.30	0.00
		Cl	8.31	0.00
2	Pump Seals	SS	1.00	197.60
		FSA	1.00	0.00
		Cl	1.00	0.00
3	PIX adsorption	SS	0.00	350000
		FSA	0.00	35000
		Cl	0.00	1000
4	PIX backwash	SS	1.00	0.00
		FSA	0.60	240.05
		Cl	1.00	0.00
5	CIP	SS	1.00	7670.35
		FSA	1.00	0.00
		Cl	1.00	0.00

D.3.4 Piping Costs

Extraction and discharge costs for the utility sources and sinks are listed in table D.2 (a) and (b). Fixed piping costs and associated parameters are listed in table D.4, below.

TABLE D.4
Additional economic parameters

Hourly cost per meter piping (based on average system diameter), K_i	4.78×10^{-3} (R·h^{-1})/m
Exponent for material of construction, n	0.9 (stainless steel)

Using the above parameters, equation D.5 may be expressed as follows:

$$C_{p\,j,i} = 4.78 \times 10^{-3} \cdot D_{j,i}^{0.9} \qquad \text{(D.6)}$$

where, $C_{p\,j,i}$ is the cost per meter of piping from source j to sink i. $D_{j,i}$ is the diameter of piping from source j to sink i. The diameter, $D_{j,i}$, is calculated by the software for each new connection, based on the assumption that the stream velocity for all connections is constant at 1m/s. A similar set of piping cost equations can be generated for all new connections.

D.3.4.1 Geographical Positions

Associated with the piping costs are the geographical positions of the operations (table D.5). These were required to calculate the length of piping needed to establish a new connection. A new connection is made only when there is no existing connection between the operations, or the flowrate supersedes the existing flow. Existing flowrates are shown in table D.6.

TABLE D.5
Geographical positions of the operations at AECI Bioproducts.

Name	X position [m]	Y position [m]	Name	X position [m]	Y position [m]
Process Sinks			**Process UnitOps**		
Fermentation	20	35	Pump seals	0	5
PIX strip rinse	20	20	CIP	40	0
SIX acid dilution	20	15	PIX ads	20	20
SIX rinse	30	15	PIX b-w	20	20
PIX NH3 dil.	20	20	Cooling tower	5	90
Process Sources			**Utility Sinks**		
UOS dilution	25	0	Sea outfall pipe	25	0
AS evap condensate	40	25	SWW	30	10
Pure condensate	40	20	**Utility Sources**		
			UOS water	0	10

D.3.5 Structural Constraints

The bounds governing the structure of the network and cost of connections are given in table D.6, below. Existing flowrate capacities were calculated from the maximum capacity of the standard pipe diameter for each existing connection. Connections that have been disallowed, are excluded by a *flow = 0* constraint. Flow demands for each operation are included in square parentheses beneath each operation name (unbounded flowrates are designated by *+INF*).

TABLE D.6
Bounds for connections between all sources and sinks (all bounds shown).

Sinks / Sources	Ferment-ation [3.99]	PIX strip rinse [12.43]	SIX acid dilution [1.38]	SIX rinse [1.30]	Pump seals in [6.50]	CIP in [6.38]	PIX ads in [14.44]	PIX b-w in [10.45]	Cooling tower in [29.76]	PIX NH3 dil. [0.16]	Sea outfall pipe [+INF]	SWW [+INF]
UOS dilution [80.14]	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0		flow = 0
AS evap condensate [6.40]								existing 8.99			existing 8.99	
Pure condensate [18.07]		existing 20.44		existing 20.44		existing 20.44				existing 20.44		
Pump seals out [6.50]	flow = 0	flow = 0	flow = 0	flow = 0			flow = 0	flow = 0	flow = 0	flow = 0	existing 8.99	
CIP out [6.38]	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0		flow = 0	flow = 0	flow = 0	flow = 0	existing 8.99	
PIX ads out [24.97]	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	existing 28.30	existing 28.30
PIX b-w out [17.43]	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	flow = 0		flow = 0	flow = 0	existing 20.44	
Cooling tower out [3.59]	flow = 0	flow = 0	flow = 0	flow = 0		flow = 0	flow = 0	flow = 0	flow = 0	flow = 0	existing 5.22	
UOS water [+INF]	Existing 5.22	existing 2.37	existing 1.44	existing 2.37	existing 8.99	existing 2.37	existing 20.44	existing 8.99	existing 35.36	existing 2.37		

D.3.6 Optimal Water-Using Strategy

The result of optimisation, subject the specified constraints and model parameters above, is summarised in table D.7, below. The *results summary* gives the objective cost.

TABLE D.7
Results summary.

Objective cost	556.3	R/hr
Utility Source	Cost, R/h	Flow, t/h
UOS water	152.37	60.95
Utility Sink	Cost, R/h	Flow, t/h
Sea outfall pipe	4.41	112.67
SWW	399.52	24.97
Bound costs	0	R/h
Geographical costs	0	R/h
Bounds:	78	

D.3.6.1 Connectivity

The design of the water-using network that satisfies the constraints is reported as a table of inter-operation flows (table D.8). The operations are classified according to type (i.e. utility or process).

TABLE D.8
Inter-operation flowrates (network design).

	From...	...to	Flow [t/h]	Existing capacity
	From Process...	...to Process		
1	AS evap condensate	PIX b-w in	4.29	8.99
2	Pure condensate	PIX strip rinse	11.53	20.44
3	Pure condensate	CIP in	6.38	20.44
4	Pure condensate	PIX NH3 dil.	0.16	20.44
5	PIX b-w out	PIX b-w in	3.48	
	From Utility...	...to Process		
6	UOS water	Fermentation	3.99	5.22
7	UOS water	PIX strip rinse	0.9	2.37
8	UOS water	SIX acid dilution	1.38	1.44
9	UOS water	SIX rinse	1.3	2.37
10	UOS water	Pump seals in	6.5	8.99
11	UOS water	PIX ads in	14.44	20.44
12	UOS water	PIX b-w in	2.68	8.99
13	UOS water	Cooling tower in	29.76	35.36
	From Process...	...to Utility		
14	UOS dilution	Sea outfall pipe	80.14	
15	AS evap condensate	Sea outfall pipe	2.11	8.99
16	Pump seals out	Sea outfall pipe	6.5	8.99
17	CIP out	Sea outfall pipe	6.38	8.99
18	PIX ads out	SWW	24.97	28.3
19	PIX b-w out	Sea outfall pipe	13.95	20.44
20	Cooling tower out	Sea outfall pipe	3.59	5.22

Figure D.10 (section D.5.4) shows the corresponding diagram of the water-using network.

D.3.6.2 Sensitivity Analysis

The initial inlet and outlet sensitivities for the model are presented in figure D.6 below. The inlet sensitivity values indicate that the objective cost is most sensitive to changing the inlet FSA constraint to the PIX backwash. For example, relaxing the inlet concentration constraint for FSA to the PIX backwash by 1ppm will reduce the objective cost by approximately 0.027 R/h.

The outlet sensitivity values indicate scope for further integration of a source through contaminant removal (e.g. by treatment or regeneration). For example, reducing the SS concentration in the AS evaporator condensate by 1ppm will result in a reduction in the objective cost of about 0.01 R/h. This is an indication of the amount that may be invested in implementing and running a facility that removes the sensitive contaminant. It must be emphasised that the objective cost sensitivity values reported by the software are *initial* values and must be tested over a concentration range in order to establish the validity of the value.

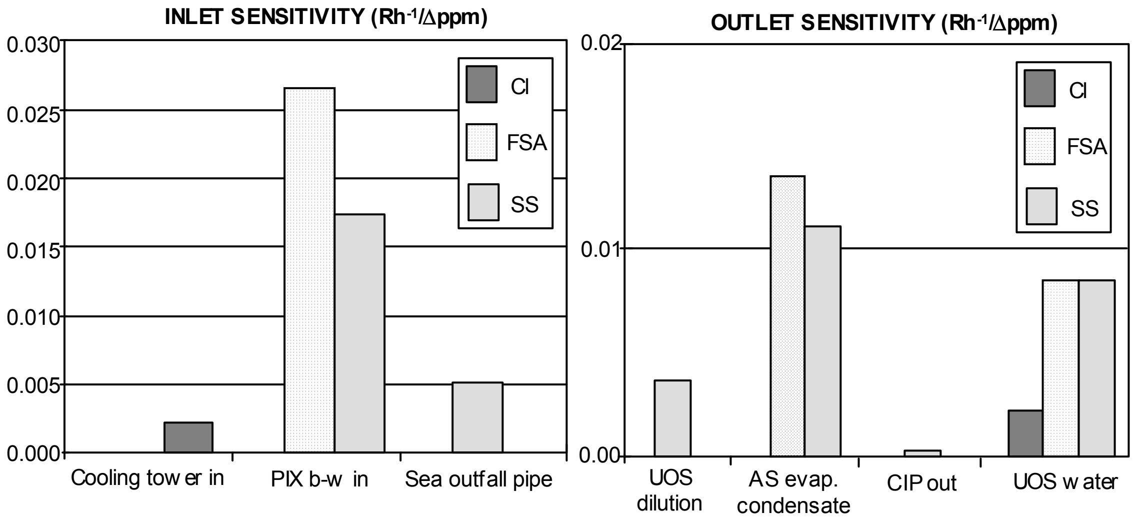

Figure D.6
Initial inlet and outlet sensitivity values.

D.4 Summary

The Linnhoff-March software suite, WaterTarget is an aid for conducting a water pinch investigation and determining the optimum economical design of water-using systems. The case study has demonstrated the following:

- WaterTracker may be used as an effective tool for assisting with data gathering and mass balance of a water-using system.

- WaterPinch uses data parameters from the mass balance as limiting for inlets to nodes so as to model the constraints and outlet conditions of the water-using system.
- Based on user specified costs, WaterPinch can determine near-optimal designs for water-using systems, subject to the specified constraints.
- The sensitivity analysis feature highlights specific areas of the network where further effort is required, with regards to determining the scope for constraint relaxation and stream regeneration or treatment.

The sensitivity analysis feature significantly reduces the effort required to determine the problematic areas of the network, which are the areas that pose the greatest barrier to saving. For this reason, WaterPinch is an effective tool for managing industrial water usage and reducing associated capital and operating costs.

D.5 Data

D.5.1 Water-Using Network (WaterTracker Mass Balance)

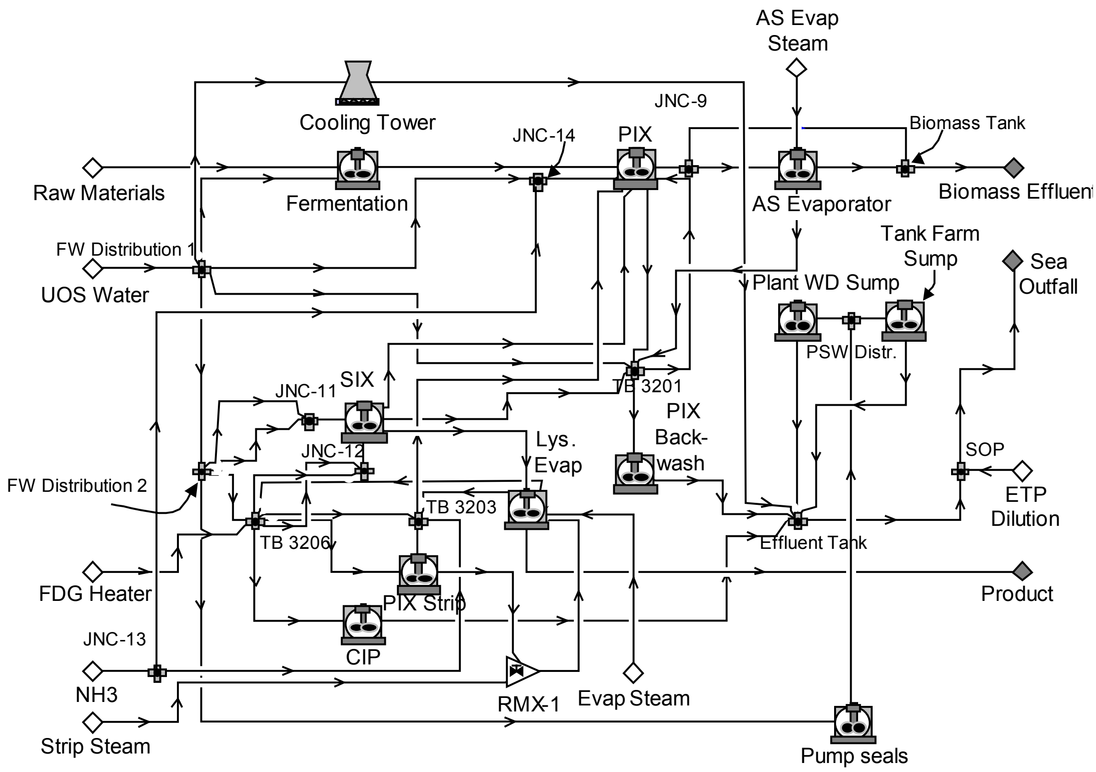

Figure D.8
The water-using network drawn on WaterTracker.

D.5.2 WaterTracker Flowrate and Contaminant Data

Table D.9 (a) and (b) gives the flowrate data tables, as they appear in WaterTracker, which correspond to the water-using network in figure D.8 (the tables have been split into two sections to accommodate the page formatting). Columns 1 and 2 show the inter-nodal connections that correspond to calculated and user-specified flowrates (column 3 and 4). Column 5, 11 and 14 is a tag that may be checked to indicate that the stream or parameter must be included in the analysis (default setting 'Yes'). Column 6, 7 and 8 give the trust category for the user-specified data. In column 6, 'Other' indicates that a user-specified maximum and minimum value is in use. Column 9 (table D.9 (b)) gives the stream linking for any mass balance relationship that is used and column 11 specifies the relationship. For example the flowrate of the cooling tower blowdown is 0.1205 times the freshwater feed flowrate. In column 12 splitting fraction data is listed. Column 13 lists physical maximum flowrate parameters.

The concentration data parameters (table D.10, D.11, D.12) are analogous to the flowrate data parameters.

TABLE D.9 (a)

Flowrate data specifications as they appear on WaterTracker.

	1	2	3	4	5	6	7	8
	From	To	Calc.'d	Flow rate	Use?	Trust	Minimum	Maximum
1	UOS Water	FW Distribution 1	63.75	67.11	Yes	+/- 5.0%	63.75	70.47
2	FW Distribution 1	Fermentation	3.99	3.99	Yes	Other	3.8	4.18
3	Fermentation	PIX	18.48	18.48	Yes	Other	17.33	19.64
4	PIX	TB 3201	21.12	22.83	Yes	Other	21.12	23.47
5	TB 3201	Backwash	17.43	17.43	Yes	Other	17.17	17.69
6	FW Distribution 1	FW Distribution 2	11.51	0				
7	FW Distribution 2	Pump seals	7.92	6.5	Yes	+/- 25.0%	4.88	8.13
8	CIP	Effluent Tank	6.38	0				
9	FW Distribution 1	TB 3201	4.05	0				
10	SIX	PIX	2.66	2.66	Yes	Other	2.57	2.75
11	Backwash	Effluent Tank	17.43	18.72				
12	ETP Dilution	SOP	80.14	80.14	Yes	+/- 2.0%	78.54	81.74
13	SOP	Sea Outfall	115.46	124.21				
14	Effluent Tank	SOP	35.32	44.07				
15	SIX	TB 3201	0.02	0.02	Yes	Other	0.02	0.02
16	TB 3201	PIX	14.17	14.17	Yes	Other	13.4	14.93
17	Raw Materials	Fermentation	14.49	0				
18	FW Distribution 2	TB 3206	1.47	0				
19	TB 3206	CIP	6.38	6.38	Yes	Other	6.08	6.69
20	AS Evaporator	Biomass Tank	9.14	9.14	Yes	Other	8.48	9.8
21	Biomass Tank	Biomass Effluent	24.97	0				
22	Plant WD Sump	Effluent Tank	5.28	0				
23	TB 3206	PIX Strip	12.43	12.43	Yes	Other	11.76	13.1
24	TB 3206	TB 3203	0.16	0				
25	TB 3203	PIX Strip	2.3	0				
26	Lys. Evap	TB 3206	17.09	16.33	Yes	Other	15.51	17.15
27	Lys. Evap	TB 3203	3.52	3.52	Yes	Other	3.34	3.7
28	TB 3203	PIX	1.85	1.85	Yes	Other	1.77	1.92
29	FDG Heater	TB 3206	1.74	1.74	Yes	Other	1.56	1.93
30	Lys. Evap	Product	1.59	1.59	Yes	Other	1.5	1.68
31	PIX	JNC-9	31.37	0				
32	JNC-9	AS Evaporator	15.54	15.54	Yes	Other	14.84	16.24
33	JNC-9	Biomass Tank	15.83	0				
34	RMX-1	Lys. Evap	18.25	0				
35	PIX Strip	RMX-1	14.73	14.74	Yes	Other	13.99	15.48
36	Strip Steam	RMX-1	3.52	3.52	Yes	Other	3.44	3.7
37	Pump seals	PSW Distr.	7.92	0				
38	PSW Distr.	Plant WD Sump	5.28	0				
39	PSW Distr.	Tank Farm Sump	2.64	0				
40	Tank Farm Sump	Effluent Tank	2.64	0				
41	Cooling Tower	[Evaporation]	26.17	0				
42	Cooling Tower	Effluent Tank	3.59	0				
43	AS Evap Steam	AS Evaporator	0	1.48				
44	Evap Steam	Lys. Evap	3.18	3.18	Yes	Other	3.01	3.35
45	FW Distribution 1	Cooling Tower	29.76	29.76	Yes	+/- 2.0%	29.16	30.36
46	FW Distribution 2	JNC-11	1.09	1.09	Yes	Other	1.08	1.11
47	FW Distribution 2	JNC-11	1.02	1.02	Yes	Other	0.97	1.08
48	JNC-11	SIX	2.12	0				
49	TB 3206	JNC-12	0.23	0.23	Yes	Other	0.21	0.24
50	TB 3206	JNC-12	1.1	1.1	Yes	Other	1.08	1.12
51	JNC-12	SIX	1.33	0				
52	SIX	Lys. Evap	0.76	0				
53	AS Evaporator	TB 3201	6.4	7.5	Yes	+/- 25.0%	5.63	9.38
54	JNC-13	TB 3203	0.46	0.46	Yes	+/- 25.0%	0.35	0.58
55	FW Distribution 1	JNC-14	14.44	14.44	Yes	Other	13.74	15.15
56	JNC-13	JNC-14	0.9	0.9	Yes	Other	0.87	0.93
57	JNC-14	PIX	15.34	0				
58	NH3	JNC-13	1.36	0				

TABLE D.9 (b)

Flowrate data specifications as they appear on WaterTracker.

	9	10	11	12	13	14
	Linked To	Use?	Value	Split Frac.	Phys.Max.	Use?
1					+inf	
2					+inf	
3	None		0		+inf	
4	None		0		63.62	Yes
5					+inf	
6					+inf	
7					+inf	
8	None		0		+inf	
9					63.62	Yes
10	None		0		+inf	
11	None		0		+inf	
12					+inf	
13					+inf	
14					74	Yes
15	None		0		0.03	Yes
16					+inf	
17					+inf	
18					+inf	
19					+inf	
20	None		0		+inf	
21					+inf	
22	None		0		+inf	
23					+inf	
24					+inf	
25					+inf	
26	None		0		+inf	
27	None		0		+inf	
28					+inf	
29					+inf	
30	None		0		+inf	
31	None		0		+inf	
32					+inf	
33					+inf	
34		Yes			+inf	
35	None		0		+inf	
36					+inf	
37	None		0		+inf	
38				0.667	+inf	
39				0.333	+inf	
40	None		0		+inf	
41	None		0		+inf	
42	FW Distribution 1 -> Cooling Tower	Yes	0.1205		+inf	
43					+inf	
44					+inf	
45					+inf	
46					+inf	
47					+inf	
48					+inf	
49					+inf	
50					+inf	
51					+inf	
52	None		0		+inf	
53	None		0		+inf	
54					+inf	
55					+inf	
56					+inf	
57					+inf	
58					+inf	

TABLE D.10 (a)

SS concentration data specifications as they appear on WaterTracker.

	1	2	3	4	5	6	7	8
	From	To	Calc.'d	Concentr.	Use?	Trust	Minimum	Maximum
1	UOS Water	FW Distribution 1	24.9	24.9	Yes	Other	0	64.3
2	FW Distribution 1	Fermentation	24.9	24.9	Yes	+/- 25.0%	18.68	31.13
3	Fermentation	PIX	1630.13	2000				
4	PIX	TB 3201	1341.12	400	Yes	+/- 25.0%	300	500
5	TB 3201	Backwash	963	0				
6	FW Distribution 1	FW Distribution 2	24.9	24.9	Yes	+/- 25.0%	18.68	31.13
7	FW Distribution 2	Pump seals	24.9	24.9	Yes	+/- 25.0%	18.68	31.13
8	CIP	Effluent Tank	7673.06	7673.06	Yes	+/- 2.0%	7519.6	7826.52
9	FW Distribution 1	TB 3201	24.9	24.9	Yes	+/- 25.0%	18.68	31.13
10	SIX	PIX	0	0				
11	Backwash	Effluent Tank	963	963	Yes	+/- 25.0%	722.25	1203.75
12	ETP Dilution	SOP	126.89	126.89	Yes	Other	100.11	153.68
13	SOP	Sea Outfall	669.32	728.44				
14	Effluent Tank	SOP	1687.65	505.09				
15	SIX	TB 3201	1805.24	0				
16	TB 3201	PIX	963	0				
17	Raw Materials	Fermentation	2588.95	0				
18	FW Distribution 2	TB 3206	24.9	24.9	Yes	+/- 25.0%	18.68	31.13
19	TB 3206	CIP	2.71	0				
20	AS Evaporator	Biomass Tank	0	0				
21	Biomass Tank	Biomass Effluent	0	0				
22	Plant WD Sump	Effluent Tank	81.5	695				
23	TB 3206	PIX Strip	2.71	0				
24	TB 3206	TB 3203	2.71	0				
25	TB 3203	PIX Strip	0.11	0				
26	Lys. Evap	TB 3206	0	0	Yes	+/- 2.0%	0	0
27	Lys. Evap	TB 3203	0	0	Yes	+/- 2.0%	0	0
28	TB 3203	PIX	0.11	0				
29	FDG Heater	TB 3206	0	0	Yes	+/- 2.0%	0	0
30	Lys. Evap	Product	0	0	Yes	+/- 2.0%	0	0
31	PIX	JNC-9	0	0				
32	JNC-9	AS Evaporator	0	0				
33	JNC-9	Biomass Tank	0	0				
34	RMX-1	Lys. Evap	0	0	Yes	+/- 2.0%	0	0
35	PIX Strip	RMX-1	0	0				
36	Strip Steam	RMX-1	0	0	Yes	+/- 2.0%	0	0
37	Pump seals	PSW Distr.	222.5	0				
38	PSW Distr.	Plant WD Sump	222.5	0				
39	PSW Distr.	Tank Farm Sump	222.5	0				
40	Tank Farm Sump	Effluent Tank	222.5	222.5	Yes	Other	77.95	367.05
41	Cooling Tower	[Evaporation]	0	0	Yes	+/- 2.0%	0	0
42	Cooling Tower	Effluent Tank	1000	1000	Yes	+/- 2.0%	980	1020
43	AS Evap Steam	AS Evaporator	0	0	Yes	+/- 2.0%	0	0
44	Evap Steam	Lys. Evap	0	0	Yes	+/- 2.0%	0	0
45	FW Distribution 1	Cooling Tower	---	0				
46	FW Distribution 2	JNC-11	---	0				
47	FW Distribution 2	JNC-11	---	0				
48	JNC-11	SIX	---	0				
49	TB 3206	JNC-12	---	0				
50	TB 3206	JNC-12	---	0				
51	JNC-12	SIX	---	0				
52	SIX	Lys. Evap	---	0				
53	AS Evaporator	TB 3201	---	1000	Yes	+/- 2.0%	980	1020
54	JNC-13	TB 3203	---	0				
55	FW Distribution 1	JNC-14	---	0				
56	JNC-13	JNC-14	---	0				
57	JNC-14	PIX	---	0				
58	NH3	JNC-13	---	0				

TABLE D.10 (b)

SS concentration data specifications as they appear on WaterTracker.

	9	10	11	12
	Linked To	Use?	Value	Link Type
1				
2				
3	None		0	<None>
4	None		0	<None>
5				
6	FW Distribution 1 -> Fermentation			Same as other outlet
7				
8	None		0	<None>
9	FW Distribution 1 -> Fermentation			Same as other outlet
10	None		0	<None>
11	None		0	<None>
12				
13				
14				
15	JNC-11 -> SIX	Yes	1	'Ccalc' = 'Cin' x Factor
16	TB 3201 -> Backwash (PIX stage 3)			Same as other outlet
17				
18	FW Distribution 2 -> Pump seals			Same as other outlet
19				
20	None		0	<None>
21				
22	None		0	<None>
23	TB 3206 -> CIP			Same as other outlet
24	TB 3206 -> CIP			Same as other outlet
25				
26	None		0	<None>
27	None		0	<None>
28	TB 3203 -> PIX Strip			Same as other outlet
29				
30	None		0	<None>
31	None		0	<None>
32				
33	JNC-9 -> AS Evaporator			Same as other outlet
34				
35	None		0	<None>
36				
37	None		0	<None>
38				
39	PSW Distr. -> Plant WD Sump			Same as other outlet
40	None		0	<None>
41	None		0	<None>
42	None		0	<None>
43				
44				
45	FW Distribution 1 -> Fermentation			Same as other outlet
46	FW Distribution 2 -> Pump seals			Same as other outlet
47	FW Distribution 2 -> Pump seals			Same as other outlet
48				
49	TB 3206 -> CIP			Same as other outlet
50	TB 3206 -> CIP			Same as other outlet
51				
52	None		0	<None>
53	None		0	<None>
54				
55	FW Distribution 1 -> Fermentation			Same as other outlet
56	JNC-13 -> TB 3203			Same as other outlet
57				
58				

TABLE D.11 (a)

FSA concentration data specifications as they appear on WaterTracker.

	1	2	3	4	5	6	7	8
	From	To	Calc.'d	Concentr.	Use?	Trust	Minimum	Maximum
1	UOS Water	FW Distribution 1	0	0	Yes	+/- 2.0%	0	0
2	FW Distribution 1	Fermentation	0	0				
3	Fermentation	PIX	2500	2500	Yes	+/- 25.0%	1875	3125
4	PIX	TB 3201	140.48	100	Yes	+/- 25.0%	75	125
5	TB 3201	Backwash	100	100	Yes	+/- 25.0%	75	125
6	FW Distribution 1	FW Distribution 2	0	0				
7	FW Distribution 2	Pump seals	0	0				
8	CIP	Effluent Tank	0	0				
9	FW Distribution 1	TB 3201	0	0				
10	SIX	PIX	0	0				
11	Backwash	Effluent Tank	300	300	Yes	+/- 25.0%	225	375
12	ETP Dilution	SOP	16.44	16.44	Yes	Other	14.82	18.07
13	SOP	Sea Outfall	96.56	96.56	Yes	Other	52.4	140.71
14	Effluent Tank	SOP	246.96	196.46				
15	SIX	TB 3201	0	0	Yes	+/- 2.0%	0	0
16	TB 3201	PIX	100	100	Yes	+/- 25.0%	75	125
17	Raw Materials	Fermentation	3993.26	0				
18	FW Distribution 2	TB 3206	0	0				
19	TB 3206	CIP	0	0				
20	AS Evaporator	Biomass Tank	53395.18	0				
21	Biomass Tank	Biomass Effluent	17080.06	0				
22	Plant WD Sump	Effluent Tank	277.67	0				
23	TB 3206	PIX Strip	0	0				
24	TB 3206	TB 3203	0	0				
25	TB 3203	PIX Strip	119000	119000	Yes	+/- 25.0%	89250	148750
26	Lys. Evap	TB 3206	0	0	Yes	+/- 2.0%	0	0
27	Lys. Evap	TB 3203	77835.11	0				
28	TB 3203	PIX	119000	119000	Yes	+/- 25.0%	89250	148750
29	FDG Heater	TB 3206	0	0	Yes	+/- 2.0%	0	0
30	Lys. Evap	Product	0	0	Yes	+/- 2.0%	0	0
31	PIX	JNC-9	12022.17	0				
32	JNC-9	AS Evaporator	12022.17	0				
33	JNC-9	Biomass Tank	12022.17	0				
34	RMX-1	Lys. Evap	15018.31	0				
35	PIX Strip	RMX-1	18608.62	0				
36	Strip Steam	RMX-1	0	0	Yes	+/- 2.0%	0	0
37	Pump seals	PSW Distr.	758.01	0				
38	PSW Distr.	Plant WD Sump	758.01	0				
39	PSW Distr.	Tank Farm Sump	758.01	0				
40	Tank Farm Sump	Effluent Tank	758.01	0				
41	Cooling Tower	[Evaporation]	0	0	Yes	+/- 2.0%	0	0
42	Cooling Tower	Effluent Tank	0	0	Yes	+/- 2.0%	0	0
43	AS Evap Steam	AS Evaporator	0	0	Yes	+/- 2.0%	0	0
44	Evap Steam	Lys. Evap	0	0	Yes	+/- 2.0%	0	0
45	FW Distribution 1	Cooling Tower	---	0				
46	FW Distribution 2	JNC-11	---	0				
47	FW Distribution 2	JNC-11	---	0				
48	JNC-11	SIX	---	0				
49	TB 3206	JNC-12	---	0				
50	TB 3206	JNC-12	---	0				
51	JNC-12	SIX	---	0				
52	SIX	Lys. Evap	---	0				
53	AS Evaporator	TB 3201	---	1500	Yes	+/- 2.0%	1470	1530
54	JNC-13	TB 3203	---	0				
55	FW Distribution 1	JNC-14	---	0				
56	JNC-13	JNC-14	---	0				
57	JNC-14	PIX	---	0				
58	NH3	JNC-13	---	68000	Yes	+/- 25.0%	51000	85000

TABLE D.11 (b)

FSA concentration data specifications as they appear on WaterTracker.

	9	10	11	12
	Linked To	Use?	Value	Link Type
1				
2				
3	None		0	<None>
4	None		0	<None>
5				
6	FW Distribution 1 -> Fermentation			Same as other outlet
7				
8	None		0	<None>
9	FW Distribution 1 -> Fermentation			Same as other outlet
10	None		0	<None>
11	None		0	<None>
12				
13				
14				
15	JNC-12 -> SIX	Yes	1	'Ccalc' = 'Cin' x Factor
16	TB 3201 -> Backwash (PIX stage 3)			Same as other outlet
17				
18	FW Distribution 2 -> Pump seals			Same as other outlet
19				
20	None		0	<None>
21				
22	None		0	<None>
23	TB 3206 -> CIP			Same as other outlet
24	TB 3206 -> CIP			Same as other outlet
25				
26	None		0	<None>
27	None		0	<None>
28	TB 3203 -> PIX Strip			Same as other outlet
29				
30	None		0	<None>
31	None		0	<None>
32				
33	JNC-9 -> AS Evaporator			Same as other outlet
34				
35	None		0	<None>
36				
37	None		0	<None>
38				
39	PSW Distr. -> Plant WD Sump			Same as other outlet
40	None		0	<None>
41	None		0	<None>
42	None		0	<None>
43				
44				
45	FW Distribution 1 -> Fermentation			Same as other outlet
46	FW Distribution 2 -> Pump seals			Same as other outlet
47	FW Distribution 2 -> Pump seals			Same as other outlet
48				
49	TB 3206 -> CIP			Same as other outlet
50	TB 3206 -> CIP			Same as other outlet
51				
52	None		0	<None>
53	None		0	<None>
54				
55	FW Distribution 1 -> Fermentation			Same as other outlet
56	JNC-13 -> TB 3203			Same as other outlet
57				
58				

TABLE D.12 (a)

Cl concentration data specifications as they appear on WaterTracker.

	1	2	3	4	5	6	7	8
	From	To	Calc.'d	Concentr.	Use?	Trust	Minimum	Maximum
1	UOS Water	FW Distribution 1	324.43	324.43	Yes	Other	308.73	340.13
2	FW Distribution 1	Fermentation	324.43	0				
3	Fermentation	PIX	121.32	0				
4	PIX	TB 3201	596.01	0				
5	TB 3201	Backwash	532.65	0				
6	FW Distribution 1	FW Distribution 2	324.43	0				
7	FW Distribution 2	Pump seals	324.43	0				
8	CIP	Effluent Tank	35.31	0				
9	FW Distribution 1	TB 3201	324.43	0				
10	SIX	PIX	0	0				
11	Backwash	Effluent Tank	532.65	0				
12	ETP Dilution	SOP	80.63	80.63	Yes	+/- 2.0%	79.02	82.24
13	SOP	Sea Outfall	172.32	0				
14	Effluent Tank	SOP	344.46	0				
15	SIX	TB 3201	23520.99	324.43	Yes	+/- 2.0%	317.94	330.92
16	TB 3201	PIX	532.65	0				
17	Raw Materials	Fermentation	0	0				
18	FW Distribution 2	TB 3206	324.43	0				
19	TB 3206	CIP	35.31	0				
20	AS Evaporator	Biomass Tank	0	0				
21	Biomass Tank	Biomass Effluent	0	0				
22	Plant WD Sump	Effluent Tank	118.84	0				
23	TB 3206	PIX Strip	35.31	0				
24	TB 3206	TB 3203	35.31	0				
25	TB 3203	PIX Strip	241.09	0				
26	Lys. Evap	TB 3206	0	0	Yes	+/- 2.0%	0	0
27	Lys. Evap	TB 3203	282.29	0				
28	TB 3203	PIX	241.09	0				
29	FDG Heater	TB 3206	0	0	Yes	+/- 2.0%	0	0
30	Lys. Evap	Product	0	0	Yes	+/- 2.0%	0	0
31	PIX	JNC-9	0	0				
32	JNC-9	AS Evaporator	0	0				
33	JNC-9	Biomass Tank	0	0				
34	RMX-1	Lys. Evap	54.47	0				
35	PIX Strip	RMX-1	67.49	0				
36	Strip Steam	RMX-1	0	0	Yes	+/- 2.0%	0	0
37	Pump seals	PSW Distr.	324.43	0				
38	PSW Distr.	Plant WD Sump	324.43	0				
39	PSW Distr.	Tank Farm Sump	324.43	0				
40	Tank Farm Sump	Effluent Tank	324.43	0				
41	Cooling Tower	[Evaporation]	0	0	Yes	+/- 2.0%	0	0
42	Cooling Tower	Effluent Tank	669.23	669.23	Yes	Other	616.11	722.35
43	AS Evap Steam	AS Evaporator	0	0	Yes	+/- 2.0%	0	0
44	Evap Steam	Lys. Evap	0	0	Yes	+/- 2.0%	0	0
45	FW Distribution 1	Cooling Tower	---	0				
46	FW Distribution 2	JNC-11	---	0				
47	FW Distribution 2	JNC-11	---	0				
48	JNC-11	SIX	---	0				
49	TB 3206	JNC-12	---	0				
50	TB 3206	JNC-12	---	0				
51	JNC-12	SIX	---	0				
52	SIX	Lys. Evap	---	0				
53	AS Evaporator	TB 3201	---	0	Yes	+/- 2.0%	0	0
54	JNC-13	TB 3203	---	0				
55	FW Distribution 1	JNC-14	---	0				
56	JNC-13	JNC-14	---	0				
57	JNC-14	PIX	---	0				
58	NH3	JNC-13	---	324.43	Yes	+/- 2.0%	317.94	330.92

TABLE D.12 (a)
Cl concentration data specifications as they appear on WaterTracker.

	9	10	11	12
	Linked To	Use?	Value	Link Type
1				
2				
3	None		0	<None>
4	JNC-14 -> PIX	Yes	1	'Ccalc' = 'Cin' x Factor
5				
6	FW Distribution 1 -> Fermentation			Same as other outlet
7				
8	None		0	<None>
9	FW Distribution 1 -> Fermentation			Same as other outlet
10	None		0	<None>
11	None		0	<None>
12				
13				
14				
15	JNC-11 -> SIX	Yes	1	'Ccalc' = 'Cin' x Factor
16	TB 3201 -> Backwash (PIX stage 3)			Same as other outlet
17				
18	FW Distribution 2 -> Pump seals			Same as other outlet
19				
20	None		0	<None>
21				
22	None		0	<None>
23	TB 3206 -> CIP			Same as other outlet
24	TB 3206 -> CIP			Same as other outlet
25				
26	None		0	<None>
27	None		0	<None>
28	TB 3203 -> PIX Strip			Same as other outlet
29				
30	None		0	<None>
31	None		0	<None>
32				
33	JNC-9 -> AS Evaporator			Same as other outlet
34				
35	None		0	<None>
36				
37	None		0	<None>
38				
39	PSW Distr. -> Plant WD Sump			Same as other outlet
40	None		0	<None>
41	None		0	<None>
42	None		0	<None>
43				
44				
45	FW Distribution 1 -> Fermentation			Same as other outlet
46	FW Distribution 2 -> Pump seals			Same as other outlet
47	FW Distribution 2 -> Pump seals			Same as other outlet
48				
49	TB 3206 -> CIP			Same as other outlet
50	TB 3206 -> CIP			Same as other outlet
51				
52	None		0	<None>
53	None		0	<None>
54				
55	FW Distribution 1 -> Fermentation			Same as other outlet
56	JNC-13 -> TB 3203			Same as other outlet
57				
58				

D.5.3 Source and Sink Elimination

TABLE D.13
Classification of WaterTracker streams for determining the WaterPinch model.

	From	To	Use?
1	UOS Water	FW Distribution 1	UOS water: Utility source
2	FW Distribution 1	Fermentation	Yes: Process sink
3	Fermentation	PIX	No
4	PIX	TB 3201	No
5	TB 3201	Backwash	Yes: Process operation (sink)
6	FW Distribution 1	FW Distribution 2	No
7	FW Distribution 2	Pump seals	Yes: Process operation (sink)
8	CIP	Effluent Tank	Yes: Process operation (source)
9	FW Distribution 1	TB 3201	No
10	SIX	PIX	No
11	Backwash	Effluent Tank	Yes: Process operation (source)
12	ETP Dilution	SOP	Yes: Process source
13	SOP	Sea Outfall	Yes: Utility sink
14	Effluent Tank	SOP	No
15	SIX	TB 3201	No
16	TB 3201	PIX	No
17	Raw Materials	Fermentation	No
18	FW Distribution 2	TB 3206	No
19	TB 3206	CIP	Yes: Process operation (sink)
20	AS Evaporator	Biomass Tank	No: Flow combined with JNC-9 to Biomass tank (33.)
21	Biomass Tank	Biomass Effluent	Yes: Utility sink (SWW)
22	Plant WD Sump	Effluent Tank	No
23	TB 3206	PIX Strip	Yes: Process sink
24	TB 3206	TB 3203	Yes: Process sink (PIX NH3 dilution)
25	TB 3203	PIX Strip	No
26	Lys. Evap	TB 3206	Yes: Process source (pure condensate)
27	Lys. Evap	TB 3203	No
28	TB 3203	PIX	No
29	FDG Heater	TB 3206	Yes: Process source (pure condensate)
30	Lys. Evap	Product	No
31	PIX	JNC-9	No
32	JNC-9	AS Evaporator	No
33	JNC-9	Biomass Tank	Yes: Process operation (source), PIX adsorption outlet combined with AS evaporator effluent (20.)
34	RMX-1	Lys. Evap	No
35	PIX Strip	RMX-1	No
36	Strip Steam	RMX-1	No
37	Pump seals	PSW Distr.	Yes: Process operation source
38	PSW Distr.	Plant WD Sump	No
39	PSW Distr.	Tank Farm Sump	No
40	Tank Farm Sump	Effluent Tank	No
41	Cooling Tower	[Evaporation]	No
42	Cooling Tower	Effluent Tank	Yes: Process operation (source)
43	AS Evap Steam	AS Evaporator	No
44	Evap Steam	Lys. Evap	No
45	FW Distribution 1	Cooling Tower	Yes: Process operation (sink)
46	FW Distribution 2	JNC-11	No
47	FW Distribution 2	JNC-11	No
48	JNC-11	SIX	Yes: Process sink (SIX acid dilution)
49	TB 3206	JNC-12	No
50	TB 3206	JNC-12	No
51	JNC-12	SIX	Yes: Process sink (SIX rinse)
52	SIX	Lys. Evap	No
53	AS Evaporator	TB 3201	Yes: Process source (AS condensate)
54	JNC-13	TB 3203	No
55	FW Distribution 1	JNC-14	No
56	JNC-13	JNC-14	No
57	JNC-14	PIX	Yes: Process operation (source), PIX adsorption.
58	NH3	JNC-13	No

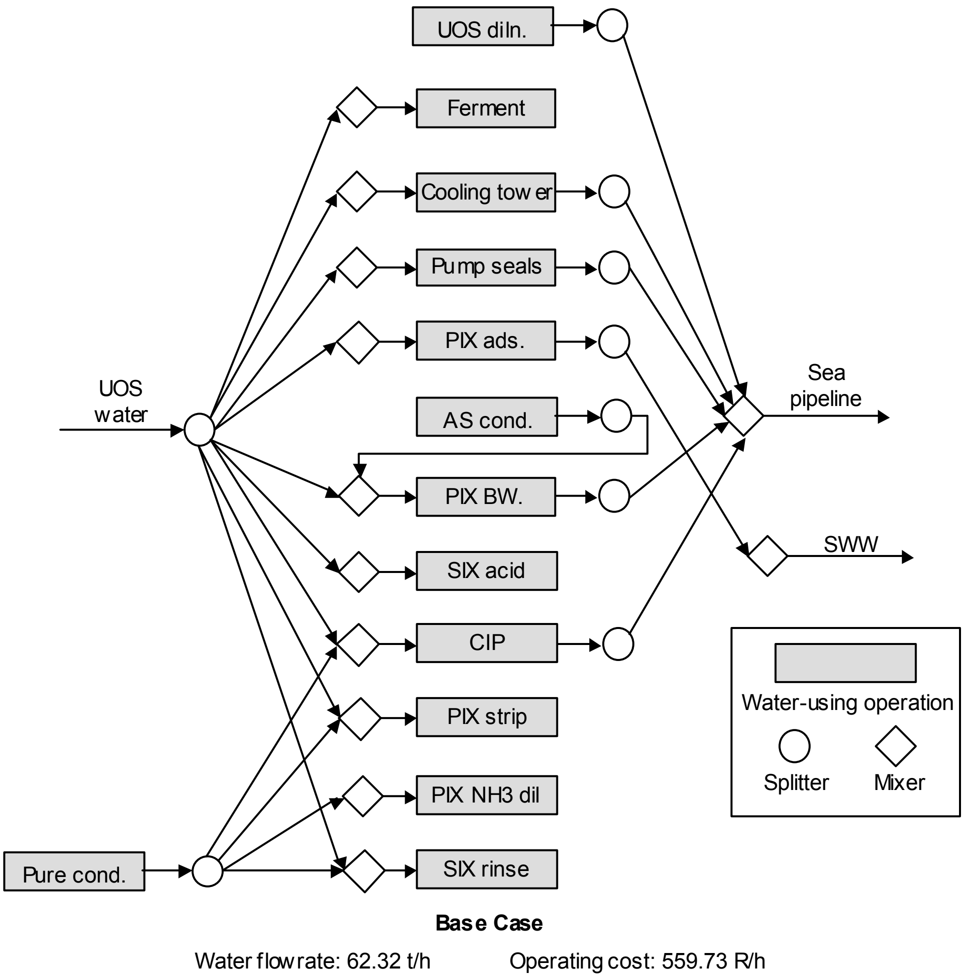

Figure D.9
Base-case water-using subsystem design for the AECI Bioproducts system.

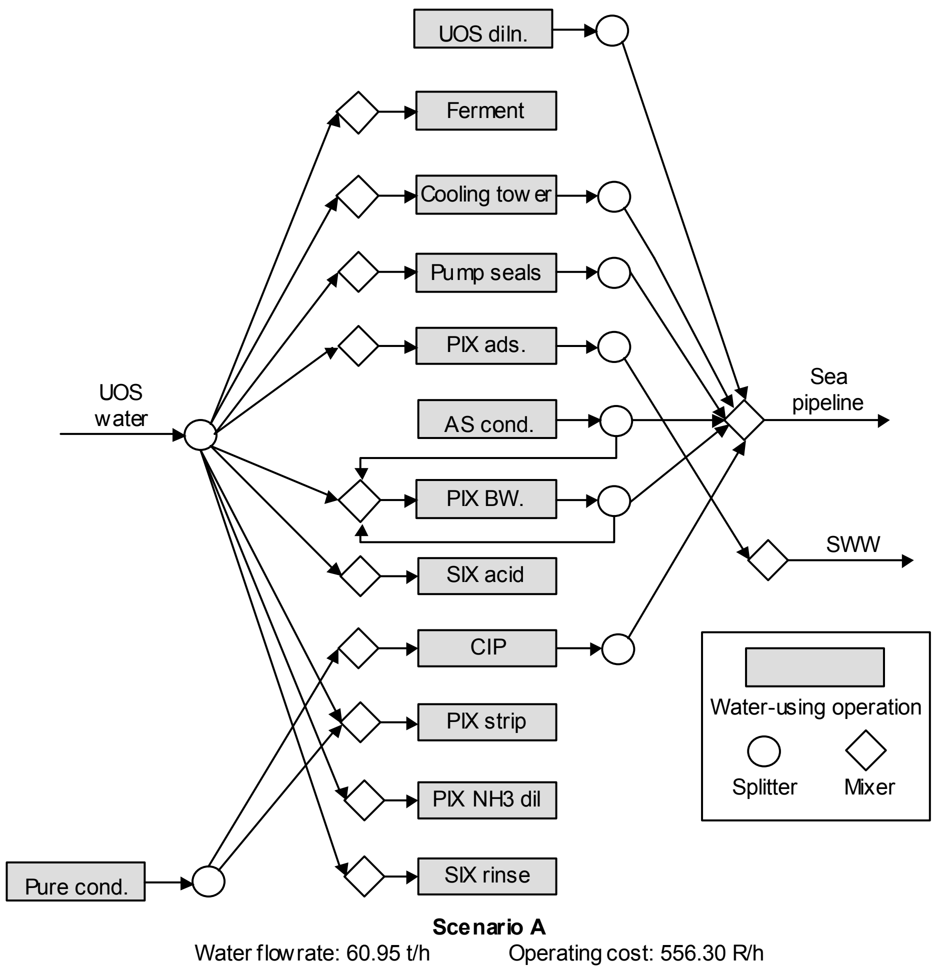

Figure D.10
Design of water-using network for optimal connectivity in table D.8

Appendix E: Data

E.1 Mass Balance Data

Table E.1 to E.4 below give the flowrate and contaminant input data that was entered into WaterTracker. The specified minimum and maximum values are given, which were calculated determining the standard deviation about the mean (Appendix B), or the 95% confidence interval where significant outliers were present. Where the uncertainty in he data is not explicitly known, a percentage tolerance is specified. Values calculated using WaterTracker are given alongside the user specified values. The stream names correspond to the nodes of the network in figure E.1.

E.1.1 Connectivity Data

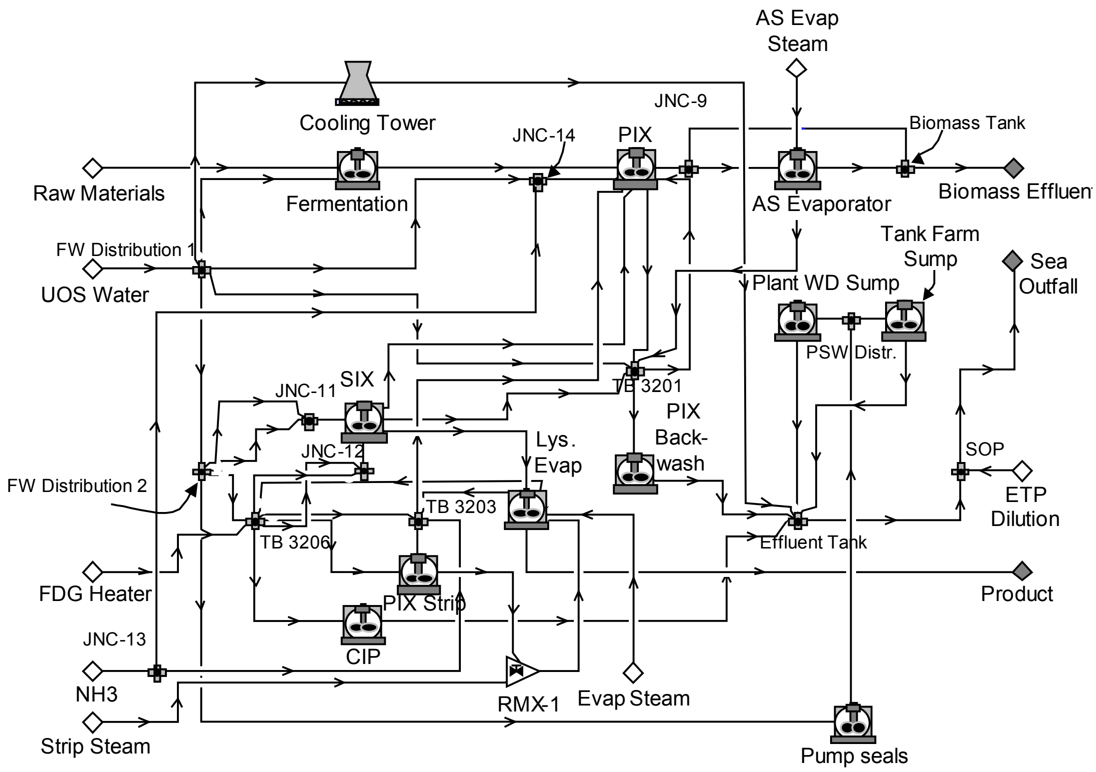

Figure E.1
The water-using network drawn on WaterTracker.

E.1.2 Flow Data

TABLE E.1
Calculated and user-specified stream flowrates.

Stream		Flowrate / [t/h]		Trust		
From	To	Calc.'d	Specified	%	Minimum [t/h]	Maximum [t/h]
UOS Water	FW Distribution 1	63.75	67.11	+/- 5.0	63.75	70.47
FW Distribution 1	Fermentation	3.99	3.99		3.8	4.18
Fermentation	PIX	18.48	18.48		17.33	19.64
PIX	TB 3201	21.12	22.83		21.12	23.47
TB 3201	Backwash	17.43	17.43		17.17	17.69
FW Distribution 1	FW Distribution 2	11.51	0			
FW Distribution 2	Pump seals	7.92	6.5	+/- 25.0	4.88	8.13
CIP	Effluent Tank	6.38	0			
FW Distribution 1	TB 3201	4.05	0			
SIX	PIX	2.66	2.66		2.57	2.75
Backwash	Effluent Tank	17.43	18.72			
ETP Dilution	SOP	80.14	80.14	+/- 2.0	78.54	81.74
SOP	Sea Outfall	115.46	124.21			
Effluent Tank	SOP	35.32	44.07			
SIX	TB 3201	0.02	0.02		0.02	0.02
TB 3201	PIX	14.17	14.17		13.4	14.93
Raw Materials	Fermentation	14.49	0			
FW Distribution 2	TB 3206	1.47	0			
TB 3206	CIP	6.38	6.38		6.08	6.69
AS Evaporator	Biomass Tank	9.14	9.14		8.48	9.8
Biomass Tank	Biomass Effluent	24.97	0			
Plant WD Sump	Effluent Tank	5.28	0			
TB 3206	PIX Strip	12.43	12.43		11.76	13.1
TB 3206	TB 3203	0.16	0			
TB 3203	PIX Strip	2.3	0			
Lys. Evap	TB 3206	17.09	16.33		15.51	17.15
Lys. Evap	TB 3203	3.52	3.52		3.34	3.7
TB 3203	PIX	1.85	1.85		1.77	1.92
FDG Heater	TB 3206	1.74	1.74		1.56	1.93
Lys. Evap	Product	1.59	1.59		1.5	1.68
PIX	JNC-9	31.37	0			
JNC-9	AS Evaporator	15.54	15.54		14.84	16.24
JNC-9	Biomass Tank	15.83	0			
RMX-1	Lys. Evap	18.25	0			
PIX Strip	RMX-1	14.73	14.74		13.99	15.48
Strip Steam	RMX-1	3.52	3.52		3.44	3.7
Pump seals	PSW Distr.	7.92	0			
PSW Distr.	Plant WD Sump	5.28	0			
PSW Distr.	Tank Farm Sump	2.64	0			
Tank Farm Sump	Effluent Tank	2.64	0			
Cooling Tower	[Evaporation]	26.17	0			
Cooling Tower	Effluent Tank	3.59	0			

TABLE E.1 (contd.)
Calculated and user-specified stream flowrates.

Stream		Flowrate / [t/h]			Trust	
From	To	Calc.'d	Specified	%	Minimum [t/h]	Maximum [t/h]
AS Evap Steam	AS Evaporator	0	1.48			
Evap Steam	Lys. Evap	3.18	3.18		3.01	3.35
FW Distribution 1	Cooling Tower	29.76	29.76		29.16	30.36
FW Distribution 2	JNC-11	1.09	1.09		1.08	1.11
FW Distribution 2	JNC-11	1.02	1.02		0.97	1.08
JNC-11	SIX	2.12	0			
TB 3206	JNC-12	0.23	0.23		0.21	0.24
TB 3206	JNC-12	1.1	1.1		1.08	1.12
JNC-12	SIX	1.33	0			
SIX	Lys. Evap	0.76	0			
AS Evaporator	TB 3201	6.4	7.5		5.63	9.38
JNC-13	TB 3203	0.46	0.46		0.35	0.58
FW Distribution 1	JNC-14	14.44	14.44		13.74	15.15
JNC-13	JNC-14	0.9	0.9		0.87	0.93
JNC-14	PIX	15.34	0			
NH3	JNC-13	1.36	0			

E.1.3 Concentration Data

TABLE E.2
Calculated and user-specified SS concentration.

Stream		Concentration [ppm]			Trust	
From	To	Calc.'d	Specified	%	Minimum [ppm]	Maximum [ppm]
UOS Water	FW Distribution 1	24.9	24.9		0	64.3
FW Distribution 1	Fermentation	24.9	24.9	+/- 25.0	18.68	31.13
Fermentation	PIX	1630.13	2000			
PIX	TB 3201	1341.12	400	+/- 25.0	300	500
TB 3201	Backwash	963	0			
FW Distribution 1	FW Distribution 2	24.9	24.9	+/- 25.0	18.68	31.13
FW Distribution 2	Pump seals	24.9	24.9	+/- 25.0	18.68	31.13
CIP	Effluent Tank	7673.06	7673.06	+/- 2.0	7519.6	7826.52
FW Distribution 1	TB 3201	24.9	24.9	+/- 25.0	18.68	31.13
SIX	PIX	0	0			
Backwash	Effluent Tank	963	963	+/- 25.0	722.25	1203.75
ETP Dilution	SOP	126.89	126.89		100.11	153.68
SOP	Sea Outfall	669.32	728.44			
Effluent Tank	SOP	1687.65	505.09			
SIX	TB 3201	1805.24	0			
TB 3201	PIX	963	0			
Raw Materials	Fermentation	2588.95	0			
FW Distribution 2	TB 3206	24.9	24.9	+/- 25.0	18.68	31.13
TB 3206	CIP	2.71	0			
AS Evaporator	Biomass Tank	0	0			

TABLE E.2 (contd.)
Calculated and user-specified SS concentration.

Stream		Concentration [ppm]		Trust		
From	To	Calc.'d	Specified	%	Minimum [ppm]	Maximum [ppm]
PSW Distr.	Tank Farm Sump	222.5	0			
Tank Farm Sump	Effluent Tank	222.5	222.5		77.95	367.05
Cooling Tower	[Evaporation]	0	0	+/- 2.0	0	0
Cooling Tower	Effluent Tank	1000	1000	+/- 2.0	980	1020
AS Evap Steam	AS Evaporator	0	0	+/- 2.0	0	0
Evap Steam	Lys. Evap	0	0	+/- 2.0	0	0
FW Distribution 1	Cooling Tower	---	0			
FW Distribution 2	JNC-11	---	0			
FW Distribution 2	JNC-11	---	0			
JNC-11	SIX	---	0			
TB 3206	JNC-12	---	0			
TB 3206	JNC-12	---	0			
JNC-12	SIX	---	0			
SIX	Lys. Evap	---	0			
AS Evaporator	TB 3201	---	1000	+/- 2.0	980	1020
JNC-13	TB 3203	---	0			
FW Distribution 1	JNC-14	---	0			
JNC-13	JNC-14	---	0			
JNC-14	PIX	---	0			
NH3	JNC-13	---	0			
Biomass Tank	Biomass Effluent	0	0			
Plant WD Sump	Effluent Tank	81.5	695			
TB 3206	PIX Strip	2.71	0			
TB 3206	TB 3203	2.71	0			
TB 3203	PIX Strip	0.11	0			
Lys. Evap	TB 3206	0	0	+/- 2.0	0	0
Lys. Evap	TB 3203	0	0	+/- 2.0	0	0
TB 3203	PIX	0.11	0			
FDG Heater	TB 3206	0	0	+/- 2.0	0	0
Lys. Evap	Product	0	0	+/- 2.0	0	0
PIX	JNC-9	0	0			
JNC-9	AS Evaporator	0	0			
JNC-9	Biomass Tank	0	0			
RMX-1	Lys. Evap	0	0	+/- 2.0	0	0
PIX Strip	RMX-1	0	0			
Strip Steam	RMX-1	0	0	+/- 2.0	0	0
Pump seals	PSW Distr.	222.5	0			
PSW Distr.	Plant WD Sump	222.5	0			

TABLE E.3
Calculated and user-specified FSA concentration.

Stream		Concentration [ppm]		Trust		
From	To	Calc.'d	Specified	%	Minimum [ppm]	Maximum [ppm]
UOS Water	FW Distribution 1	0	0	+/- 2.0	0	0
FW Distribution 1	Fermentation	0	0			
Fermentation	PIX	2500	2500	+/- 25.0	1875	3125
PIX	TB 3201	140.48	100	+/- 25.0	75	125
TB 3201	Backwash	100	100	+/- 25.0	75	125
FW Distribution 1	FW Distribution 2	0	0			
FW Distribution 2	Pump seals	0	0			
CIP	Effluent Tank	0	0			
FW Distribution 1	TB 3201	0	0			
SIX	PIX	0	0			
Backwash	Effluent Tank	300	300	+/- 25.0	225	375
ETP Dilution	SOP	16.44	16.44		14.82	18.07
SOP	Sea Outfall	96.56	96.56		52.4	140.71
Effluent Tank	SOP	246.96	196.46			
SIX	TB 3201	0	0	+/- 2.0	0	0
TB 3201	PIX	100	100	+/- 25.0	75	125
Raw Materials	Fermentation	3993.26	0			
FW Distribution 2	TB 3206	0	0			
TB 3206	CIP	0	0			
AS Evaporator	Biomass Tank	53395.18	0			
Biomass Tank	Biomass Effluent	17080.06	0			
Plant WD Sump	Effluent Tank	277.67	0			
TB 3206	PIX Strip	0	0			
TB 3206	TB 3203	0	0			
TB 3203	PIX Strip	119000	119000	+/- 25.0	89250	148750
Lys. Evap	TB 3206	0	0	+/- 2.0	0	0
Lys. Evap	TB 3203	77835.11	0			
TB 3203	PIX	119000	119000	+/- 25.0	89250	148750
FDG Heater	TB 3206	0	0	+/- 2.0	0	0
Lys. Evap	Product	0	0	+/- 2.0	0	0
PIX	JNC-9	12022.17	0			
JNC-9	AS Evaporator	12022.17	0			
JNC-9	Biomass Tank	12022.17	0			
RMX-1	Lys. Evap	15018.31	0			
PIX Strip	RMX-1	18608.62	0			
Strip Steam	RMX-1	0	0	+/- 2.0	0	0
Pump seals	PSW Distr.	758.01	0			
PSW Distr.	Plant WD Sump	758.01	0			
PSW Distr.	Tank Farm Sump	758.01	0			
Tank Farm Sump	Effluent Tank	758.01	0			
Cooling Tower	[Evaporation]	0	0	+/- 2.0	0	0

TABLE E.3 (contd.)
Calculated and user-specified FSA concentration.

Stream		Concentration [ppm]			Trust	
From	To	Calc.'d	Specified	%	Minimum [ppm]	Maximum [ppm]
Cooling Tower	Effluent Tank	0	0	+/- 2.0	0	0
AS Evap Steam	AS Evaporator	0	0	+/- 2.0	0	0
Evap Steam	Lys. Evap	0	0	+/- 2.0	0	0
FW Distribution 1	Cooling Tower	---	0			
FW Distribution 2	JNC-11	---	0			
FW Distribution 2	JNC-11	---	0			
JNC-11	SIX	---	0			
TB 3206	JNC-12	---	0			
TB 3206	JNC-12	---	0			
JNC-12	SIX	---	0			
SIX	Lys. Evap	---	0			
AS Evaporator	TB 3201	---	1500	+/- 2.0	1470	1530
JNC-13	TB 3203	---	0			
FW Distribution 1	JNC-14	---	0			
JNC-13	JNC-14	---	0			
JNC-14	PIX	---	0			
NH3	JNC-13	---	68000	+/- 25.0	51000	85000

TABLE E.4
Calculated and user-specified Cl concentration.

Stream		Concentration [ppm]			Trust	
From	To	Calc.'d	Specified	%	Minimum [ppm]	Maximum [ppm]
UOS Water	FW Distribution 1	324.43	324.43		308.73	340.13
FW Distribution 1	Fermentation	324.43	0			
Fermentation	PIX	121.32	0			
PIX	TB 3201	596.01	0			
TB 3201	Backwash	532.65	0			
FW Distribution 1	FW Distribution 2	324.43	0			
FW Distribution 2	Pump seals	324.43	0			
CIP	Effluent Tank	35.31	0			
FW Distribution 1	TB 3201	324.43	0			
SIX	PIX	0	0			
Backwash	Effluent Tank	532.65	0			
ETP Dilution	SOP	80.63	80.63	+/- 2.0	79.02	82.24
SOP	Sea Outfall	172.32	0			
Effluent Tank	SOP	344.46	0			
SIX	TB 3201	23520.99	324.43	+/- 2.0	317.94	330.92
TB 3201	PIX	532.65	0			
Raw Materials	Fermentation	0	0			
FW Distribution 2	TB 3206	324.43	0			
TB 3206	CIP	35.31	0			
AS Evaporator	Biomass Tank	0	0			

TABLE E.4 (contd.)
Calculated and user-specified Cl concentration.

Stream		Concentration [ppm]		Trust		
From	To	Calc.'d	Specified	%	Minimum [ppm]	Maximum [ppm]
Biomass Tank	Biomass Effluent	0	0			
Plant WD Sump	Effluent Tank	118.84	0			
TB 3206	PIX Strip	35.31	0			
TB 3206	TB 3203	35.31	0			
TB 3203	PIX Strip	241.09	0			
Lys. Evap	TB 3206	0	0	+/- 2.0	0	0
Lys. Evap	TB 3203	282.29	0			
TB 3203	PIX	241.09	0			
FDG Heater	TB 3206	0	0	+/- 2.0	0	0
Lys. Evap	Product	0	0	+/- 2.0	0	0
PIX	JNC-9	0	0			
JNC-9	AS Evaporator	0	0			
JNC-9	Biomass Tank	0	0			
RMX-1	Lys. Evap	54.47	0			
PIX Strip	RMX-1	67.49	0			
Strip Steam	RMX-1	0	0	+/- 2.0	0	0
Pump seals	PSW Distr.	324.43	0			
PSW Distr.	Plant WD Sump	324.43	0			
PSW Distr.	Tank Farm Sump	324.43	0			
Tank Farm Sump	Effluent Tank	324.43	0			
Cooling Tower	[Evaporation]	0	0	+/- 2.0	0	0
Cooling Tower	Effluent Tank	669.23	669.23		616.11	722.35
AS Evap Steam	AS Evaporator	0	0	+/- 2.0	0	0
Evap Steam	Lys. Evap	0	0	+/- 2.0	0	0
FW Distribution 1	Cooling Tower	---	0			
FW Distribution 2	JNC-11	---	0			
FW Distribution 2	JNC-11	---	0			
JNC-11	SIX	---	0			
TB 3206	JNC-12	---	0			
TB 3206	JNC-12	---	0			
JNC-12	SIX	---	0			
SIX	Lys. Evap	---	0			
AS Evaporator	TB 3201	---	0	+/- 2.0	0	0
JNC-13	TB 3203	---	0			
FW Distribution 1	JNC-14	---	0			
JNC-13	JNC-14	---	0			
JNC-14	PIX	---	0			
NH3	JNC-13	---	324.43	+/- 2.0	317.94	330.92

E.2 Pipe Capacities

The pipe capacities in table E.5 and E.6 were used to determine the *existing capacity* above which a new connection is specified (which would incur a piping and installation cost).

TABLE E.5
Pipe diameters and capacities for existing connections.

From	To	Flow / [m^3/h]	Required pipe diameter / [in]	Capacity / [m^3/h]
CIP	Sea pipeline	6.38	4	8.99
Pump seals	Sea pipeline	6.5	4	8.99
Cooling tower	Sea pipeline	3.59	3	5.22
PIX b-w	Sea pipeline	18.72	6	20.44
PIX ads	SWW	12.485	5	14.15
AS condensate	PIX b-w	7.5	4	8.99
	Sea pipeline	7.5	4	8.99
UOS water	Fermentation	3.99	3	5.22
	Pump seals	6.5	4	8.99
	Cooling tower	29.76	8	35.36
	PIX ads	14.44	6	20.44
	PIX b-w	8.83	4	8.99
	SIX acid	1.38	1.5	1.44

TABLE E.6
Pipe diameters and capacities for existing connections from condensate tank

From	To	Tank feeds / [m^3/h]	Required pipe diameter / [in]	Capacity / [m^3/h]
Pure condensate	CIP PIX strip SIX rinse PIX NH_3 dilution	18.07	6	20.44
UOS water	CIP SIX rinse PIX strip	2.20	2	2.37

E.3 Solution Flow Data

The flowrate data for the configurations in Scenario B, C, and the case when the FSA and SS are relaxed in the sea pipeline, are given in table E.7, E8, and E.9 below.

TABLE E.7
Matrix of inter-operation flows for the configuration of the Scenario B water system; flows in t/h (figure 3.6).

From \ To	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH_3 dil.	PIX ads.	PIX b-w	SIX rinse	SIX acid	Sea pipeline	SWW
CIP											6.38	
Pump seals											6.50	
Cooling tower											3.59	
Pure condensate		6.38			11.69							
UOS dilution											80.14	
PIX b-w								3.48			13.95	
PIX ads												24.97
AS cond.								6.40				
UOS water	3.99		6.50	29.76	0.74	0.16	14.44	0.57	1.30	1.38		

Existing connection

TABLE E.8
Matrix of inter-operation flows for the configuration of the Scenario C water system; flows in t/h (figure 3.8).

From \ To	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH_3 dil.	PIX ads.	PIX b-w	SIX rinse	SIX acid	Sea pipeline	SWW
CIP											6.38	
Pump seals											6.50	
Cooling tower											3.59	
Pure condensate		6.38			11.69							
UOS dilution											80.14	
PIX b-w								3.48			13.95	
PIX ads												24.97
AS cond.											6.40	
UOS water	3.99		6.50	29.76	0.74	0.16	14.44	6.97	1.30	1.38		

Existing connection

TABLE E.9
Matrix of inter-operation flows for the configuration of the water system with SS unconstrained in the sea pipeline and FSA ≤ 5000ppm; flows in t/h (figure 3.18).

From \ To	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH_3 dil.	PIX ads.	PIX b-w	SIX rinse	SIX acid	Sea pipeline	SWW
CIP											6.38	
Pump seals											6.50	
Cooling tower											3.59	
Pure condensate		6.38			10.39				1.30			
UOS dilution											80.14	
PIX b-w								1.00			16.43	
PIX ads											19.65	5.32
AS cond.								0.46			5.94	
UOS water	3.99		6.50	29.76	2.04	0.16	14.44	8.99		1.38		

Existing connection

E.4 Scenario A, B, and C Solution Concentration Data

The sink (water-using operation inlet) and source (water-using operation outlet) flowrate and contaminant concentration conditions for each scenario are listed in table E.10 to E.15, below. The values annotated with an asterisk indicate that the sink concentration is not at its limit.

TABLE E.10
Scenario A sink conditions.

Name	Flow / [t/h]	SS / [ppm]	FSA / [ppm]	Cl / [ppm]
Fermentation	3.99	24.90	0.00	80.63*
PIX strip rinse	12.43	1.80*	0.00	5.84*
SIX acid dil.	1.38	24.90	0.00	80.63*
SIX rinse	1.30	24.90	0.00	80.63*
Pump seals	6.50	24.90	0.00	80.63
CIP	6.38	0.00*	0.00	0.00*
PIX ads	14.44	24.90	0.00*	80.63*
PIX b-w	10.45	625.00	100.00	31.01*
Cooling tower	29.76	24.90	0.00	80.63
PIX NH3 dil.	0.16	0.00*	0.00	0.00*
Sea outfall pipe	112.67	665.52*	48.85*	87.19*
SWW	24.97	3.50×10^{5}*	3.50×10^{4}*	1.00×10^{3}*

TABLE E.11
Scenario A source conditions.

Name	Flow / [t/h]	SS / [ppm]	FSA / [ppm]	Cl / [ppm]
UOS dilution	80.14	126.89	16.44	80.63
AS evap. cond.	6.40	1.00×10^{3}	0.00	0.00
Pure cond.	18.07	0.00	0.00	0.00
Pump seals	6.50	222.50	0.00	80.63
CIP	6.38	7670.35	0.00	0.00
PIX ads.	24.97	3.50×10^{5}	3.50×10^{4}	1.00×10^{3}
PIX b-w	17.43	625.00	300.05	31.01
Cooling tower	3.59	1000	0.00	670.04
UOS water	60.95	24.90	0.00	80.63

TABLE E.12
Scenario B sink conditions.

Name	Flow / [t/h]	SS / [ppm]	FSA / [ppm]	Cl / [ppm]
Fermentation	3.99	24.90	0.00	80.63*
PIX strip rinse	12.43	4.09*	0.00	13.23*
SIX acid dil.	1.38	24.90	0.00	80.63*
SIX rinse	1.30	0.00*	0.00	0.00*
Pump seals	6.50	24.90	0.00	80.63
CIP	6.38	0.00*	0.00	0.00*
PIX ads	14.44	24.90	0.00*	80.63*
PIX b-w	10.45	2.03	100.00	6.56*
Cooling tower	29.76	24.90	0.00	80.63
PIX NH3 dil.	0.16	24.90	0.00	80.63*
Sea outfall pipe	110.59	678.05*	59.53*	86.03*
SWW	24.94	3.50×10^{5}*	3.50×10^{4}*	1.00×10^{3}*

TABLE E.13
Scenario B source conditions.

Name	Flow / [t/h]	SS / [ppm]	FSA / [ppm]	Cl / [ppm]
UOS dilution	80.14	126.89	16.44	80.63
AS evap cond.	6.40	0.00	0.00	0.00
Pure cond.	18.07	0.00	0.00	0.00
Pump seals	6.50	222.5	0.00	80.63
CIP	6.38	7.67×10^{3}	0.00	0.00
PIX ads	24.97	3.50×10^{5}	3.50×10^{4}	1.00×10^{3}
PIX b-w	17.43	2.03	300.05	6.56
Cooling tower	3.59	1.00×10^{3}	0.00	670.04
UOS water	58.84	24.90	0.00	80.63

TABLE E.14
Scenario C sink conditions.

Name	Flow / [t/h]	SS / [ppm]	FSA / [ppm]	Cl / [ppm]
Fermentation	3.99	24.90	0.00	80.63*
PIX strip rinse	12.43	1.48*	0.00	4.80*
SIX acid dil.	1.38	24.90	0.00	80.63*
SIX rinse	1.30	24.90	0.00	80.63*
Pump seals	6.50	24.90	0.00	80.63
CIP	6.38	0.00*	0.00	0.00*
PIX ads	14.44	24.90	0.00*	80.63*
PIX b-w	10.45	24.90*	100.00	80.63*
Cooling tower	29.76	24.90	0.00	80.63
PIX NH3 dil.	0.16	24.90	0.00	80.63*
Sea outfall pipe	116.96	606.11*	47.05*	89.91*
SWW	24.97	3.50×10^{5}*	3.50×10^{4}*	1.00×10^{3}*

TABLE E.15
Scenario C source conditions.

Name	Flow / [t/h]	SS / [ppm]	FSA / [ppm]	Cl / [ppm]
UOS dilution	80.14	126.89	16.44	80.63
AS evap. cond.	6.40	$\leq2.00\times10^{3}$	0.00	0.00
Pure cond.	18.07	0.00	0.00	0.00
Pump seals	6.50	222.50	0.00	80.63
CIP	6.38	7.67×10^{3}	0.00	0.00
PIX ads.	24.97	3.50×10^{5}	3.50×10^{4}	1.00×10^{3}
PIX b-w	17.43	24.90	300.05	80.63
Cooling tower	3.59	1.00×10^{3}	0.00	670.04
UOS water	65.24	24.90	0.00	80.63

E.5 Sensitivity Analysis Data

Table E.16 to E.21 gives the data that corresponds to the initial sensitivity graphs in section 3.6. The data used to plot the sensitivity of the objective function to changing freshwater costs, inlet constraints and outlet conditions (section 3.7) is given in table E.22 to E.26

E.5.1 Initial Sensitivity Values

TABLE E.16
Initial objective cost sensitivity values for Scenario A inlet constraints (figure 3.5 (a)).

Contaminant	Objective cost sensitivity / $[R \cdot h^{-1}/\Delta ppm]$		
	Cooling tower inlet	PIX backwash inlet	Sea outfall pipeline inlet
SS	0.00	1.73×10^{-2}	5.16×10^{-3}
FSA	0.00	2.65×10^{-2}	0.00
Cl	2.20×10^{-3}	0.00	0.00

TABLE E.17
Initial objective cost sensitivity values for Scenario A outlet concentrations (figure 3.5 (b)).

Contaminant	Objective cost sensitivity / $[R \cdot h^{-1}/\Delta ppm]$				
	UOS dilution	PIX adsorption outlet	AS evap. condensate	CIP outlet	UOS water
SS	3.67×10^{-3}	2.00×10^{-9}	1.12×10^{-2}	2.92×10^{-4}	8.57×10^{-3}
FSA	0.00	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	0.00	2.20×10^{-3}

TABLE E.18
Initial objective cost sensitivity values for Scenario B inlet constraints (figure 3.7 (a)).

Contaminant	Objective cost sensitivity / $[R \cdot h^{-1}/\Delta ppm]$	
	PIX backwash inlet	Sea outfall pipeline inlet
SS	0.00	5.06×10^{-3}
FSA	6.89×10^{-2}	0.00
Cl	0.00	0.00

TABLE E.19
Initial objective cost sensitivity values for Scenario B outlet concentrations (figure 3.7 (b)).

Contaminant	Objective cost sensitivity / $[R \cdot h^{-1}/\Delta ppm]$			
	UOS dilution	PIX adsorption outlet	CIP outlet	UOS water
SS	3.67×10^{-3}	1.23×10^{-6}	2.92×10^{-4}	1.71×10^{-3}
FSA	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	2.15×10^{-1}

TABLE E.20
Initial objective cost sensitivity values for Scenario C inlet constraints.

Contaminant	Objective cost sensitivity / $[R \cdot h^{-1} / \Delta ppm]$	
	PIX backwash inlet	Sea outfall pipeline inlet
SS	0.00	5.06×10^{-3}
FSA	6.89×10^{-2}	0.00
Cl	0.00	0.00

TABLE E.21
Initial objective cost sensitivity values for Scenario C outlet concentrations.

Contaminant	Objective cost sensitivity / $[R \cdot h^{-1} / \Delta ppm]$			
	UOS dilution	PIX adsorption outlet	CIP outlet	UOS water
SS	3.67×10^{-3}	1.23×10^{-6}	2.92×10^{-4}	1.71×10^{-3}
FSA	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	2.15×10^{-1}

E.5.2 Data for Model Sensitivity Analysis

TABLE E.22
Sensitivity of the objective cost, and FW flowrate to the FW cost (figure 3.9 and 3.10).

	FW cost / [R/t]	FW flowrate / [t/h]	Objective cost / [R/h]
1	2.50	60.95	556.3
2	3.00	60.95	586.78
3	3.50	60.95	617.25
4	4.00	60.95	647.73
5	4.50	60.95	678.2
6	5.00	60.95	708.68
7	5.50	60.95	739.15
8	6.00	60.95	769.63
9	6.50	60.95	800.01
10	7.00	60.95	830.58
11	10.00	60.95	1013.42
12	16.00	60.95	1379.12

TABLE E.23
Sensitivity of the objective cost, and FW flowrate SS concentration constraint for the inlet to the PIX backwash (figure 3.11 and 3.12).

	$C_{SS,PIX\,bw}^{in,MAX}$ / [ppm]	Objective cost[1] / [R/h]	Objective cost[2] / [R/h]	FW flowrate / [t/h]
1	625	560.71	556.3	60.95
2	630	560.62	556.21	60.91
3	640	560.45	556.04	60.84
4	660	560.09	555.68	60.7
5	700	559.37	554.96	60.41
6	750	558.48	554.07	60.06
7	800	557.59	553.18	59.7
8	850	556.69	552.28	59.34
9	900	555.8	551.39	58.98
10	920	555.44	551.03	58.84
11	925	555.43	551.02	58.84

1. SS constraint in sea pipeline fixed at 74984.29g/h.
2. SS constraint in sea pipeline relaxed.

TABLE E.24
Sensitivity of the objective cost to SS concentration in the sea pipeline (figure 3.13 and 3.14).

	SS Mass-flowrate / [g/h]	Objective cost / [R/h]	Flow to sea pipeline / [t/h]	FSA conc. in sea pipeline / [ppm]
1	7.50×10^{4}	556.30	112.67	48.85
2	7.50×10^{4}	556.30	112.67	48.86
3	8.00×10^{4}	556.07	112.68	53.29
4	9.00×10^{4}	555.62	112.71	62.15
5	1.00×10^{5}	555.16	112.74	71.01
6	1.50×10^{5}	552.87	112.88	115.21
7	2.00×10^{5}	550.59	113.03	159.30
8	2.50×10^{5}	548.30	113.17	203.28
9	3.00×10^{5}	546.02	113.31	247.15
10	3.50×10^{5}	543.73	113.46	290.91
11	3.60×10^{5}	543.26	113.49	300.00

TABLE E.25
Sensitivity of the objective cost, FW flowrate and sea pipeline flowrate to FSA concentration in the sea pipeline (figure 3.15, 3.16, and 3.17).

	FSA concentration / [ppm]	Objective cost / [R/h]	Flow to sea pipeline / [t/h]	FW flowrate / [t/h]
1	300	543.26	113.49	60.95
2	1000	505.87	115.82	60.95
3	1500	478.21	117.55	60.95
4	2000	449.72	119.33	60.95
5	2500	420.34	121.17	60.95
6	3000	390.05	123.06	60.95
7	3500	358.8	125.01	60.95
8	4000	326.54	127.03	60.95
9	4500	293.22	129.11	60.95
10	5000	257.73	138.63	67.26
11	5250	238.8	139.79	67.26
12	5500	220.14	140.98	67.26
13	5750	200.86	142.18	67.26
14	6000	181.25	143.41	67.26
15	6389.54	160.21	139.01	62.32

TABLE E.26
Sensitivity of the objective cost, and AS cond. reuse flowrate to the SS concentration in the AS evaporator condensate (figure 3.19 and 3.20 and equation 4.1).

	$C_{SS,AS\ evap}^{out}$ / [ppm]	Objective cost / [R/h]	AS cond. Reuse flowrate / [t/h]	p / [t/(h·ppm)]
1	0	551.02	6.4	-
2	500	551.02	6.4	-
3	600	551.02	6.4	-
4	700	551.54	6.19	4333
5	750	552.61	5.77	4327.5
6	850	554.35	5.07	4309.5
7	900	555.08	4.78	4302
8	1000	556.3	4.29	4290
9	1100	557.3	3.89	4279
10	1300	558.83	3.28	4264
11	1500	559.94	2.83	4245
12	1700	560.78	2.5	4250
13	2000	561.73	2.12	4240
14	2500	562.8	1.69	-
15	3000	563.51	1.41	-
16	3500	564.02	1.2	-
17	4000	564.39	1.05	-
18	5000	564.92	0.84	-