

THE APPLICATION OF PINCH ANALYSIS FOR WATER AND EFFLUENT MANAGEMENT

**Report to the
WATER RESEARCH COMMISSION**

by

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**"The Further Application of Pinch Analysis for Water and Effluent
Management"**

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EXECUTIVE SUMMARY

This report is a sequel to WRC Report No. 851/1/03 entitled *The Application of Pinch Analysis for the Rational Management of Water and Effluent in an Industrial Complex*. The earlier report set out the basis and methodology, together with some practical guidelines, for applying water pinch analysis to an industrial system, and presented some case studies as practical examples. This report is mostly concerned with further case studies which had not been completed at the time of the previous report. However these case studies do reflect some development in theoretical understanding which occurred during the intervening period. Thus the two reports are complementary to one another, and should be considered together. In particular, the literature survey and general theoretical background to water pinch analysis are contained in the previous report, while this report starts to address some issues which were raised in the previous report.

1 Background and Motivation

Industrial processes usually require water with a range of qualities, and produce several effluents with a range of qualities, which allow the possibility of a hierarchical use of water.

Possible strategies for reducing the consumption of fresh water and the production of wastewater include:

- **reuse:** wastewater from one process can be directly reused in others, provided the level of contamination is sufficiently low to meet the requirements of the subsequent processes;
- **regenerative reuse:** wastewater can be treated to reduce the levels of contaminants before being reused in other processes. In this option, the water is not recycled to the process from it came;
- **regenerative recycling:** after regeneration, water can be recycled to the process from which it came. This is generally more difficult than reuse, because recycling tends to build up contaminants.

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

Water Pinch Analysis thus involves a set of systematic formal techniques to handle the complex problem of hierarchical water allocation to a system consisting of a number of processes, and choosing the best combination of strategies. The theory that appears in the literature is still developing. The practical application of this theory is not as well established in the open literature, and particularly not in a South African context.

2 Project Objectives

As originally stated, the project objectives were:

- to promote the wide spread application of pinch analysis for the management of water and effluents;
- to develop the technique for the specific problems associated with South African industry;
- to promote better water management by undertaking pinch analysis studies at selected sites;
- to enhance the capacity within South Africa to undertake pinch analysis studies and to promote the wider understanding of the technique within educational institutions, industry and government by training people in the technique.

These objectives were pursued chiefly through undertaking case studies at a number of factories. Some of these were carried out by full time students at the University of Natal, whereas a number involved part-time students who were also working as engineers at the factories which were the subjects of study. Chapter 4 concerning the Mondi Merebank Paper Mill is based on one of these part-time student projects.

3 Overall course of the project

The history of this project is inextricably interwoven with that of WRC project that preceded it: K5/851 *The Application of Pinch Analysis for the Rational Management of Water and Effluent in an Industrial Complex*, so a single account of both is given.

The original project was envisaged as concerning only factories in the Umbogintwini industrial complex, located south of Durban. At the start in 1997, a preliminary survey identified AECI Bioproducts (lysine), SA Tioxide (titanium dioxide pigment) and Sasol Polymers (chlor-alkali) as the three largest water users in the complex, and these were selected for the initial investigations.

At the same time, the Canelands factory of Sanachem, a subsidiary of Sentrachem, producing agrochemical (principally herbicides and pesticides) requested to join the project. One of their chemical engineers, Thokozani Majozi, was assigned to undertaking the pinch analysis of processes at their site. This work was undertaken as a MScEng project, for which he was allowed to devote 50 % of his time.

A collaborative relationship was also established with Linnhoff-March, the UK consulting firm developing and marketing the *WaterTarget*TM suite of software for water pinch analysis.

Later in the project, other case studies were initiated as a result of interest from industry. The first of these was a study of the Eskom Lethabo Power Station near Vereeniging, in which the objective was to use pinch analysis to determine the best way to use a reverse osmosis plant within the power station water system. Three studies were started at paper mills: the Mondi Merebank paper mill with Gladys Naylor (née Crampton), the Sappi Ngodwana mill with Eric Slabbert and the Sappi Tugela mill with Maryna Mansfield. All three investigators were process engineers associated with the mills, who registering as part-time MScEng students. A similar arrangement was made with Annelie Lourens, a Sasol process engineer who worked on the water systems at the Natref refinery and the Secunda oil-from-coal complex. Finally, a study was commissioned by the South African branch of ILSI, the International Life Sciences Institute, to produce a monograph on the application of water pinch analysis in the food industry, after undertaking a pilot study at the Ceres Fruit Juice factory in Ceres. This

was carried out by Janos Schneider after completing his thesis on the AECI Bioproducts plant.

Not all of these investigations reached successful conclusions during the course of the project. The initial studies at SA Tioxide and AECI Bioproducts stopped as a result of the resignation of key personnel; however the AECI Bioproducts study was subsequently restarted and completed successfully by a different student, Janos Schneider. The Sasol study halted when Mrs. Lourens resigned from Sasol to emigrate. The Sappi Ngodwana and Sappi Tugela studies were not completed by the end of the project, largely because of the pressure of other work commitments on the part-time students involved. This report and WRC Report 851/1/03, between them present those case studies which reached a sufficient degree of closure. These were:

- i) The Sasol Polymers Chlor-alkali plant. This in fact provided two case studies, the first carried out by Grant Gardner during the earlier project, and reported in WRC Report 851/1/03. In the follow-up project the plant was revisited by Paolo Gianadda in the light of the advances in pinch analysis theory which had occurred, as well as changes which had taken place in the factory. The later case study appears in the present report (chapter 6)
- ii) The Sanachem agrochemical plant (WRC Report 851/1/03).
- iii) The Lethabo Power Station (WRC Report 851/1/03).
- iv) The Ceres Fruit Juice factory (chapter 3 of this report).
- v) The AECI Bioproducts Lysine plant (chapter 4 of this report).
- vi) The Mondi Merebank paper mill (chapter 5 of this report).

Although the other case studies do not appear explicitly in the reports, they are represented implicitly in that they provided valuable experience which contributed greatly to the general understanding of pinch analysis, which in turn influenced the more successful projects.

4 Structure of the report

The principal matter of this report is contained in the four case studies, which present pinch analyses applied to different factories, involving widely varying circumstances. The factories involved were Ceres Fruit Juices, (chapter 3), the AECI Bioproducts lysine plant (chapter 4), the Mondi Merebank paper mill (chapter 5) and the Sasol Polymers chlor-alkali plant (chapter 6). Each of these case studies has its own discussion and conclusions related to issues specific to the system involved. These are preceded by chapter 2 devoted to those aspects of the methodology which were common to the investigations. In particular, it describes the Linnhoff-March *WaterTarget* software which was the principal tool used for the lysine plant and the paper mill, and which was also used in a subsidiary role for the chlor-alkali plant. Chapter 7 presents activities which aimed to promote water pinch analysis to industry during the course of the project. The conclusions and recommendations of chapter 8 concern issues which emerge from considering the various case studies together, and the overall experience of applying water pinch analysis to South African industries.

5 Methodology

The chief *modus operandi* of this project was to promote the water pinch concept to industries, and wherever possible to recruit engineering personnel from the companies involved to enrol for part-time MScEng degrees, undertaking water pinch analysis studies in their factories. Two conventional academic projects involving full-time students served to

generate theoretical support for situations where the current techniques are not completely adequate.

During the project a relationship was established with the British company Linnhoff-March, which has been associated with the development of both thermal and water pinch analysis. The *WaterTarget*[®] suite of software from Linnhoff-March was used for several of the studies.

The Linnhoff-March software is aimed at the analysis of systems in which water is used only as a utility to a process, and is not an intrinsic part of the core process technology. The *combined water and materials pinch analysis* which was developed during the study of the Sasol Polymers chlor-alkali process required a different framework.

The distinction made between process streams and water streams in the pinch analysis formulation is more precisely a distinction between process streams and *utility-water* streams. It often happens that some of the process streams are also water streams. Making the distinction between process streams and water streams in the usual manner therefore results in some of the streams involving water being excluded from the analysis. In addition, some of the dissolved species present in the process-water streams may not be undesirable contaminants, but instead necessary elements of the process technology.

To properly optimise the use of water in such systems requires an approach which considers both the process-water streams and the utility-water streams. Given that the present techniques and tools only consider the utility-side of the problem, we coined the terms *utility-water pinch analysis* for the situation where only utility streams are considered, and *process-water pinch analysis* where process-water streams are also included. Process-water pinch analysis is a superset of utility-water pinch analysis since utility-water streams are also included in the analysis.

6 Results of the case studies

6.1 Ceres Fruit Juices

The South African branch of the International Life Sciences Institute (ILSI) commissioned the preparation a monograph on the application of water pinch analysis in the food industry. ILSI is a non-profit, world-wide foundation established in 1978 to advance the understanding of scientific issues relating to nutrition, food safety, toxicology, and the environment. It was part of the terms of reference of the commission that the studies should present straightforward applications of pinch analysis, using the simplest and most easily understood version of the technique. The Ceres Fruit Juices (CFJ) study is included in this report to represent this relatively simple end of the pinch analysis spectrum.

CFJ is located in the town of Ceres, approximately 200 km east of Cape Town. CFJ manufacture fruit juice for both the local and export market. Fruit juice from blending is heat sterilised to form the final product for packaging. Blending requires ultra pure water from the water treatment plant. Chlorinated water from the treatment plant is used for the sterilisation process and for cooling. Finally, effluent is treated in the effluent treatment plant to comply with municipal standards.

The study largely followed the general methodology for applying pinch analysis to an existing process set out in chapter 3 of the previous WRC Report No. 851/1/03. The steps in the process were:

- 1) selection of the system boundaries;
- 2) identification of water sources and sinks;
- 3) pre-screening;

- 4) data gathering;
- 5) pinch problem formulation
 - modeling of unit operations
 - optimisation,
 - identification of bottlenecks - relax constraints or regenerate,
 - integrated network design;

The final step 6), implementing the suggested design changes, was not achieved during the project period.

The pinch analysis was based on a single contaminant, total solids (TS) which included dissolved and suspended solids. A straightforward application of the pinch analysis method identified the minimum fresh water supply rate as 3 t/h, compared with the current figure of 9.5 t/h. However, this did not take into account a number of restrictions on where water could be recycled which were related to the requirements of food processing. After eliminating reuse options which were considered to involve unacceptable contamination risks, the fresh water requirement was determined to be 4.7 t/h, which still represented a reduction of almost 50 % on the current usage. The study ended at this point, so it was not possible to confirm whether this could be implemented in practice. This would require a detail assessment of each reuse option to check that it was in fact appropriate: for instance it might happen that some contaminant that was not fully represented by the TS could prevent reuse of water from one particular part of the process to another.

6.2 The AECI Bioproducts Lysine Plant

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 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.

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 environmental regulations limit the concentration of pollutants expelled in this manner. What remained after lysine extraction was broth effluent, which was removed from the site and handled by the 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.

The aims of this project were to:

- i) apply water pinch analysis at Bioproducts, which consisted 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 were the greatest barriers to further saving and improvement, and in so doing, suggest possible improvements that would aid in the implementation of similar projects in the future.

The results of this case study had the following notable features:

- 1) The analysis was carried out using the Linnhoff-March WaterTarget software and the mathematical programming approach to water pinch analysis. It was limited to utility water streams, considered multiple contaminants, and optimised an economic objective function, i.e. it sought to minimise costs associated with the water system rather than the volumetric use of water.
- 2) Although it was not able to identify significant *water* savings, it did identify significant *cost* savings, which was in strong contrast to the classical pinch analysis methodology.
- 3) The nature of these cost savings raised some interesting issues. The pinch analysis demonstrated that savings were prevented by the external limit on the concentration of suspended solids (SS) constraint at the sea pipeline. Saving could be achieved by relaxing this constraint and allowing for discharge of broth effluent to the sea. At R16 /t, the hourly cost of disposing the broth effluent at the local wastewater treatment works amounted to R400 /h, approximately 72% of the total water-using network operating cost of R 556 /h. Thus, the DWAF effluent discharge permit concerning the broth effluent, with its SS constraint of 400 mg/L at the sea outfall, was established as the major barrier to further savings. Subsequently to the study, the factory applied to DWAF to allow the discharge of broth effluent to sea, and to increase the 400 mg/L SS limit. The reason for setting this limit had been purely to avoid an unsightly stain of the sea surface, and the scientific basis for the value of 400 mg/L was far from certain. However, DWAF would not consider environmental arguments for relaxing it until the factory had demonstrated that it had reached the limit of what could be achieved by improving its operation. The pinch analysis was accepted as evidence that this was the case, so it was agreed to relax the limits, subject to monitoring the resulting condition of the sea. To date no adverse effects resulting from the discharge have been detected.
- 4) This outcome suggests a useful role for pinch analysis in the interaction between industries and regulatory authorities in establishing the parameters of water use permits. It offers systematic and transparent analysis of the industry's water needs which could provide the basis for trust between the parties. However, it does require a capacity in both parties to understand and question the basis of the analysis.

7 The Mondi paper mill at Merebank, Durban

The Mondi Paper mill at Merebank in south Durban is an integrated pulp and paper mill, producing three types of pulp, supercalendered magazine paper, uncoated woodfree paper, newsprint, telephone directory and carbonless coated paper. The three types of pulp produced at Mondi Paper are:

- Thermomechanical pulp

- Groundwood pulp
- Recycled fibre pulp

The groundwood and thermomechanical pulps are produced by mechanically separating the fibres from other wood constituents, by means of log grinding in the groundwood process and chip refining in the thermomechanical process.

The fibre sources used in the production of the pulp and paper are:

- Logs and chips - Pine
- Recycled paper - newspapers and magazines
- Chemical pulp - hardwood pulp produced from Eucalyptus wood and softwood pulp produced from Pine

There are five paper machines at Mondi Paper producing the following paper grades:

Paper Machine 1	Supercalendered magazine paper
Paper Machines 2 and 3	Uncoated woodfree paper
Paper Machines 4 and 5	Newsprint and telephone directory

Some of the uncoated woodfree paper produced at the mill is coated with microcapsules, on a separate coating machine, to produce carbonless coated paper.

The steam requirements of the mill are supplied by the power plant which comprises two coal fired boilers, two standby oil boilers and two standby gas boilers. The coal boilers supply the steam required to produce the pulp and dry the paper.

Water has many vital functions in all the sections of the mill, and is indeed integral to the process. However, the water in the main process streams was excluded from the analysis, except where it left the process as an effluent. As with the lysine plant case study, the Linnhoff-March *WaterTarget* software was used for the analysis.

In order to perform a Water Pinch analysis on a site which is as complicated as the Merebank mill, the operation was divided into manageable sections. The sections chosen were the *Recycled Fibre Plant*, the *Thermo-mechanical Pulp Plant* and the *Paper Machines*. A flow sheet model of each sections was then developed, and a water and contaminant balance was established. Once a sufficiently accurate water and contaminant balance was achieved, the streams which were not variable, and therefore did not form part of the water pinch analysis (e.g. product streams), were not considered further. Once the streams which did not form part of the water pinch analysis had been removed and the water pinch model of the plant had been developed, this model was tested by forcing the stream flows to correspond to the actual plant situation as closely as possible by introducing flow constraints. This constrained model formed the baseline to compare subsequent results against. The next step involved removing those constraints which appeared not to be absolutely required in terms of process considerations, and allowing the model to re-route streams in order to achieve a minimum fresh water consumption.

The results of the optimisation of the individual plants were disappointing: no significant saving in water usage was identified at all. In retrospect this was understandable in that each individual plant was set up essentially as a countercurrent process treating a pulp stream, which is well known to be the most efficient configuration. The only possibility for discovering further efficiencies lay in considering the different sections as an integrated system, and exploiting inter-section transfers of water.

The results of the analysis of the integrated process were to reduce the total fresh water consumption from 636.3 t/h to 584.5 t/h, and the total effluent generated from 954.4 t/h to 902.9 t/h (8.1 % reduction in fresh water consumption and 5.4 % in effluent generation).

From this investigation of the application of water pinch analysis in an integrated pulp and paper mill, the following can be concluded:

- i) Scope for optimisation and water savings within individual sections of the mill was insignificant. There were a number of reasons for this namely:
 - Only utility water was considered in this analysis
 - There has been a considerable amount of effort already put into reducing water consumption at the mill over a number of years.
 - Water is already recycled and reused within the process to some extent
- ii) By application of single contaminant analysis to a larger section of the mill it was possible to reduce the fresh water requirement by 51.54 t/h (8.1%) and effluent generated by the same amount (5.4%).
- iii) These reductions translated into a saving of R1 548 593 /annum. The savings was calculated by the objective function which included fresh water costs and effluent costs, but did not include engineering costs or piping costs. In addition, the objective function did not take geographical costs into account, the distance between the sections in the plant was not included in the analysis.
- iv) There are operability constraints which could prevent these savings from being achieved, since they involve the transfer of water from processes which are not always operated on the same schedule.
- v) Thirty two new connections were generated in the optimised model, however the same savings could be achieved with just three. These three streams were identified using a novel approach to implementing water pinch analysis which involved the evaluation of sensitivity coefficients of the flow constraints in combination with the magnitude of the streams involved. The top three new connections identified in this manner corresponded to the three streams which were responsible for the fresh water savings in the optimised model generated by the water pinch analysis.

This study did not consider the use of treatment options to reduce the fibre content in the existing streams and thereby reduce the fresh water consumption further. Removal of fibre from streams will allow further reuse and recycling within the process and thus a further reduction in the amount of fresh water required.

During the course of the study, the water supply situation for the mill was changed substantially with the commissioning of the Durban Water Recycling Plant. This treats recovered domestic and industrial wastewater to a standard which makes it suitable for industrial use. Mondi is the scheme's main customer, and is supplied recycled water in terms of a "take or pay" agreement. The mill uses the recycled water for all the process requirements and in terms of the agreement with the Recycling Plant the mill pays for a minimum amount of water per day, whether this amount of water is used or not. Currently the mill consumption of water is slightly below the "take or pay" minimum specification, so the commercial incentive to implement water saving measures has disappeared.

8 The Sasol Polymers chlor-alkali process at Umbogintwini

The application of Pinch Analysis to water and wastewater management at the Sasol Polymers chlor-alkali complex was first addressed as part of WRC Project K5/851. As part of that project, a Water Pinch Analysis study at the chlor-alkali complex was conducted by

Gardner, starting in 1997 . Motivated by the results from this study and with a number of process changes that had been made to the chlor-alkali complex, the follow-up study reported here was undertaken by Paolo Gianadda and began in 1999.

The Sasol Polymers chlor-alkali complex, formerly operated by Polifin Limited and previously by AECI Chlor-Alkali and Plastics Limited, was located within the Umbogintwini Industrial Site some 25 km south of Durban, South Africa. During its period of operation, from 1955 to 2001, the complex produced chlorine and caustic soda, together with a range of other derived products. It was also in this period that the complex underwent a number of changes as processes were upgraded and decommissioned. As it stood at the time of its closure, the complex produced caustic soda, chlorine, hydrogen, hydrochloric acid and sodium hypochlorite. Otherwise indicated, references to the plant refer to its configuration as it stood when it was closed in 2001.

Central to the activities of the complex was the brine circuit which converts raw salt to caustic soda, chlorine and hydrogen. Part of the chlorine and hydrogen generated from the circuit was used for the production of hydrochloric acid in the hydrochloric acid synthesis plant. Chlorine was further used, along with caustic soda, in the manufacture of sodium hypochlorite in the sodium hypochlorite synthesis plant. Two other plants located within the complex were the demineralisation plant, which produced a high quality water for use within the complex, and the Hydecats destruction plant which destroyed surplus or below-specification sodium hypochlorite along with other chlorine-containing effluents.

Results from Gardner's study (presented in WRC report 851/1/03) showed that there was significant potential for savings to be effected on the chlor-alkali complex through the reuse and recovery of **both** water and reagents. However, the approach adopted at the time resulted in the problem being considered from a *single contaminant* perspective; as such the optimality and even the feasibility of the proposed network configurations could not be guaranteed from the *multiple contaminant* perspective. The chlor-alkali complex also did not correspond to the typical situation associated with the application of Water Pinch Analysis. Existing Water Pinch Analysis tools, and the theory from which they developed, rely on the assumption that a clear distinction can be made between so-called *water streams* and *process streams*. With this distinction in place, only the water-side of the problem is considered in the Pinch Analysis: the process-side is not represented explicitly. However, it was not possible to distinguish between process streams and water streams in the chlor-alkali complex.

There were three key aspects to the problem presented by the chlor-alkali complex which made the application of current water pinch analysis theory to the situation unsatisfactory. These were:

- The lack of distinction between process streams and water streams;
- The presence of multiple resources, in this case reagents and raw materials, in addition to water. These resources carried species which had an economic value to the system, and could not be treated in the same way as contaminants; and
- The chemical reactions taking place between the various species in the system.

An extension of the theory was needed to address these issues, and the term *Combined Water and Materials Pinch Analysis* was coined to describe the new methodology.

Species considered in the combined water and materials pinch analysis

Species	Status	Justification for Selection
Ca ²⁺	Undesirable	Precipitates as hydroxide in electrolyser membranes
CaCO ₃	Undesirable	A precipitate which can foul electrolyser membranes
Cl ₂	Desirable Undesirable	Product produced and raw material used by the complex Destroys cation-exchange resin in brine circuit
H ₂	Desirable	Product produced and raw material used by the complex
HCl	Desirable Undesirable	Product produced and reagent/raw material used by the complex Contaminant where caustic soda is required
H ₂ O	-	Involved in chemical reactions
Mg ²⁺	Undesirable	Precipitates as hydroxide in electrolyser membranes
Mg(OH) ₂	Undesirable	A precipitate which can foul electrolyser membranes
NaCl	Desirable Undesirable	Raw material used in the complex Contaminant in demineralised water production
NaClO ₃	Undesirable	Damages cation-exchange resin in brine circuit
Na ₂ CO ₃	Desirable Undesirable	Used as a reagent to precipitate calcium in brine circuit Affects electrolyser membranes at high concentrations
NaHSO ₃	Desirable Undesirable	Destroys Cl ₂ in brine stream Converts to sulphate which is undesirable
NaOCl	Desirable Undesirable	Product produced by the complex Cl ₂ releasing species - problematic in brine circuit and effluent
NaOH	Desirable Undesirable	Product produced and reagent/raw material used by the complex Contaminant where hydrochloric acid is required
Na ₂ SO ₄	Undesirable	Diffuses through electrolyser membranes with some precipitation taking place
O ₂	-	Product of chemical reactions
Insolubles	Undesirable	Fouling of equipment
TDS	Undesirable	Of significance in the cooling towers

The analysis followed the mathematical programming approach, along roughly similar lines to the Linnhoff-March *WaterTarget* software, but new software had to be developed to take all the additional considerations into account. This was implemented using the GAMS (General Algebraic Modelling System) modelling framework.

This study represented the most comprehensive attempt to provide a thorough theoretical and practical treatment of the *process water pinch analysis* problem. The issue of utility water pinch analysis *vs.* process water pinch analysis was one which was encountered in some form in all the case studies undertaken during this project and WRC Project K5/851 that preceded it. It seems that, at least in the context of a water-poor country like South Africa, that the limitation to considering only utility water is a significant restriction. Clearly the extended theory is more complex and requires much more effort to apply. The individual process modules have to be individually crafted, and require much more insight and modelling skill than those which have been found adequate for utility water pinch analysis. The risks of making changes which will adversely affect the process involved are also greater.

Some perspective on these issues can be obtained from a utility water pinch analysis of the same chlor-alkali system carried out using the Linnhoff-March WaterPinch software, based on the same input data. A comparison between the results of the (utility) water pinch analysis results and the combined water and materials pinch analysis are shown in the table below

The Water Pinch Analysis study was able to realise 57% of the total saving achieved by Combined Water and Materials Pinch Analysis. In terms of water abstraction and effluent generation, relatively small changes are observed between these two studies with the Combined Water and Materials Pinch Analysis achieving a further 3 % reduction in the total amount of water used and an additional 10 % reduction in terms of the amount of effluent generated. It is however in the area of chemical recovery and reuse where Combined Water and Materials Pinch Analysis outperforms Water Pinch Analysis and much of the additional cost saving is attributable to this.

Comparison of potential savings achieved by Utility Water Pinch Analysis and Combined Water and Materials Pinch Analysis

	Water Pinch Analysis [%]	Combined Water and Materials Pinch Analysis [%]
Umbogintwini River Water	7	0.9
Umgeni Water	42	100
Total Water	11	14
Demineralised Water	34	34
Caustic Soda (32% m/m NaOH)	0.2	1.6
Hydrochloric Acid (31% m/m HCl)	1.9	8.3
Raw Salt	0	0.17
Sodium Carbonate	0	-0.53
Sodium Bisulphite	0	1.6
Chlorine	0	0.05
Hydrogen	0	0
Steam	0	-1.2
Flocculant	0	-3.3
Alpha-Cellulose	0	6.6
Effluent	32	42
Solid Waste	0	5.6
Annual Saving [R/y]	542 881	945 727

9 Conclusions and recommendations

In addition to the individual conclusions pertaining to each case study, which appear in the relevant chapters, the range and scope of the case studies undertaken during the project allows some broad conclusions to be drawn about water pinch analysis as a technique.

9.1 An assessment of the status of water pinch analysis theory and practice

Pinch analysis, whether applied to energy or water, is a special case of the more general technique of process optimisation. In most cases the problem of fully optimising all aspects

of a process is so large that it is impractical to tackle as a whole. The strategy commonly adopted is to break up the full optimisation problem into a set of more manageable sub-problems which can be solved independently; pinch analysis seeks to address one of these sub-problems. It considers the optimisation of the utility systems in the process - either the thermal utility system or the water utility system.

The experience of the case studies undertaken in this project has been repeatedly that the standard assumptions of pinch analysis are somewhat restrictive. The continuous pressure to conserve water in South Africa means that many industries have already introduced measures to use water more efficiently, so the easy savings reported in the literature are often not available, and it becomes necessary to venture into more difficult areas to make further progress.

9.1.1 What pinch analysis promises

Pinch analysis was originally developed for the design of energy utility systems. One of the more important features of pinch analysis is its ability to target minimum utility requirements for any process. Such *targets* may be set without the need for detailed design. The design of the utility can therefore be undertaken in two stages: determining the targets, for which only physical data are required, followed by detailed design, where all the other factors, such as economics, safety and operability must be taken into account.

Pinch analysis methods have also been developed for redesigning a utility system to improve efficiency: the so-called *retrofit* situation. Here the process design units are in place, and would not be expected to change. What pinch analysis offers in this case are the targets which show how much improvement in efficiency can possibly be achieved by the redesign, and the design rules which allow one to pinpoint where structural inefficiencies exist in the current design, and so where to focus effort and investment to the best advantage.

9.1.2 Theoretical limitations encountered

The resounding success of numerous applications of energy pinch analysis suggests that its underlying assumptions work well in practice; the more limited success of water pinch analysis suggests that its assumptions are not as useful in many cases. Part of the reason for this is that water pinch analysis is based on an analogy between water and energy which is not exact. The first problem with the analogy is that, while the quality of energy is uniquely represented by temperature, the quality of water is an altogether more complex and less well-defined concept. The second problem is that the boundary assumptions in terms of fixed contaminant loads and concentrations are less often appropriate in practice.

In energy pinch analysis, the formalism allows one to identify a *thermodynamic limit* to energy recovery, which is independent of any economic considerations related to the energy utility system. Optimising the system can thus be handled in two steps: the first identifies the thermodynamic limit, and then the second examines how close one can get to this limit economically. It is this clear separation of the physical and economic effects that has contributed greatly to the conceptual appeal and practical acceptance of the technique.

When it comes to water pinch analysis, the lack of rigour in the thermodynamic analogy means that the equivalent of thermodynamic limit does not really exist independently of economic factors. The crucial issue is that of *quality regeneration*. In the case of energy, quality is regenerated by means of a heat pump, which is driven by an input of energy, and so can be analysed on the same thermodynamic basis as the rest of the system. In the case of water, quality is regenerated essentially by the input of energy (including chemical energy), which cannot be represented in terms of contaminant load and concentration. Reductions in the use of fresh water have to be balanced against the use of energy and/or chemicals in

treating used water, and economic considerations are the usual means for determining the relative weighting of such disparate physical inputs. *Thus, the separation of physical and economic effects in the analysis is not possible, unless quality regeneration is excluded as a design option.*

This brings into question the nature of the “pinch” itself. In the energy pinch analysis the pinch is a limiting temperature, and in the simplest form of water pinch analysis it is a limiting concentration, but this depends on interpreting the limit in terms of the thermodynamic analogy. In response to the problem of water quality being a function of multiple contaminant concentrations rather than a single variable, the Linnhoff-March WaterPinch software, that features in chapters 2, 4 and 5 of this report, uses the sensitivities or *marginal costs* of the concentration limits to take the place of the pinch, however in chapter 5 it was demonstrated that these do not suffice, and that flow rate constraints also need to be considered. This leads to a concept of the pinch as *the set of all constraints which are active at the optimum*. (Active constraints are those for which the relevant variables are at their limiting values). Unfortunately this does not have the elegance and intuitive appeal of the original pinch concept. Furthermore, the utility target values that it provides do not have the certainty associated with the original pinch concept, because they depend on what factors were included in the pinch analysis model.

When considering the question of the boundary assumptions for the subsystems to be analysed, the considerations are fundamentally similar for both energy and water pinch analysis. However, it does seem that in practice precluding process changes in the optimisation is more limiting in the case of water, perhaps because water is used for such diverse purposes.

The effect of these three issues (having to include economic effects early in the analysis; the consequent absence of a purely physical pinch limit; and the pressure to include process streams in the optimisation) is that water pinch analysis tends towards full process optimisation, which dilutes its status as a separate discipline. From a practical viewpoint, this means that the one cannot accept the general procedures and conclusions of the standard pinch analysis theory, and that each application needs to be evaluated on its particular merits.

It must be acknowledged that the above conclusions mostly reflect the experience of applying the analysis in the retrofit mode: i.e. to improving water utilisation in existing, well established processes. In the case of a new design where process conditions have not yet been fixed, it may well be that the assumptions and approximations involved in the standard version of pinch analysis would be quite justified in view of the uncertainties about what the process conditions will be.

9.1.3 Practical strategies for applying water pinch analysis

How can water pinch analysis be applied so as to circumvent its theoretical limitations and realise its promise as far as possible? The case studies presented in this report suggest that there is no single answer to the question, and that an approach must be formulated according to the nature of the process involved.

The case study of **Ceres Fruit Juices** (chapter 3) demonstrated the most straightforward application of water pinch analysis, as the process conformed most closely to the classical assumptions of pinch analysis. The water involved is used for utility purposes of equipment washing and sterilisation and cooling (although some water is blended into the products, this could easily be excluded from the analysis). No wastewater treatment for quality regeneration was practised or contemplated. Total solids was considered as the single contaminant representing water quality.

From this example the first strategy for applying water pinch analysis can be formulated as:

- i) include only utility water streams in the analysis;
- ii) use a single, non-reactive contaminant to represent water quality.
- iii) exclude water treatment for the purpose of making it fit for reuse (treating the water to meet discharge standards may be considered);

This strategy avoids all the theoretical difficulties noted above, and allows one to use the classical pinch analysis methodology. This comes at the potential expense of the accuracy in locating the true optimum for the system design. Each option may be evaluated for its possible effect:

- i) Since this is a food process, risk factors would tend to preclude water reuse in any streams which come into direct contact with the product, so excluding process streams from the analysis is advisable in any case.
- ii) The use of a single contaminant could make the predicted water savings over-optimistic, in that specific contaminants might prevent the reuse of water for specific purposes. This issue was noted in the case study, with the caution that the results should be seen as a first assessment, with such issues requiring further investigation. The justification for using a single contaminant is not really theoretical, as the methods for using multiple contaminants are readily available, it is more about the effort and expense of gathering the necessary data.

The case studies of the **AECI Bioproducts Lysine Plant** and the **Mondi Merebank Paper Mill** (chapters 4 and 5) illustrate a second possible strategy. These also considered only utility water, excluding process from the analysis, however they deviated from the simple strategy in several respects, thereby requiring the use of mathematical programming software. These deviations were:

- i) Excluding certain connections between specific sources and specific sinks. This is not the same as excluding a source or a sink: the source and sink involved remain in the analysis, and a constraint is added to the optimisation problem which is of a different kind to the concentration constraints in the standard pinch analysis.
- ii) The objective function was not simply the amount of fresh water supplied, but included costs of water supply and effluent discharge. Although neither of these case studies happened to involve regeneration for reuse, these factors had the same effect of moving away from considering the thermodynamic minimum for water use.
- iii) In the case of the lysine plant, multiple contaminants were considered.

These examples can be taken as representing the second strategy for approaching a water pinch analysis, in which mathematical programming is used to address all the restrictions except the exclusion of process streams and chemically reactive species. These exclusions allow the system to be modelled in terms of simple standardised elements, which makes it possible to use a generalised software package, such as WaterTarget used in these two studies.

The final case study of the **Sasol Polymers Chlor-alkali Plant** (chapter 6) accepted none of the restrictions noted above. While this resulted in the most rigorous approach to the problem, it was also the most complex and time consuming. In particular for process water containing reacting species, individual models of each process unit had to be developed which adequately represented process constraints and economics, which means that the development of a generalised software solution is much more difficult. It could be argued that this approach is no longer really pinch analysis, but borders on full process optimisation.

Although the three approaches were applied to different case studies in this project, the above argument suggests that they could be used sequentially as a progressive overall approach in a single project, in which one only moves to the next level of complexity if the results of the simpler analysis indicate that it is justified.

9.1.4 Other considerations

There are some observations concerning the application of water pinch analysis that are not related to its theoretical structure:

- 1) The direct economic drivers for water conservation are not as great as those for energy conservation, so industries are not as easily motivated to undertake water pinch analysis as energy pinch analysis.
- 2) In water-scarce situations, not uncommon in South Africa, there are indirect drivers related to the value chain of water, i.e. the economic value derived from activities which could not take place without a sufficient supply of water of adequate quality.
- 3) In such situations regulators have the responsibility of balancing the water requirements of different users in an equitable way. The systematic and transparent methodology of water pinch analysis could be useful for establishing the water requirements of industrial systems for regulatory purposes. It must be emphasised that, in its present form, it is unlikely to be useful for non-industrial systems.

9.2 Recommendations

Recommendations that can be made fall into two categories: those that concern the application of water pinch analysis according to the current state of the art, and those that concern in what directions further development of water pinch is needed .

9.2.1 The application of water pinch analysis

- 1) A water pinch analysis of a system needs to be approached with a very clear understanding of the conceptual basis of the technique, its underlying assumptions, its range of applicability and its limitations.
- 2) Water pinch analysis is essential a *design tool*; it is useful for deciding how a water using system should be configured, or perhaps reconfigured. It does not have a useful role in managing the operation of a water using system.
- 3) As the case studies of this report demonstrate, pinch analysis encompasses a range of variants of the technique, each with a different set of modelling assumptions, and a different set of strengths and weaknesses. Care should be taken to select the most appropriate variant for a particular system, and a particular purpose. All the variants have been developed for application to industrial systems, and are intended to optimise the use of water in an industrial context. Any attempt to use it in a different context (for instance, in an environmental context) should be approached with great care to evaluate the appropriateness of its underlying assumptions.
- 4) A pinch analysis of a system is usually an iterative process with much uncertainty in the early iterations. It seems logical to start with the simplest form of the analysis, in spite of the sweeping assumptions involved; and bring in more sophisticated considerations as they are shown to be required.

9.2.2 The further development of water pinch analysis

- 1) Further efforts are required to encourage wider acceptance of water pinch analysis by South African industry. This should be undertaken in conjunction with industry on a case study basis.

- 2) Further work is needed to extend the water pinch analysis methodology to account for chemically reacting solutes and aqueous reagents.
- 3) Techniques for the early identification of the applicability of water pinch need to be further developed.
- 4) Techniques need to be developed to reduce the time and effort required to gather the data needed for a water pinch analysis.
- 5) The use of water pinch analysis as a tool for co-regulation should be explored. This will require studies in which regulatory authorities are involved as partners, and the development of a protocol for reporting the modelling assumptions and process limits used in an analysis in a transparent and auditable way, so that it can be used with confidence in negotiations between industrial and regulatory parties.
- 6) Local consultants should be encouraged to set up a water pinch analysis service to industry.
- 7) The energy efficiency of a process has a significant impact on its water use for cooling and the concomitant generation of saline effluents. The simultaneous optimisation of water and energy use is therefore an important direction for further investigation.

10 Technology transfer

The main thrusts of this project were technology evaluation and technology transfer. Water pinch analysis appeared in the literature as a technique that held much promise in the South African context, and the project sought to test it on South African processes, and promote its use by South African industries. Any theoretical aspects arose purely in response to problems encountered along the way. The chief *modus operandi* was to promote the water pinch concept to industries, and wherever possible to recruit engineering personnel from the companies involved to enrol for part-time MScEng degrees, undertaking water pinch analysis studies in their factories. Some more conventional academic projects involving full-time MScEng students and one PhD have served to generate theoretical support for situations where the current techniques were not completely adequate. In all cases the projects were centred on industrial case studies.

10.1 Industry based part time MScEng projects

The success of Thokozani Majozi's project at Sanachem, which was undertaken during the preceding water pinch project and presented in WRC report 851/01/03, prompted us to adopt the idea of enrolling process engineers who wanted to further their technical studies as part time postgraduate students on studies based at their own factories. The concept was that the project should be related to their normal work, and should be of interest to the company, to minimise conflicting priorities between work and study time. Four projects of this kind were started : Gladys Naylor (née Crampton) at Mondi Merebank, Maryna Mansfield at Sappi Tugela, Eric Slabbert at Sappi Ngodwana and Annelie Lourens at Sasol Secunda.

The concept appeared to work well at first, with good support from the companies involved. However, it seems that the 2 to 3 year time scale for a part time MScEng is significantly longer than the interest span of many companies. In most cases the priorities of the companies changed with time, and when the projects did not yield quick results, the students/engineers came under pressure to devote their attention to different areas which were considered to be more urgent or important than improving water efficiency. At the time of compiling this report, only Gladys Naylor had completed, and she did so in spite of the fact that company had by then completely lost interest in water efficiency, because of the way its supply contract with the Durban Water Recycling Scheme had been structured.

Clearly this is not a satisfactory state of affairs, and the concept needs to be rethought for the future. However it was successful in making the companies aware of water pinch analysis and exposing them to some of its practicalities.

A significant later outcome was that, after completing his PhD, Paolo Gianadda was employed by Sappi in an R&D position dealing with optimisation of their operations, which includes the application of pinch analysis.

10.2 Workshops and courses

A pre-conference workshop for WISA delegates was also held at the University of Natal on the 19th of May, entitled *Water Pinch Analysis: A tool for the rational management of water and effluent in an industrial complex*. It was attended by 14 persons. A similar workshop was held at the University of Cape Town as part of WISA 2004. This was presented by Chris Brouckaert and Duncan Fraser, and attended by 10 persons.

At WISA 2002 there was a WRC sponsored workshop on *Tools for Cleaner Production*, in which a presentation was made on *Water Pinch Analysis as a Transparent Tool for the Co-regulation of Industrial Processes* (BROUCKAERT, C.J., SCHNEIDER, J., MANSFIELD, M. and BUCKLEY, C.A.). This forum gave the project and the technique very important exposure.

10.3 Conference presentations

The following paper was presented at *The International Water Association Conference on Water and Wastewater Management for Developing Countries*, Putra World Trade Centre, Kuala Lumpur, Malaysia, 29-31 October 2001, and subsequently accepted for publication in *Water Science and Technology*.

GIANADDA, P., BROUCKAERT, C.J., SAYER, R and BUCKLEY, C.A., The Application of Pinch Analysis to Water, Regent and Effluent Management in a Chlor-Alkali Facility

at the *Water Institute of Southern Africa Biennial WISA Conference and Exhibition*, Durban, 19-23 May 2002, the following posters and presentations were made:

LOURENS, A., The Application of Water Pinch at a Petrochemical Industry (Paper)

GIANADDA, P., BROUCKAERT, C.J., SAYER, R. and BUCKLEY, C.A., Process Water Pinch Analysis Guides Water, Reagent and Effluent Management in the Chlor-alkali Industry (Paper).

BROUCKAERT, C.J., SCHNEIDER, J., MANSFIELD, M. and BUCKLEY, C.A., Water Pinch Analysis as a Transparent Tool for the Co-regulation of Industrial Processes (Poster).

The last topic was also used as a presentation as part of a WRC sponsored workshop on Tools for Cleaner Production. This forum gave the project and the technique very important exposure.

At the *International Seminar on Advanced Achievements in Pinch Technology and Industrial Resource Management for Energy Savings, Pollution Reduction and Sustainable Development in Africa*, University of Durban-Westville, Durban, 18 - 20 November 2002 the following presentations were made:

BUCKLEY, C.A., BROUCKAERT, C.J., MANSFIELD, M. And GIANADDA, P. , Applying Water Pinch Analysis in the South African Context

GIANADDA, P., BROUCKAERT, C.J. And BUCKLEY, CA., Conceptual Developments in the Field of Water Pinch Analysis - Selected Case Studies from the Chlor-Alkali

MANSFIELD, M., BROUCKAERT, C.J. And BUCKLEY, C.A., Water Pinch Analysis at the Sappi Tugela Paper Mill.

BROUCKAERT, C.J., BUCKLEY, C.A., HANEKOM, D.* and WOODHOUSE, C.*, Optimal Location of a Membrane Treatment Plant in a Power Station

At the South African Chemical Engineering Congress, Chemical Engineers Competing in the Global Economy, Sun City, South Africa, 3-5 September 2003

GIANADDA, P., BROUCKAERT, C.J. AND BUCKLEY, C.A., The Application of Combined Water and Materials Pinch Analysis to a Chlor-alkali Plant, (Paper)

GIANADDA, P., BROUCKAERT, C.J. And BUCKLEY, C.A., The Optimisation of an Ion-exchange Demineralisation Plant Using Combined Water and Materials and Pinch Analysis (Poster)

At the Waste Management Emissions & Recycling in the Metallurgical and Chemical Process Industries Conference, Mintek Conference Centre, Randburg, Gauteng, South Africa, 18-19 March 2004 :

BROUCKAERT, C.J., GIANADDA, P. and BUCKLEY, C.A., Process Integration for Water and Energy Management (Paper)

10.4 Publication

GIANADDA, P., BROUCKAERT, C.J., SAYER, R. and BUCKLEY, C.A., The Application of Pinch Analysis to Water, Regent and Effluent Management in a Chlor-Alkali Facility, *Water Science & Technology*, 46 (9), pp. 21-28, October 2002, ISBN 1843394286.

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ABBREVIATIONS

AS	Ammonium sulphate
CIP	Clean-in-place
CFJ	Ceres Fruit Juices
COD	Chemical oxygen demand
DWAF	Department of Water Affairs and Forestry
FSA	Free and saline ammonia
HD	High density
PIX	Primary ion exchange
PM	Paper machine
ppm	Parts per million
RF	Recycled fibre
RFP	Recycled fibre plant
SIX	Secondary ion exchange
SS	Suspended solids
SWW	Southern Wastewater Treatment Plant (in Durban)
UOS	Umbogintwini Operating Services

1 INTRODUCTION

This report is a sequel to WRC Report No. 851/1/03 entitled *The Application of Pinch Analysis for the Rational Management of Water and Effluent in an Industrial Complex*. The earlier report set out the basis and methodology, together with some practical guidelines, for applying water pinch analysis to an industrial system, and presented some case studies as practical examples. This report is mostly concerned with further case studies which had not been completed at the time of the previous report. However these case studies do reflect some development in theoretical understanding which occurred during the intervening period. Thus the two reports are complementary to one another, and should be considered together. In particular, the literature survey and general theoretical background to water pinch analysis are contained in the previous report, while this report starts to address some issues which were raised in the previous report.

While the reader is referred to the earlier report for a fuller discussion, a brief introduction to the nature and scope of water pinch analysis is repeated here.

1.1 The nature and scope of water pinch analysis

Industrial processes usually require water with a range of qualities, and produce several effluents with a range of qualities, which allow the possibility of a hierarchical use of water.

Possible strategies for reducing the consumption of fresh water and the production of wastewater include:

- reuse:** wastewater from one process can be directly reused in others, provided the level of contamination is sufficiently low to meet the requirements of the subsequent processes;
- regenerative reuse:** wastewater can be treated to reduce the levels of contaminants before being reused in other processes. In this option, the water is not recycled to the process from it came;
- regenerative recycling:** after regeneration, water can be recycled to the process from which it came. This is generally more difficult than reuse, because recycling tends to build up contaminants.

Pinch analysis is a process integration tool, which was first developed for the design of heat recovery systems during the late 1970s. Using the analogies between heat and mass-transfer, a similar approach was developed for the design of mass-exchange systems (El-Halwagi, 1995). This work formed the basis for the design of water-using systems that conform to the usage patterns envisaged by Smith (1995) and illustrated in Figure 1.1. It took the design objective to be to minimise water consumption by maximising the reuse of water, using a graphical technique (Wang and Smith, 1994) which was termed *Water Pinch Analysis* (Buehner and Rossiter, 1996). However the technique was difficult (although possible) to extend to accommodate the practical constraints and characteristics of water-using systems, such as multiple contaminants, flow rate constraints, piping costs, etc. The added desire to introduce cost optimisation required that the problem be formulated using mathematical programming techniques (Doyle and Smith, 1997).

Water Pinch Analysis thus involves a set of systematic formal techniques to handle the complex problem of hierarchical water allocation to a system consisting of a number of processes, and choosing the best combination of strategies. The theory that appears in the

literature is still developing. The practical application of this theory is not as well established in the open literature, and particularly not in a South African context.

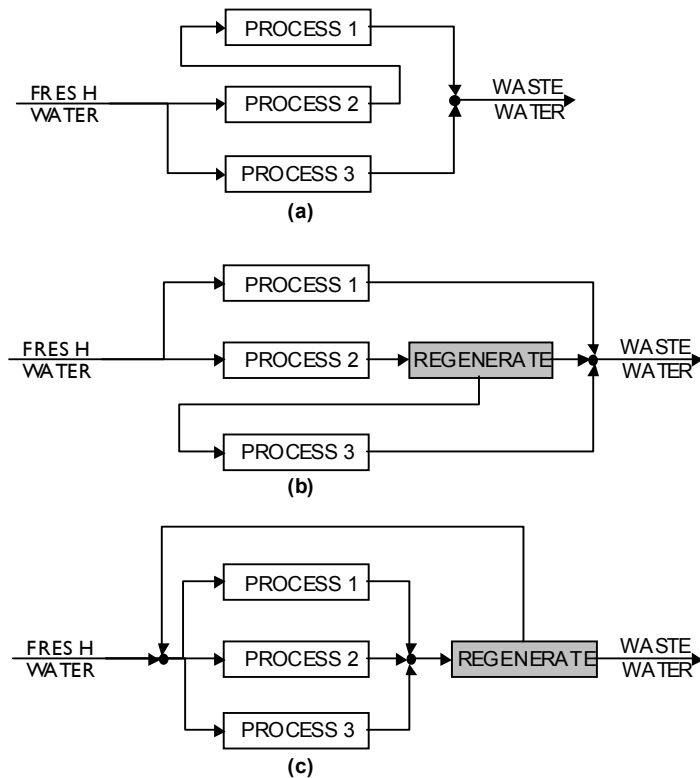


Figure 1.1: Water minimisation through (a) reuse, (b) regeneration reuse, and (c) regeneration recycling (Smith, 1995)

1.2 Project Objectives

As originally stated, the project objectives were:

- to promote the wide spread application of pinch analysis for the management of water and effluents;
- to develop the technique for the specific problems associated with South African industry;
- to promote better water management by undertaking pinch analysis studies at selected sites;
- to enhance the capacity within South Africa to undertake pinch analysis studies and to promote the wider understanding of the technique within educational institutions, industry and government by training people in the technique.

These objectives were pursued chiefly through undertaking case studies at a number of factories. Some of these were carried out by full time students at the University of Natal, whereas a number involved part-time students who were also working as engineers at the factories which were the subjects of study. Chapter 4 concerning the Mondi Merebank Paper Mill is based on one of these part-time student projects.

1.3 Overall course of the project

The history of this project is inextricably interwoven with that of WRC project that preceded it: K5/851 *The Application of Pinch Analysis for the Rational Management of Water and Effluent in an Industrial Complex*, so a single account of both is given.

The original project was envisaged as concerning only factories in the Umbogintwini industrial complex, located south of Durban. At the start in 1997, a preliminary survey identified AECI Bioproducts (lysine), SA Tioxide (titanium dioxide pigment) and Sasol Polymers (chlor-alkali) as the three largest water users in the complex, and these were selected for the initial investigations.

At the same time, the Canelands factory of Sanachem, a subsidiary of Sentrachem, producing agrochemical (principally herbicides and pesticides) requested to join the project. One of their chemical engineers, Thokozani Majozi, was assigned to undertaking the pinch analysis of processes at their site. This work was undertaken as a MScEng project, for which he was allowed to devote 50 % of his time.

A collaborative relationship was also established with Linnhoff-March, the UK consulting firm developing and marketing the WaterTarget™ suite of software for water pinch analysis.

Later in the project, other case studies were initiated as a result of interest from industry. The first of these was a study of the Eskom Lethabo Power Station near Vereeniging, in which the objective was to use pinch analysis to determine the best way to use a reverse osmosis plant within the power station water system. Three studies were started at paper mills: the Mondi Merebank paper mill with Gladys Naylor (née Crampton), the Sappi Ngodwana mill with Eric Slabbert and the Sappi Tugela mill with Maryna Mansfield. All three investigators were process engineers associated with the mills, who registering as part-time MScEng students. A similar arrangement was made with Annelie Lourens, a Sasol process engineer who worked on the water systems at the Natref refinery and the Secunda oil-from-coal complex. Finally, a study was commissioned by the South African branch of ILSI, the International Life Sciences Institute, to produce a monograph on the application of water pinch analysis in the food industry, after undertaking a pilot study at the Ceres Fruit Juice factory in Ceres. This was carried out by Janos Schneider after completing his thesis on the AECI Bioproducts plant.

Not all of these investigations reached successful conclusions during the course of the project. The initial studies at SA Tioxide and AECI Bioproducts stopped as a result of the resignation of key personnel; however the AECI Bioproducts study was subsequently restarted and completed successfully by a different student, Janos Schneider. The Sasol study halted when Mrs. Lourens resigned from Sasol to emigrate. The Sappi Ngodwana and Sappi Tugela studies were not completed by the end of the project, largely because of the pressure of other work commitments on the part-time students involved. This report and WRC Report 851/1/03, between them present those case studies which reached a sufficient degree of closure. These were:

- i) The Sasol Polymers Chlor-alkali plant. This in fact provided two case studies, the first carried out by Grant Gardner during the earlier project, and reported in WRC Report 851/1/03. In the follow-up project the plant was revisited by Paolo Gianadda in the light of the advances in pinch analysis theory which had occurred, as well as changes which had taken place in the factory. The later case study appears in the present report (chapter 6)
- ii) The Sanachem agrochemical plant (WRC Report 851/1/03).
- iii) The Lethabo Power Station (WRC Report 851/1/03).

- iv) The Ceres Fruit Juice factory (chapter 3 of this report).
- v) The AECI Bioproducts Lysine plant (chapter 4 of this report).
- vi) The Mondi Merebank paper mill (chapter 5 of this report).

Although the other case studies do not appear explicitly in the reports, they are represented implicitly in that they provided valuable experience which contributed greatly to the general understanding of pinch analysis, which in turn influenced the more successful projects.

1.4 Structure of the report

The principal matter of this report is contained in the four case studies, which present pinch analyses applied to different factories, involving widely varying circumstances. The factories were Ceres Fruit Juices, (chapter 3), the AECI Bioproducts lysine plant (chapter 4), the Mondi Merebank paper mill (chapter 5) and the Sasol Polymers chlor-alkali plant (chapter 6). Each of these case studies has its own discussion and conclusions related to issues specific to the system involved. These are preceded by chapter 2 devoted to those aspects of the methodology which were common to the investigations. In particular, it describes the Linnhoff-March *WaterTarget* software which was the principal tool used for the lysine plant and the paper mill, and which was also used in a subsidiary role for the chlor-alkali plant. Chapter 7 presents activities which aimed to promote water pinch analysis to industry during the course of the project. The conclusions and recommendations of chapter 8 concern issues which emerge from considering the various case studies together, and the overall experience of applying water pinch analysis to South African industries.

2 METHODOLOGY

The chief *modus operandi* of this project was to promote the water pinch concept to industries, and wherever possible to recruit engineering personnel from the companies involved to enrol for part-time MScEng degrees, undertaking water pinch analysis studies in their factories. Two conventional academic projects involving full-time students served to generate theoretical support for situations where the current techniques are not completely adequate. In all cases the projects centred around industrial case studies. Chapters 3, 4, 5 and 6 present the four major case studies which were completed during the project.

During the project a relationship was established with the British company Linnhoff-March, which has been associated with the development of both thermal and water pinch analysis. The *WaterTarget*[®] suite of software from Linnhoff-March was used for several of the studies, (in particular those of chapter 4 and 5) and this chapter is largely devoted to explaining the modelling framework which the software provides. The Linnhoff-March software is aimed at the analysis of systems in which water is used only as a utility to a process, and is not an intrinsic part of the core process technology. The *combined water and materials pinch analysis* of chapter 6 requires a different framework, which is developed and explained in chapter 6.

2.1 Outline of a Water Pinch Analysis investigation

As outlined in WRC Report No. 851/1/03, a water pinch investigation consists of several steps that are required to create a satisfactory design, as follows:

- i) Determine the water-using network.
- ii) Undertake a *pre-screening* or *rapid-scoping* exercise to identify the parts of the network which should be included in the analysis.
- iii) Establish flowrate and concentration data (measured data) and mass balance data (model data) for sources, water-using operations and discharge points.
- iv) 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.
- v) Simplify the network to exclude process streams that do not offer any scope for integration.
- vi) Determine the optimal design assuming current operating conditions are limiting.
- vii) Establish sensitive operations close to the pinch that offer further scope for saving by relaxation of constraints or by regeneration of streams.
- viii) 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.
- ix) Check suitability of design e.g. by simulation.
- x) Implement design if economically feasible.

The Linnhoff-March *WaterTarget*[®] suite provides software tools to assist in these tasks.

2.2 Utility Water Pinch Analysis and Process Water Pinch Analysis

Up to now, the literature on water pinch analysis has focused on problems where mass loads of contaminants are removed from process streams by water streams (Wang and Smith, 1994; Doyle and Smith 1997). Accordingly, the factor which limits the reuse of this water is the

presence of these contaminants in the water. Inherent in this approach, a number of assumptions are apparent - these are that:

- a clear distinction can be made between water streams and process streams;
- water behaves as a utility in the process system; and
- contaminants are exclusively undesirable

With the distinction being made between the process streams and water streams, only the water side of the problem is considered in the pinch analysis. The process-side of the problem is represented simply as contaminant *mass loads* with contaminant *concentration limits* applied to the water streams (to take the place of the equilibrium and kinetic relationships that govern the mass-exchange between these process streams and the water streams).

The distinction made between process streams and water streams in the pinch analysis formulation is more precisely a distinction between process streams and *utility-water* streams. It often happens that some of the process streams are also water streams. Making the distinction between process streams and water streams in the usual manner therefore results in some of the streams involving water being excluded from the analysis. In addition, some of the dissolved species present in the process-water streams may not be undesirable contaminants, but instead necessary elements of the process technology.

To properly optimise the use of water in such systems requires an approach which considers both the process-water streams and the utility-water streams. Given that the present techniques and tools only consider the utility-side of the problem, we coined the terms *utility-water pinch analysis* for the situation where only utility streams are considered, and *process-water pinch analysis* where process-water streams are also included. Process-water pinch analysis is a superset of utility-water pinch analysis since utility-water streams are also included in the analysis.

The practical problem facing an investigator is that process-water pinch analysis is a largely undeveloped field, whereas proven techniques are available for utility-water pinch analysis. In many cases the pragmatic approach is to limit the analysis to utility-water, and accept that the result will not be a fully optimal solution. On the other hand, there are industrial processes where this limitation severely restricts what can be achieved.

The following section describes the commercial software package that was used in several of the case studies of this report for utility-water pinch analysis.

2.3 The Linnhoff-March *WaterTarget* software

The Linnhoff-March *WaterTarget* software consists of two programs, *WaterTracker*, for data gathering and reconciliation, and *WaterPinch* for determining optimal water network designs and analysis of sensitive operations. Figure 2.1 is a flowchart illustrating how a water pinch analysis might be undertaken using this software.

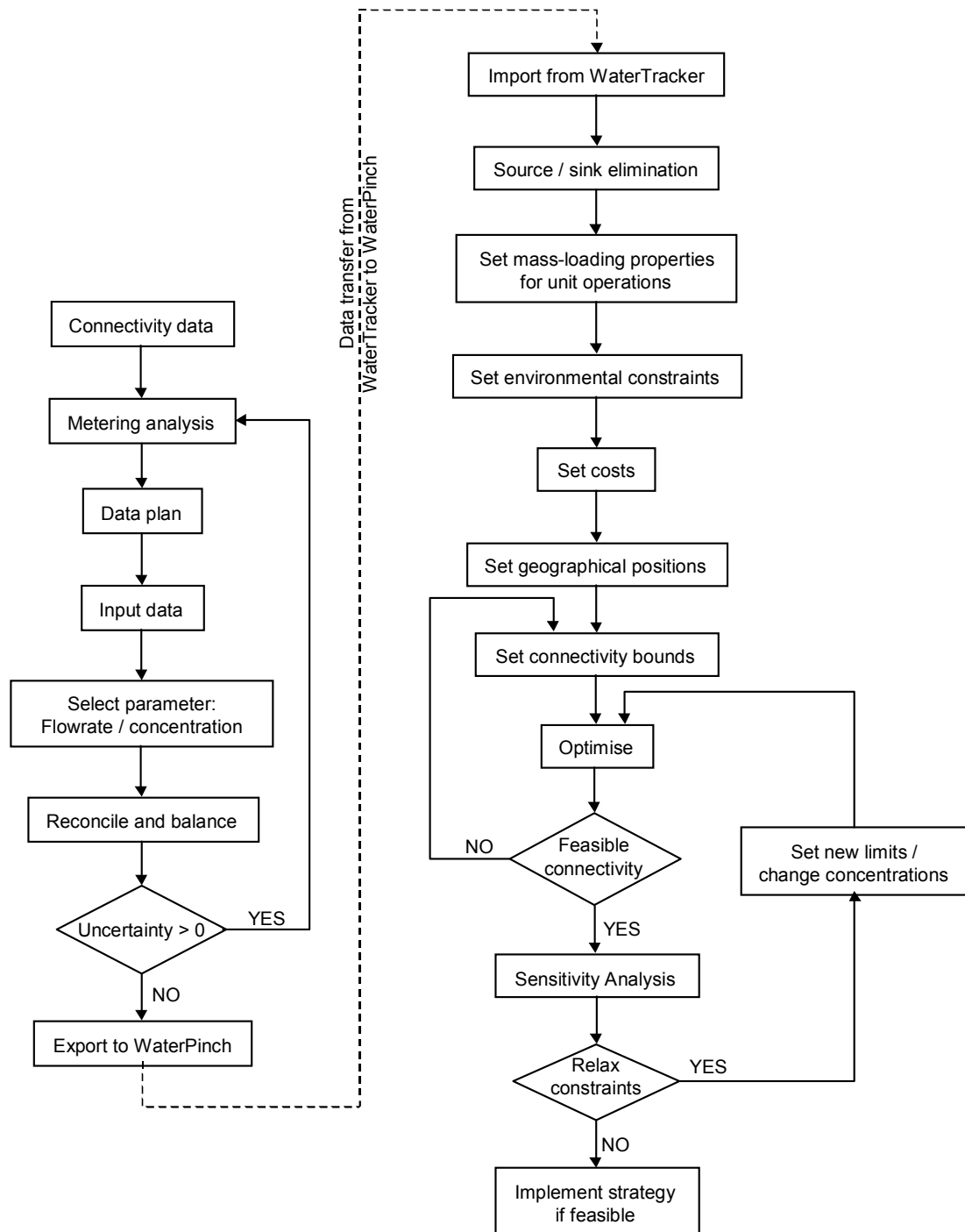


Figure 2.1: Outline of a water pinch investigation carried out using *WaterTarget*

2.3.1 The *WaterTarget* modelling framework

The water-using system (figure 2.2 (a)) consists 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:

- 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 2.2 (b)).
- 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 2.2 (c)).
 - Streams: Connections between nodes that represent material flow from one node to another.

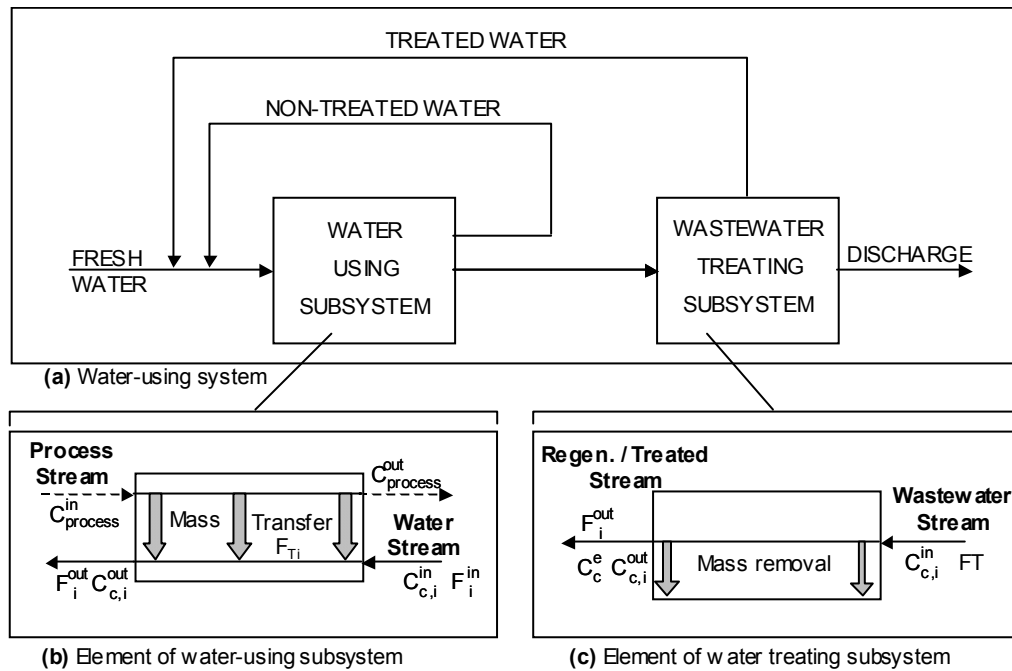


Figure 2.2 : A conceptual view of an industrial water-using system (a). Processes (b) and treatment / regeneration (c) unit operations. The dashed inlet and outlet line in (b) denotes the process stream.

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.

2.3.2 The WaterTracker program

WaterTracker assists with the tasks involved in gathering a consistent, mass-balanced data set from a water using plant

2.3.2.1 Types of Data

A set of 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.

2.3.2.2 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 where in structure 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*.

2.3.2.3 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:

- *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.
- A discontinuity exists between two determinations of a parameter (such as the directly measured value and a value determined by material balance from other measurements in the network), i.e.. a region of agreement cannot be identified within the ranges of related determinations. This type of discrepancy is illustrated in figure 2.3, below. Figure 2.3 (a) illustrates the case where the ranges of possible values according to the two determinations overlap. However, a discrepancy is reported when there is a gap between the ranges (figure 2.3 (b)).

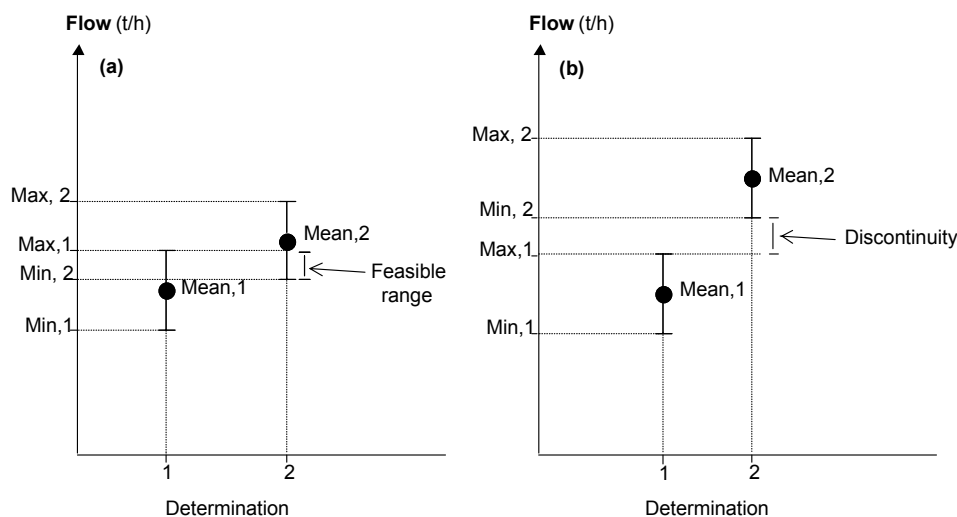


Figure 2.3 : Illustration of feasible (a) and infeasible (b) related measured information.

Data reconciliation determines a set of 'corrected measurements' that the best fits the measurement information within the ranges between the specified minimum and maximum

values, while maintaining water and contaminant balances across each node, subject to the specified model information.

2.3.3 The *WaterPinch* program

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*.

2.3.3.1 Inlet and Outlet Classification

In *WaterTracker*, some sources, sinks and associated operation inlets and outlets, may have been included to complete the balance that are not required for the pinch analysis, as they are inherent part of the process, and therefore 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 minimum and maximum limits.

2.3.3.2 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:

$$c_{ji}^{out} = A \cdot c_{ji}^{in} + B \quad (2.1)$$

where c_{ji}^{out} is the outlet concentration and c_{ji}^{in} the inlet concentration of contaminant j in operation i . The terms A and B are constants that describe the way in which contaminant mass is added or removed. For example, for process unit operations (figure 2.4 (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 :

$$F_i^{out} \cdot c_{ji}^{out} = F_i^{in} \cdot c_{ji}^{in} + \Delta m_i \quad (2.2)$$

from which the constant A and B may be calculated.

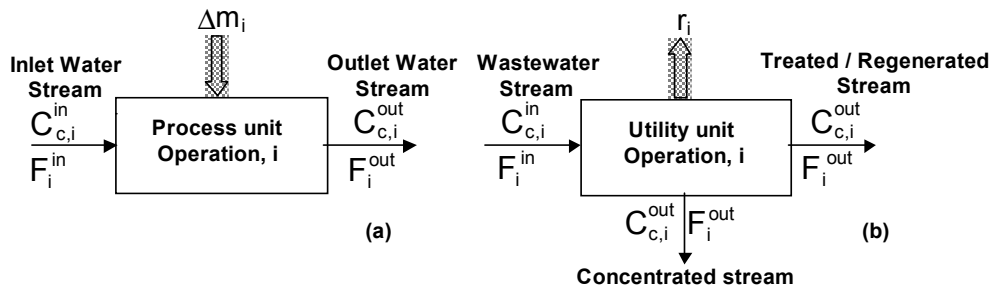


Figure 2.4 : Process (a) and utility (b) unit operation models.

Utility unit operations typically remove contaminant mass (figure 2.4 (b)). Outlet concentrations for utility unit operation i , may be related to the inlet concentration using a contaminant fractional removal term, r_i ($0 < r_i < 1$):

$$c_{ji}^{out} = c_{ji}^{in} \cdot (1 - r_i) \quad (2.3)$$

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

$$F_i^{out} = s_i \cdot F_i^{in} \quad (2.4)$$

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

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).

2.3.3.3 Environmental and Discharge Constraints

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

- **Flowrate:** constrained between a minimum and maximum or unconstrained.
- **Concentration:** limited to a maximum value or unconstrained.
- **Contaminant mass flowrate:** or Flowrate×Concentration, which is limited to a maximum value or is unconstrained.

Typically, environmental constraints are limited in terms of concentration. 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).

2.3.3.4 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 special 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). Piping costs per unit pipe length may be specified by the following equation:

$$c_{pipe} = K_i \cdot D_i^n \quad (2.5)$$

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 variables* 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.

2.3.3.5 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*.

2.3.3.6 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.

2.3.3.7 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.

3 CERES FRUIT JUICES

The South African branch of the International Life Sciences Institute (ILSI) commissioned the preparation a monograph on the application of water pinch analysis in the food industry. ILSI is a non-profit, world-wide foundation established in 1978 to advance the understanding of scientific issues relating to nutrition, food safety, toxicology, and the environment.

Two case studies were conducted, at Ceres Fruit Juices and Peninsula Beverages in the Western Cape,. It was part of the terms of reference of the commission that the studies should present straightforward applications of pinch analysis, using the simplest and most easily understood version of the technique. The Ceres Fruit Juices (CFJ) study is included in this report to represent this relatively simple end of the pinch analysis spectrum.

3.1 Process description

CFJ is located in the town of Ceres, approximately 200 km east of Cape Town. CFJ manufacture fruit juice for both the local and export market. During the data-gathering phase of the investigation (5 August - 8 August 2002) they produced approximately 1 538 325 litres of fruit juice.

Fruit juice from blending is heat sterilised to form the final product for packaging. Blending requires ultra pure water from the water treatment plant. Chlorinated water from the treatment plant is used for the sterilisation process and for cooling. Finally, effluent is treated in the effluent treatment plant to comply with municipal standards.

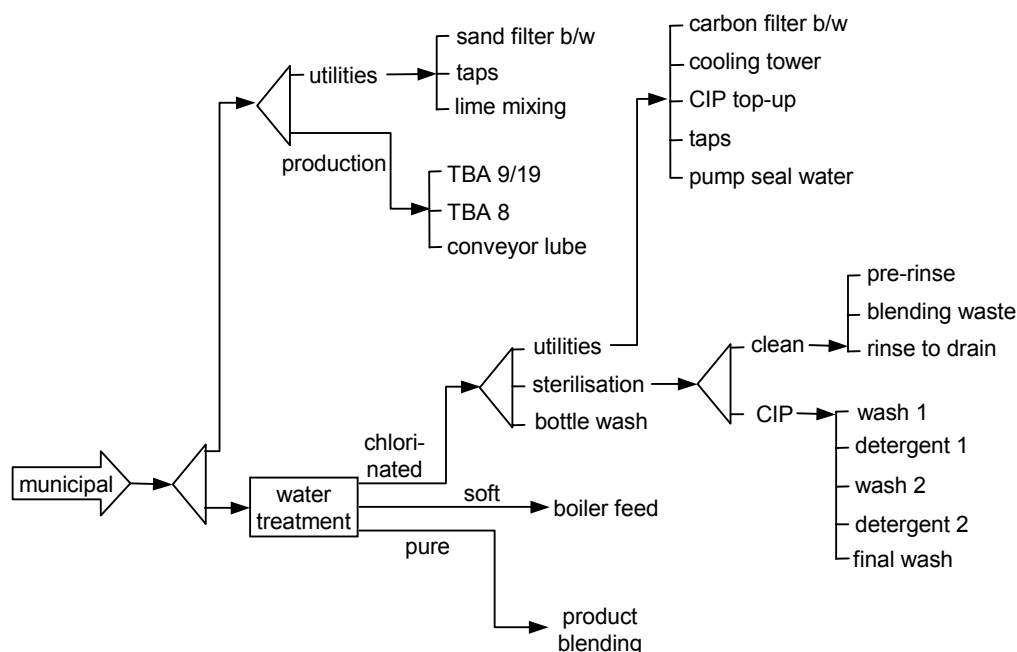


Figure 3.1 : The water distribution network at Ceres Fruit Juices

The water distribution network is shown in Figure 3.1. This was used as a guide to completing the flow balance. Municipal water is the primary source, which is either used directly or treated to produce a secondary fresh water source. At CFJ there are three

secondary fresh water sources produced by the water treatment plant: *chlorinated*, *pure*, and *soft* water.

3.1.1 Water treatment

In the water treatment plant, municipal water is initially flocculated in a clarifier, followed by sand filtration for solids removal. Sand filter filtrate is stored and chlorinated in a chlorination tank. This chlorinated water is predominantly used for washing and cleaning, or is further purified by activated carbon filtration and ultraviolet irradiation to produce pure water, which is used for product blending. A small softening unit softens municipal water for the boiler feed makeup. The sand filter is back washed with municipal water and the carbon filter with chlorinated water.

3.1.2 Municipal water users

Although not in related areas of the plant, six operations were identified as municipal water users, which use this source for:

- i) cooling of the filling machines;
- ii) lubrication of the conveyor system within the filling section;
- iii) floor and machine surface cleaning (taps);
- iv) backwash of the sand filters;
- v) makeup of the lime-mixing unit in the effluent treatment plant.

3.1.3 Blending

Pure water from the water treatment plant was used for blending with fruit juice concentrate. For a single flavour, individual batches ranged in volume from 5 m³ to 125 m³, during the period of the investigation.

3.1.4 Sterilisation and cleaning

10 lines were used for the sterilisation of the blended fruit juice, before filling. Sterilisation took place at approximately 140°C for 25 minutes by means of heat exchange with steam. After sterilisation the fruit juice was cooled with chilled water. After each batch, the sterilisation units were cleaned and a *clean in place* (CIP) routine was carried out once per day on each unit. Chlorinated water was used for cleaning, which consisted of the following steps:

- i) product push-out: fruit juice was displaced (results in blending waste)
- ii) rinse with water (contains some sugars and fruit solids)
- iii) circulation of water at 140°C (practically clean water)

The CIP routine used chlorinated water and cleaning reagents, and consisted of the following steps (after the product had been emptied):

- i) Initial wash
- ii) Detergent wash: NaOH solution
- iii) Second wash
- iv) Second detergent wash
- v) Final water rinse

3.1.5 Filling

After cooling, the sterilised fruit juice was filled into variety of package sizes, which ranged from 200 ml to 5 litres. Packaging varied in volume and type according to the juice brand.

Glass bottles (350 ml) required cleaning before filling, for which chlorinated water was used. As mentioned above, the filling machines required municipal water for cooling, which was used on a once-through basis.

Two boilers provided on-site steam, which was used for the most part for sterilisation. Soft water was used to make up evaporative and blowdown losses.

A cooling water system was in place for the cooling of juice after sterilisation. This water was circulated to cooling towers for heat removal. Chlorinated water was used to make up evaporative and blowdown losses.

3.1.6 Effluent treatment

An anaerobic digester was used for the reduction of COD in the final effluent. Lime was required for the neutralisation of the final effluent, which was slightly acidic. For this purpose, municipal water was used to make up the lime slurry.

3.1.7 Automatic CIP

An automatic CIP system (distinct from the CIP described for the sterilisation stage) was used for cleaning of the blending tanks, lines, fillers and juice pipelines. This CIP system used an internal reuse strategy, based on a countercurrent regime. After the cleaning agents had undergone several cycles of reuse, they were discharged. Chlorinated water was used to make up this water loss (together with the cleaning reagents).

3.2 Methodology

The study largely followed the general methodology for applying pinch analysis to an existing process set out in chapter 3 of the previous WRC Report No. 851/1/03 (Brouckaert and Buckley, 2003). The steps in the process were:

- 1) selection of the system boundaries;
- 2) identification of water sources and sinks;
- 3) pre-screening;
- 4) data gathering;
- 5) pinch problem formulation
 - modelling of unit operations
 - optimisation,
 - identification of bottlenecks - relax constraints or regenerate,
 - integrated network design;
- 6) implementation.

Points 1) and 2) have been covered in the process description (section 3.1). The pre-screening step 3) was identified as a need in the previous report, the approach taken in this study provides a possible way of dealing with it. The final step 6), implementing the suggested design changes, was not achieved during the project period.

3.3 Pre-screening

For relatively large water-using systems the data required for a pinch investigation (step 4) can be copious. Although some of the necessary information may be readily available, much of it may be difficult or costly to ascertain. For this reason, it is useful to obtain a quick indication of whether there is scope to realise significant benefits from the analysis *before* the detailed data-gathering stage.

The complete set of possible connections between all individual sources and sinks of water can be represented by arranging the sources and sinks in a matrix form, as shown in Figure 3.2.

			SINKS							
			1	2		j			n	d
			Sink 1	Sink 2	.	Sink j	.	.	Sink n	Sink d
SOURCES	1	Source 1	0	0						
	2	Source 2	1	0						
		.		0						
	i	Source i		0						
		.		0						
		.		0						
	m	Source m		0						
	k	Source k								

Figure 3.2 : Connectivity matrix for a general water using process. Connectivity between the sources i , and the sinks j , are represented by a '1' or a '0'

Sources, $i = 1, 2, \dots, m$ are arranged in the rows. The final rows are used to represent the freshwater sources, k . The sinks $j = 1, 2, \dots, n$ are arranged in the columns, with the final columns reserved for the available discharge points, d . The matrix entry in a given row and column is used to identify whether the connection between the correspond source and sink is possible (1) or not possible (0).

The pre-screening then is carried out by using a person experienced in the operation of the process to assess each potential connection (matrix entry) and judge whether it is likely to be possible in terms of the process requirements.

For example, if it is known that no portion of Source 1 may be used as feed for Source 2, row 1, column 1 is marked with a '0'. If it is possible that some portion of Source 2 may be used in Sink 1, row 2, column 1 is marked with a '1'.

Furthermore, the situation may arise where only freshwater may be used for a particular sink (e.g. Sink 2 in Figure 4). For such a case, it is possible to exclude this sink entirely from the pinch analysis. Similarly, a source may be excluded if it cannot be used anywhere. In the extreme case, it is conceivable that many operations may be excluded in such a way, or the matrix becomes so sparse (i.e.. full of zeros) that the identification of the remaining options for reuse becomes trivial. In this case it may be assumed that a rigorous analysis is unnecessary, and the pinch investigation may be terminated at this point.

3.3.1 General pre-screening considerations

In general the following considerations should be taken into account during pre-screening:

- Water quality requirements - some operations require freshwater in order to function properly, particularly boilers and cooling systems. These sinks may be excluded from the analysis.
- Highly variable sources - these are sources that pose a significant risk due to their unpredictable concentration fluctuations and therefore may not be deemed suitable for reuse.

- **Internal optimisation** - some processes are internally optimised, such as automatic CIP systems for example. Such systems often require freshwater and discharge water of an unsuitable quality for use elsewhere.

3.3.2 Pre-screening considerations for food and beverage operations

The following aspects should be taken into account during the pre-screening stage, which would influence the viability of reuse specifically for food and beverages:

- **Product contamination** - any activity that may result in product contamination should be avoided. For the case of multi-stage machine cleaning procedures, for machines directly involved with production, freshwater must be used in the final rinse stage.
- **Biological considerations** - any streams containing organic material such as sugars and foodstuffs, are susceptible to fermentation. Reuse options that imply significant retention times (e.g. greater than 1 day) may therefore need to be avoided.
- **Product blending requirements** - any water streams entering the product should be excluded from the analysis as final product quality will be affected.

It is important that each the pre-screening exclusions is very carefully considered, as this will preclude any further integration of the stream involved. Unsuitable connections will be re-examined at a later stage after the initial optimisation (see 3.5).

3.3.3 Pre-screening at Ceres Fruit Juices

The very large size of the pre-sceneing connectivity matrix for CFJ made it impractical to present in this report: the main outcomes are stated below. A smaller connectivity matrix resulted from the consideration of network restrictions (see Figure 3.4 in section 3.5.2); it conveys the same kind of information, but fits onto the page because of the smaller number of sources and sinks involved.

The following options were eliminated from the model during pre-screening:

- **Automatic CIP:** the CIP system was regarded as internally optimised, in terms of water usage. It was assumed that the system required freshwater and that the effluent was unsuitable for reuse elsewhere.
- **Boiler makeup and blowdown:** the makeup stream concentration requirements were fixed hence it was assumed that this could not be substituted. The blowdown was assumed to be of unsuitable quality for use elsewhere.
- **Machine cooling and conveyor lubrication:** these operations use small amounts freshwater and do not add any contamination hence internal recycle is most feasible here.
- **Product blending:** This requires ultra pure water only.
- **Taps:** used for surface cleaning (machine and floor) require freshwater and discharge a waste of highly variable and unpredictable quality, which was deemed unsuitable for reuse.

It was concluded that the remainder of the process provided sufficient potential for water saving to make it worth proceeding with the pinch analysis.

3.4 Data Gathering

There were two main objectives of the data gathering stage of the investigation. The primary objective was to obtain the parameters that adequately represent the requirements of the

water-using system. The secondary objective was to determine the current operating characteristics, which were used as a benchmark against which future savings could be measured. As productivity and associated water usage and stream concentrations fluctuate throughout the year, it was desirable to obtain data that is most representative of the average processing characteristics.

The basic information required for completing the data-gathering exercise may be summarised as follows:

- i) sink volumetric requirement;
- ii) source volume discharged;
- iii) frequency and duration of use or occurrence of sink and source flows i) and ii);
- iv) reagents used for each processing stage;
- v) water quality characteristics of the sources, such as temperature, pH, total solids (TS), suspended solids (SS), turbidity, conductivity, etc.

3.4.1 Water flow rates

The water flow rates calculated from a water balance over 1 week are given for certain key users in Table 3.1.

Table 3.1 : Flowrate data for Ceres Fruit Juices

Operation	Symbol	Water flowrate [m ³ /h]	Fresh-water Source
1. Cleaning of steriliser:			
a) rinse	F ₁	0.90	Chlorinated
b) blending waste	F ₂	0.62	Chlorinated
c) rinse to drain	F ₃	1.32	Chlorinated
2. CIP of steriliser:			
a) wash 1	F ₄	0.41	Chlorinated
b) detergent 1	F ₅	0.28	Chlorinated
c) wash 2	F ₆	0.47	Chlorinated
d) detergent 2	F ₇	0.28	Chlorinated
e) final wash	F ₈	0.30	Chlorinated
3. Sand filter backwash	F ₉	1.25	Municipal
4. Carbon filter backwash	F ₁₀	1.25	Chlorinated
5. Pump seal water	F ₁₁	2.00	Chlorinated
7. Lime mixing	F ₁₂	1.00	Municipal
8. Miscellaneous †		33.24	
Total		43.32	

† The miscellaneous water requirements include all the uses that were excluded from the analysis during pre-screening.

3.4.2 Contaminants

In the context of a water pinch investigation, the waterborne species, which restrict the reuse of water in the system, are termed contaminants. The identification of these species is done by questioning what prevents the reuse of a water stream in a particular area of the system.

Contaminants may be single entities such as ions or molecules (e.g. Ca^{2+} ions) or aggregated groups e.g. total dissolved solids (TDS).

In some cases it becomes necessary to distinguish between contaminants and reagents that are introduced deliberately. Some like sodium hydroxide for example, may be a reagent in one part of a process, and a contaminant in another.

The contaminants that were considered as restricting the extent of water reuse at CFJ were classified as follows:

- Dissolved / suspended fruit solids: sugars, pith, etc. These arise during steriliser cleaning and CIP.
- Cleaning reagents: NaOH, peroxil. These are introduced into the system during automatic CIP.
- Suspended solids: arise from the raw municipal water feed (suspended solids were flocculated in the clarifier, removed by sand filtration, and finally discharged during backwash of the sand filters).
- Chlorine / water flavours: dissolved chlorine arises from the chlorination of filtered municipal water in the chlorination tank (flavours are adsorbed in the carbon filters and discharged during backwash).
- Conductivity: dissolved ionic solids, such as chloride ions that promote corrosion. These are seen to be problematic in cooling towers, where they accumulate by evaporation concentration.

It is conceivable that numerous other contaminants, not listed above, affected the way in which water was used. However, the above discussion does serve to illustrate that some contaminants:

- i) affect water usage in localised areas only, e.g. suspended solids in water treatment.
- ii) may be viewed as reagents in some areas and contaminants in others. This is clear when considering the chlorine in water treatment and cleaning reagents for CIP.
- iii) may be grouped according to their nature and / or the way in which they affect water usage. For example, considering total solids (TS) as a contaminant, allows for suspended solids, dissolved ionic solids, caustic soda (for cleaning), and sugars to be grouped under this classification. This has the benefit of reducing the costs associated with the analysis of water and effluent streams. In addition, by considering only one contaminant, single contaminant optimisation techniques may be used, which simplifies the analysis of the model considerably. Lastly, it was decided to restrict the analysis to a single contaminant for clarity of presentation in the monograph, even though this might be an over-simplification of the situation.

Total solids (TS) was used as an indicator for contamination, hence the non-volatile solids: suspended solids, caustic soda, and sugars were grouped together as total solids.

The outlet concentration (c_{out}^*) was measured in samples taken from of effluent and water streams. The maximum inlet concentration (c_{in}^{max}) was estimated by assuming that 20% of the measured outlet concentration was allowed at the inlet. The maximum outlet concentration (c_{out}^{max}) was calculated by assuming that a linear relationship between inlet and outlet existed. The existing concentration of TS at the inlet (c_{in}) was assumed to be that of fresh water, which was measured at 60 ppm.

Table 3.2 summarises the TS data obtained in this way.

Table 3.2 : Total solids data for Ceres Fruit Juices

Operation	Process Number	C_{in} ppm	C_{in}^{max} ppm	C_{out}^* ppm	C_{out}^{max} ppm	ΔM kg/h
Steriliser cleaning						
rinse	1	60	80	10	120	0.036
Blending to waste	2			105 000		
Rinse to drain	3	60	161	503	604	0.585
CIP of Steriliser						
Wash 1	4	60	92	159	191	0.041
Detergent 1	5	60	3,180	15 600	18 720	4.351
Wash 2	6	60	1 334	6 372	7 647	2 967
Detergent 2	7	60	3 180	15 600	18 720	4.351
Final wash	8	60	554	2,471	2 965	0.723
Sand filter backwash	9	60	360	1 500	1 800	1.800
Carbon filter backwash	10	60	80	100	120	0.050
Pump seal water	11	60	100	90	130	0.060
Lime mixing †	12	60	500 000			

† The concentration constraint for the lime mixing (for effluent neutralisation) was set to high value as it was assumed that this sink could use a poor quality of water and hence could accept the effluent from any of the operations.

3.5 Pinch Analysis

The water pinch analysis in this study used the basic graphical approach, as outlined by Wang and Smith (1994)

3.5.1 Composite curve

The composite curve for the process at CFJ (Figure 3.3) was used to determine the freshwater target and pinch point. The minimum water flowrate of 2.96 t/h corresponds to the water requirement for the system where the TS concentration limits provide the only restrictions on water reuse, and may be considered as the *fresh water target* to aim for while generating water-using network designs. The pinch concentration is 120 ppm, which corresponds to the outlet of the carbon filter backwash and the rinse stage for steriliser cleaning.

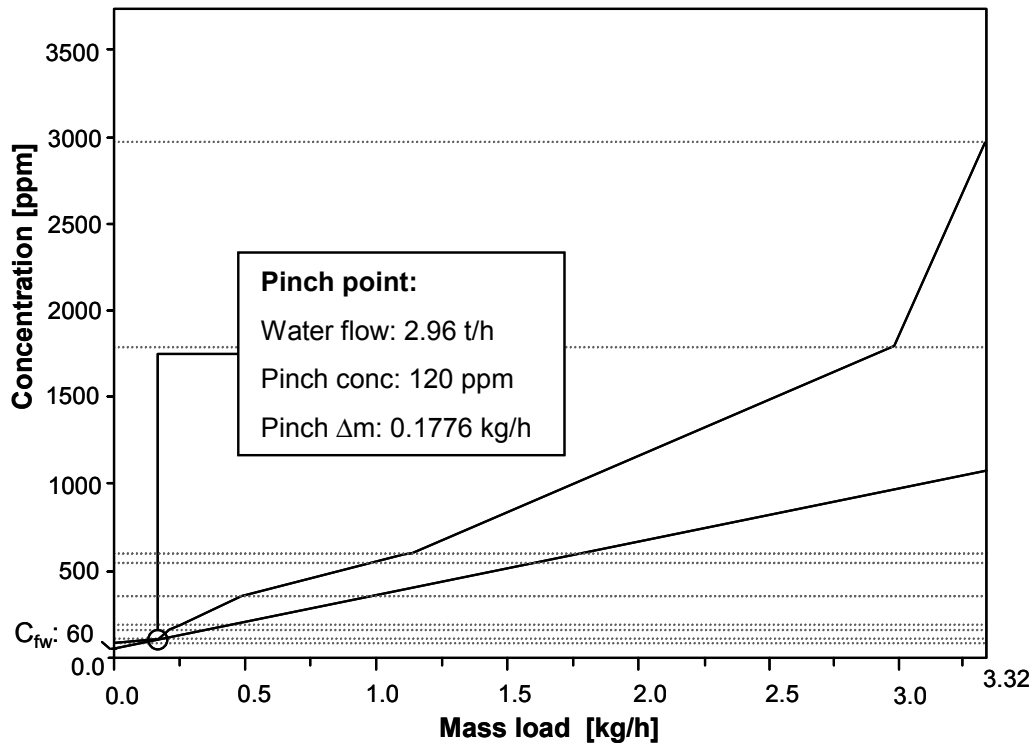


Figure 3.3 : *The composite curves for Ceres Fruit Juices*

3.5.2 Reuse restrictions

The pinch point indicated in Figure 3.3 was determined on the assumption that the only factors limiting reuse were the total solids limits of Table 3.2. Several further restrictions had to be added the CFJ model to avoid any risk associated with product contamination or equipment damage:

- i) The initial rinse before sterilisation had to use fresh water, in order to reduce the risk of product contamination.
- ii) The final wash after CIP had to use freshwater for the same reason as (i).
- iii) An individual CIP stage (wash 1, detergent, etc.) could use only water from itself or from subsequent stages.
- iv) Utilities (filters and pump seals) could not use any water associated with machine cleaning.
- v) Sand filter backwash effluent could not be used in the pump seals or the carbon filters.

These restrictions are shown as a connectivity matrix in Figure 3.3. The rows represent the sources, and the columns represent the sinks (this matrix may be viewed as the reduced form of the pre-screening matrix mentioned in section 3.3.2)

			SINKS											
			1	3	4	5	6	7	8	9	10	11	12	
			Rinse	Rinse to drain	Wash 1	Detergent 1	Wash 1	Detergent 2	Final wash	Sand filter backwash	Carbon filter backwash	Pump seals	Lime makeup	Effluent
SOURCES	1	Rinse												
	2	Blending waste												
	3	Rinse to drain												
	4	Wash 1												
	5	Detergent 1												
	6	Wash 2												
	7	Detergent 2												
	8	Final wash												
	9	Sand filter backwash												
	10	Carbon filter backwash												
	11	Pump seals												
		Freshwater												

Reuse not allowed
 Reuse allowed

Figure 3.4 : Connectivity matrix showing allowed and disallowed reuse options

3.5.3 Source-sink matching

The network configuration that satisfies the fresh water target is usually not unique. There are a number of different techniques which allow one to establish a set of connections between the available sources and sinks. The method chosen for this study uses a *source-sink mass mapping diagram* (El-Halwagi, 1997). The source and sink streams are assumed to be at their maximum inlet and outlet concentrations. The streams are plotted as single points on a source-sink mass mapping diagram as indicated in Figure 3.4.

The steps for using the mapping diagram to identify the water-recycling network are summarised below:

- i) Start with sinks requiring fresh water.
- ii) Redraw the mass mapping diagram as matches occur (if necessary).
- iii) Satisfy the sinks with the strictest water concentration requirements (cleanest water needed) first, in sequential order using sources with the lowest compositions, to minimise wastewater discharge and freshwater flows.
- iv) Try to recycle the source back to the sink of that unit, if possible (this always requires dilution with freshwater or another source stream).
- v) In applying these steps, only the allowed connections shown in Figure 3.3 could be selected. These restrictions meant that the minimum target of 2.96 t/h could not be realised.

The results of applying this procedure to the Ceres Fruit Juices system are shown in Figure 3.5 (b) with the existing configuration in Figure 3.5 (a) for comparison.

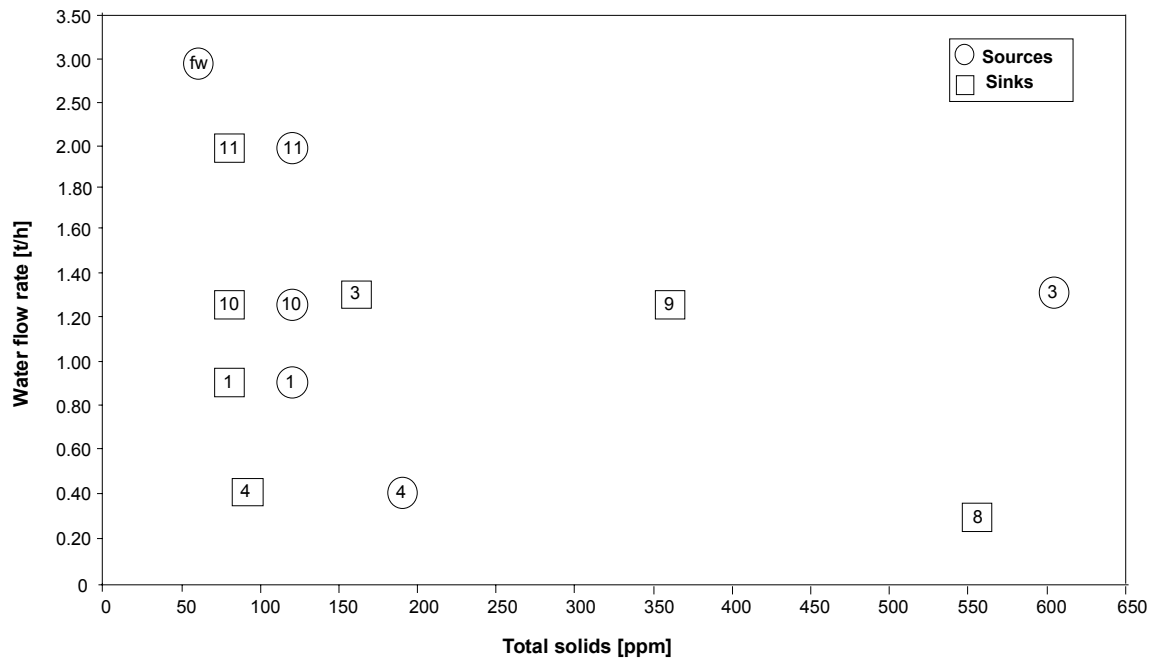


Figure 3.5 : Source-sink map for Ceres Fruit Juices. The numbers in the blocks refer to the process numbers Table 3.2. Processes 2, 5, 6, 7, and 12 fall off the scale of the diagram, however they were included in the analysis.

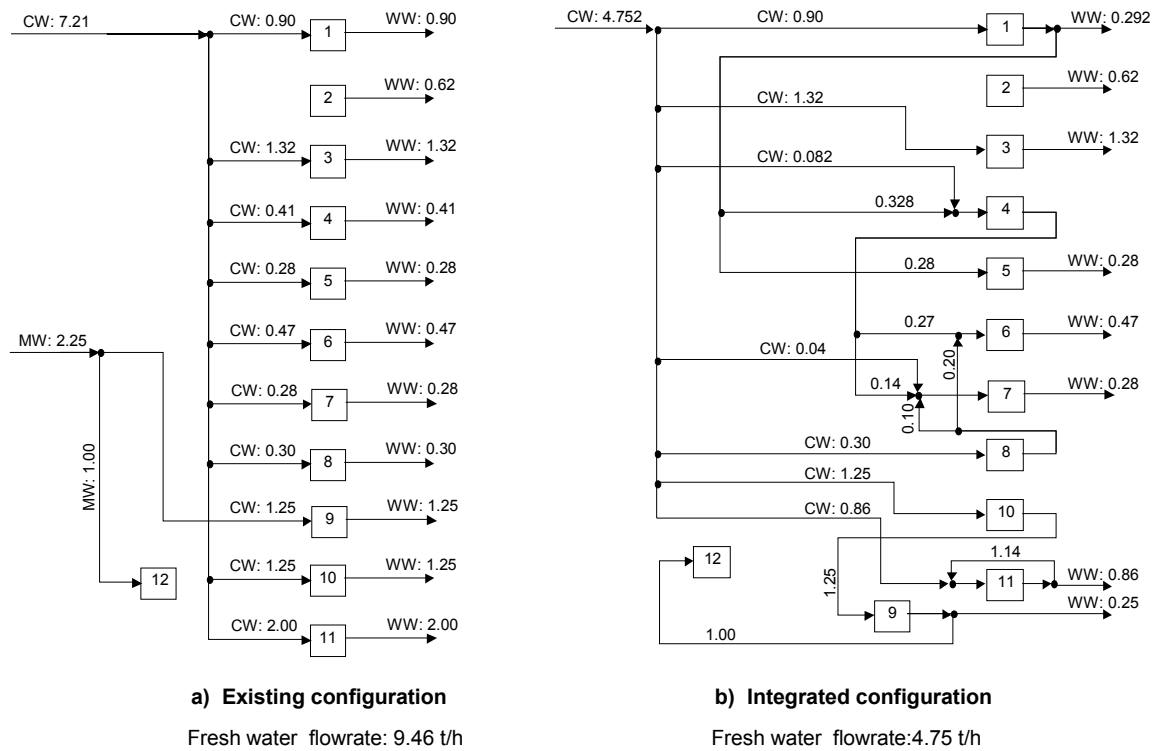


Figure 3.6 : Comparison of the existing water allocation configuration (a) at Ceres Fruit Juices with the integrated configuration resulting from the pinch analysis (b).

3.6 Discussion and conclusions

The pinch analysis identified a potential reduction of 4.7 t/h of fresh water, a saving of very nearly 50 %. The study ended at this point, so it was not possible to confirm whether this could be implemented in practice.

From the composite curve (Figure 3.2) it can be seen that the pinch occurs at a concentration of 120 ppm, which corresponds to the outlet of the carbon filter backwash and the initial rinse stage of the steriliser cleaning. Because the analysis depends so critically on this point, it also corresponds to where future engineering effort should be focused.

The first step would be to verify the data: check the flow rate and concentration parameters for these two critical operations. If they were significantly different than the initial estimates, the optimisation procedure would have to be repeated to establish a new pinch point. When satisfied with the data, the possible users of the water (sinks) need to be examined more closely; bearing in mind the stream characteristics that were not included in the single contaminant analysis. For example, the steriliser rinse takes place at 140 °C - what are the limitations or benefits of having a source at this temperature? It is useful at this stage to return to the source / sink matrix that was used to represent the structural restrictions (Figure 3.3). The integrated network solution (Figure 3.5 b)) splits the rinse effluent (Source 1) between Sink 4 and 5 with freshwater dilution, which makes the system more complex to operate, but is necessary in order to satisfy the imposed concentration constraint. It is possible that the entire source may be reused in only one of the CIP stages. Note that the concentration constraints derived for the system were not absolute limits, but were estimates based on measured outlet concentrations (section 3.4.2). Therefore, it is quite possible that the inlet concentration constraints might be relaxed for one or more of the operations considered as potential sinks.

For the carbon filter backwash effluent (Source 10), the solution identified in the integrated network used this entirely as feed to the sand filter backwash (Sink 9), effectively replacing the municipal water feed. The sand filter backwash effluent (Source 9) was in turn used for lime mixing at the effluent treatment plant (Sink 12).

Other opportunities identified include use of the final CIP rinse (Source 8) in the preceding rinse stages (with freshwater makeup).

From the above discussion it can be seen that the simple form of water pinch analysis does have a number of theoretical limitations. On the other hand, in a relatively uncomplicated system such as the one considered here, they can often be addressed by carefully considering their implications for the particular process in question. The resulting design might not strictly optimal, but should be close enough for practical purposes.

4 THE AECI BIOPRODUCTS LYSINE PLANT AT UMBOGINTWINI

This chapter is based on the University of Natal MScEng thesis by Janos Schneider entitled *The Application of Water Pinch Analysis at AECI Bioproducts*, submitted in 2002.

4.1 Introduction

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 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.

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 environmental regulations limit the concentration of pollutants discharged to the sea. What remained after lysine extraction was broth effluent, which was removed from the site and handled by the 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 operates at the industrial complex. Umbogintwini river water is treated by UOS for use in the plants at the complex. Some industries use 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 on-site 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 use reduction had not been implemented at any stage during the design or subsequent process modifications.

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 Umbogintwini industrial complex. For this reason, AECI Bioproducts was selected as a suitable candidate for a water pinch investigation.

4.2 Aims of the investigation

The aims of this project were to:

- i) apply water pinch analysis at Bioproducts, which consisted 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 were the greatest barriers to further saving and improvement, and in so doing, suggest possible improvements that would aid in the implementation of similar projects in the future.

4.3 Process overview

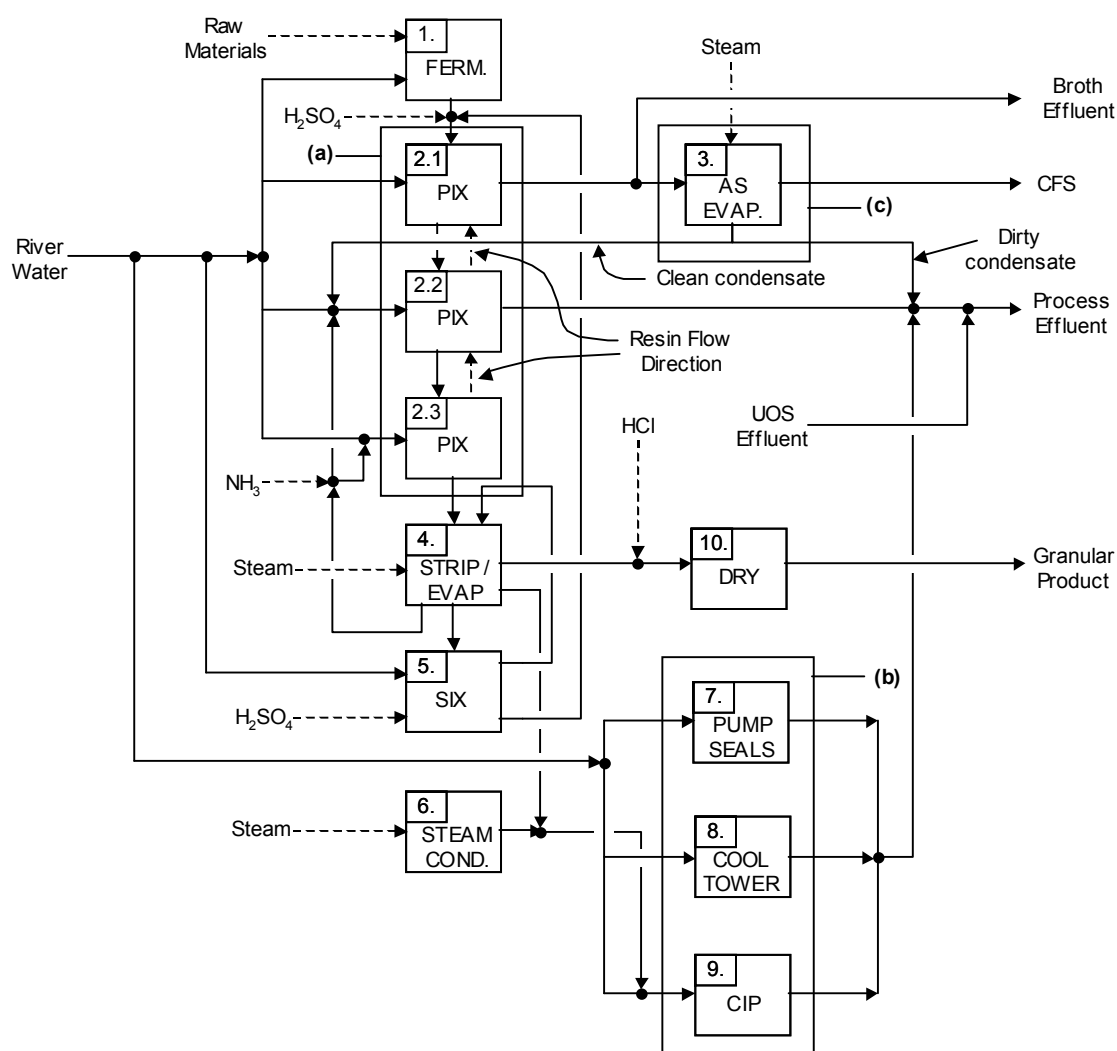


Figure 4.1 : Flow sheet outlining water and raw material distribution, and process streams in the manufacture of l-lysine at AECI Bioproducts.

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 4.1 presents a simplified view 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 for clarity.

4.3.1 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 water supplied by Umgeni Water. The most significant contaminant present in the UOS water supply is chloride, which presents corrosion problems if allowed to accumulate.

4.3.2 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.

4.3.3 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 anti foam, 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.

4.3.4 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 18 m³ pre-fermenter, where the biomass increases to approximately 250 kg, after 30 to 40 h. The pre-fermenter feeds the main fermentation stage. Four 200 m³ tanks are operated cyclically, each fermentation batch lasting 3-5 days. During the first 8 to 12 hours, the biomass increases to 4 to 5 t. Changing the balance of substrate nutrients during the remainder of the period, causes the cell population to stop increasing and the micro-organisms begin to overproduce lysine.

4.3.5 Sterilisation

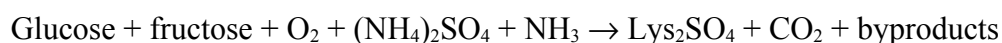
Foreign micro-organisms must not enter the fermentation process. The mutated lysine producing micro-organism cannot compete with natural micro-organisms, and the fermentation batch must be discarded if contamination of this nature occurs. For this reason, all nutrients and anti foam required for pre-fermentation 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 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 in 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 to 13 t/h.

Lysine production may be summarised by the following (unbalanced) chemical equation:

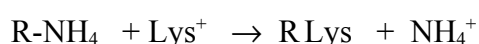
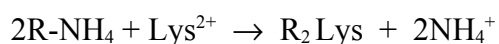


4.3.6 Primary ion exchange

The primary ion exchange (PIX) process (figure 4.1 (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.

4.3.6.1 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 countercurrent 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:



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 in

Figure 4.1) 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 from releasing this biomass-rich effluent to the sea. The effluent was transported off-site to the Durban Southern Wastewater Treatment Works (SWW).

4.3.6.2 Backwash phase

The loaded resin is rinsed to remove any product entrained on and between the resin beads. The beds are subsequently back washed 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.

4.3.6.3 Strip phase

The lysine is displaced from the resin during the strip phase, by feeding a 4M ammonia solution, countercurrent 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.

4.3.7 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 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 paragraph 4.7) for further purification. The pure lysine solution from the SIX process is further concentrated in the first and second stages of the evaporation process.

4.3.8 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.

4.3.9 Ammonium sulphate evaporator

About a third of the broth effluent is fed to the single-effect AS evaporator (Figure 4.1 (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. 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 1000 ppm is used as part of the PIX backwash feed. However, if the suspended solids concentration rises above 1000 ppm, 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.

4.3.10 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 Figure 4.1. 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.

4.3.11 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.

4.3.12 Cleaning and cooling utilities and pump-seal water

The auxiliary processes (figure 4.1 (b)) use UOS water either from the process water tank or directly, as is the case for the cooling tower. The clean-in-place (CIP) system uses condensate, made up with process water. All of these water-using operations discharge their effluent via the sea pipeline.

4.3.12.1 Clean-in-place system

Clean-in-place (CIP) is an automatic tank cleaning system. The water for the feed consists 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.

4.3.12.2 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.

4.3.12.3 Cooling tower

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

4.4 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.

4.4.1 PIX: Broth effluent

At 16 R/t, the PIX broth effluent had 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 consists mainly of AS, as the broth effluent is acidified with sulphuric acid. The concentrated nature of this effluent source makes it unsuitable 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. Broth effluent has not been considered at AECI Bioproducts, since a broth effluent recycle would lead to accumulation of charged ash particles (that arise from the HTM), which would reduce the PIX adsorption efficiency.

4.4.2 PIX: Backwash effluent

The main contaminants present in the backwash effluent are 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 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.

4.4.3 Condensate

As process steam is imported, pure condensate is not recycled to the boiler; hence it is a source of high quality water. Current water saving practices see this source being used as part of the feed to the CIP process, as well as making up 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 makes reuse of this source risky. This has been 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 4.6).

4.4.4 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.

4.4.5 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.

4.4.6 Clean-in-place system

The overall quality of the *Clean-In-Place* (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.

4.4.7 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 (Alva-Argaez, 1999). Feed to the cooling tower must be as pure as possible in order to reduce the blowdown rate.

4.5 Water pinch model of the water-using system

The Linnhoff-March Waterpinch software was used for the analysis of the system. The software is described in chapter 2.

4.5.1 Key contaminants

Three contaminants were selected: free and saline ammonia (FSA), suspended solids (SS) and chlorides (Cl).

4.5.1.1 Free and Saline Ammonia

Dissolved ammonium species, predominantly $(\text{NH}_3)_2\text{SO}_4$ and $\text{NH}_3(\text{aq})$ (depending on the pH) are collectively classified as FSA. The concentration of this contaminant must be below 300 ppm 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.

4.5.1.2 Suspended Solids

This is a broad-spectrum contaminant, which is limited to below 400 ppm 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. Pickup 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.

4.5.1.3 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 2 000 mS/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.

4.5.2 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 AECI Bioproducts can be omitted. This is shown in figure 4.2, which interprets the simplified process representation in figure 4.1 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 intrinsic 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.

4.5.2.1 PIX strip

Two separate water sources were used to feed the PIX strip phase (figure 4.2 (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.

4.5.2.2 Evaporators and condensate

In the analysis, all the pure condensate sources (figure 4.2 (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.

4.5.2.3 SIX

As with the PIX strip phase, two water supplies at different contaminant concentration levels were used in the SIX operation (figure 4.2 (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 was 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.

4.5.2.4 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 4.2 (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 6.38 t/h, the demand from the CIP system is small compared to the demand of the entire system.

4.5.2.5 Pump seals

As with the CIP system, the pump seals were treated as a single water-using operation, with a total demand of 6.5 t/h .

4.5.3 Water users

From figure 4.2, the water users considered in this study consist of:

- AS condensate;
- Fermentation;
- Cooling tower;
- Pump seals;
- PIX adsorption;
- PIX backwash;
- Steam condensate (pure condensate producers grouped together);
- SIX acid dilution;
- PIX strip water;
- CIP;
- SIX rinse;
- 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 cattle feed supplement 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 shown in figure 4.3. The flowrates that achieve this configuration are given in table 4.1.

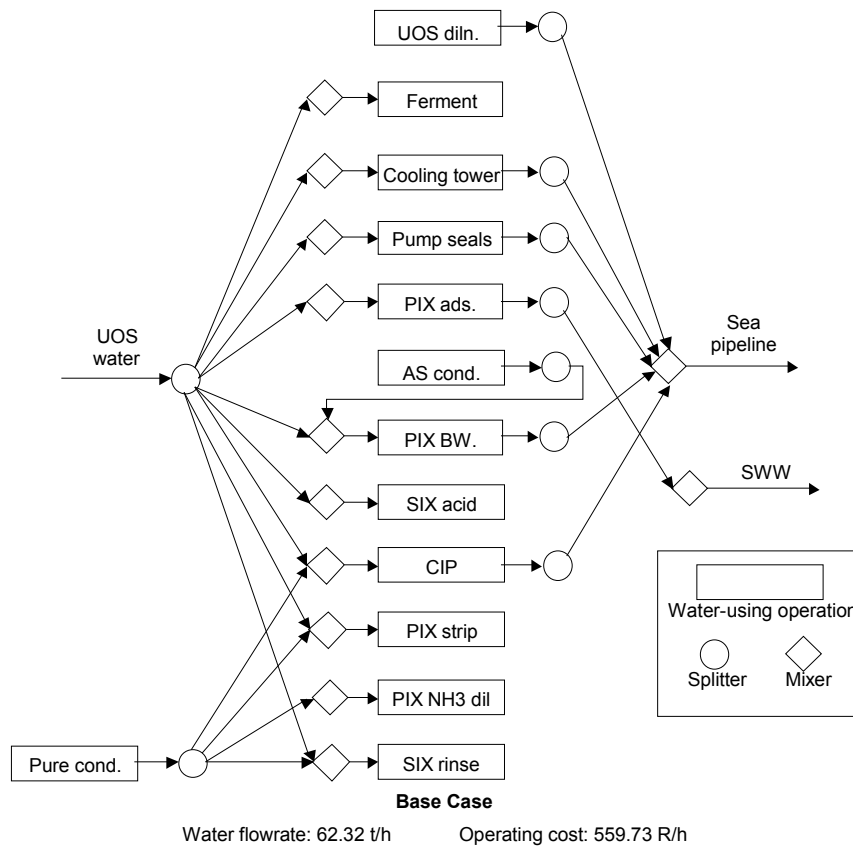


Figure 4.3: Base-case model configuration for the AECl Bioproducts system.

Table 4.1: Inter-operation flowrates for base-case configuration; flows in t/h.

To From	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH ₃ dil.	PIX ads.	PIX bw	SIX rinse	SIX acid	Sea pipeline	SWW
CIP											6.38	
Pump seals											6.50	
Cooling tower											3.59	
Pure condensate		5.67			11.08	0.16			1.16			
UOS dilution											80.14	
PIX backwash											17.43	
PIX adsorption												24.97
AS condensate								6.40				
UOS water	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 became one of determining the configuration of the water-using subsystem. Three contaminants were included: FSA, SS and Cl. Equation 2.1, was used to relate the outlet conditions to the inlet concentration for each operation. The coefficients A and B were assumed constant for all operating scenarios investigated in section 4.6. The coefficient values for each operation that has a wastewater outlet are presented in table 4.2, 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 4.5 is unconstrained and zero respectively), as it is dependent on the configuration of the water-using system. Table 4.3 lists the flow and concentration characteristics of each of these sources.

Table 4.2: Mass loading relationships and flowrates for the water-using operations

Operation	Contaminant	A (-)	B (ppm)	F _i ⁱⁿ (t/h)	F _i ^{out} (t/h)
Cooling Tower	SS	8.30	793.3	29.76	3.59
	FSA	8.30	0.0		
	Cl	8.31	0.0		
Pump seals	SS	1.00	197.6	6.5	6.5
	FSA	1.00	0.0		
	Cl	1.00	0.0		
PIX Adsorption	SS	0.00	35 0000	14.44	24.97
	FSA	0.00	35 000		
	Cl	0.00	1 000		
PIX backwash	SS	1.00	0.0	10.45	17.43
	FSA	0.60	240.1		
	Cl	1.00	0.0		
CIP	SS	1.00	7 670.3	6.38	6.38
	FSA	1.00	0.0		
	Cl	1.00	0.0		

Table 4.3 : Flow rates and concentrations of water sources

Source	Flow (t/h)	Contaminant	c ^{out} (ppm)
UOS fresh water	Variable	SS	793.3
		FSA	0.0
		Cl	0.0
Condensate	18.07	SS	197.6
		FSA	0.0
		Cl	0.0
UOS dilution	80.14	SS	350 000
		FSA	35 000
		Cl	1 000

The positions of the water-using operations are given in table 4.4. These were used to calculate the cost of installing new piping wherever a new connection was identified.

Table 4.4 : Approximate positions of the operations at AECI Bioproducts

Operation	X position [m]	Y position [m]	Operation	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 NH ₃ dilution	20	20	Cooling tower	5	90
UOS dilution	25	0	Sea outfall pipe	25	0
AS evaporation	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 4.5. The cost of using the SWW was based on the mass-flowrate of effluent (i.e.. R/t of effluent). This contrasts with the sea pipeline: an annual license fee was charged by the water authorities for its use, which was translated to an hourly usage fee (i.e.. R/h).

Table 4.5 : Cost parameters used in the analysis

Freshwater cost, α_i	R2.50 /t
Discharge cost to SWW, a_i	R6.00 /t
Discharge to sea pipeline, b_i	R4.41 /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 4.1 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 :

$$c_{pji} = 4.78 \times 10^{-3} \cdot D_{ji}^{0.9} \cdot L_{ji} \quad (4.1)$$

The length of piping, L_{ji} is calculated from the X,Y positions in table 4.4. 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.

4.6 Water-using system model analysis

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

Scenario A. This scenario looked at the scope for reusing the AS condensate for the SS s at a concentration of 1 000 ppm.

Scenario B. The reuse of pure condensate was investigated in this scenario, i.e. where no contaminant is present.

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

4.6.1 Scenario A

This scenario looked at the water-using system with the inlet constraints to the operations and discharge points set to the current operating concentration (table 4.9). A conservative approach to water reuse was adopted, which is reflected in the table of prohibited inter-process flows (table 4.6). In this scenario, the AS condensate was set to 1 000 ppm, which reflects a worst-case scenario for the concentration of this source (table 4.7) before reuse is prohibited on the plant (see section 4.2.8). The average conditions of the effluent discharged to the sea, taken for the month during which the study was made, violated the constraint for SS. Hence, the limit was adjusted to reflect this (table 4.8).

TABLE 4.6 : 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 bw	SIX rinse	SIX acid	Sea pipeline	SWW
CIP			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 bw	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		

0 Flow prohibited

Flow allowed

The general assumption was that effluent from operations where the concentration is unpredictable may not be reused as feed to sensitive operations (section 4.3), 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 was allowed in all operations. Reuse of CIP and pump seal effluent was limited to local recycling; reuse of the pump seal effluent was allowed in the CIP process. Cooling tower blowdown was deemed suitable for reuse in the pump seals only. UOS effluent dilution was constrained to the sea outfall pipe and could not be used anywhere else. Discharge of the broth effluent was constrained to the SWW for off-site treatment, in accordance with the DWAF effluent agreement in force at the time. *Note that this last constraint was later relaxed to determine the sensitivity of the configuration to relaxation of the environmental constraint for the sea pipeline.*

Table 4.7: Conditions for the AS evaporator (Scenario A)

Operation	F _{out} (t/h)	Contaminant	C ^{out}
AS Condensate	6.40	SS	0.00
		FSA	1.00
		Cl	0.00

The FSA concentration was assumed to be zero (table 4.7) for this scenario; however small quantities of this contaminant may have been present, but the concentration was not measured. The chloride concentration was very low in this source, and was assumed to be zero.

Table 4.8: Sea pipeline discharge constraints (Scenario A)

Discharge point	Contaminant	C ^{in MAX} (ppm)	M ^{in MAX} (kg/h)
Sea pipeline	SA	300	-
	SS	-	75
	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 666 ppm in the sea pipeline, which violated the environmental constraint of 400 ppm, but reflected the average discharge conditions during the period of the investigation.

In this scenario, current operating conditions determined the maximum inlet concentration constraints for each operation (equation 2.2). The maximum outlet concentration was calculated using equation 2.1, by setting:

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

Table 4.9 : Inlet and outlet flowrate and maximum inlet and outlet concentration constraints (Scenario A)

Operation	F^{in}	F^{out} (t/h)	Contaminant	$C^{in MAX}$ (ppm)	$C^{in MAX}$ (ppm)
Cooling Tower	29.76	3.59	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	80.63
Pump Seals	6.5	6.5	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	80.63
PIX adsorption	14.44	24.97	FSA	3,990	3,990
			SS	24.9	24.9
			Cl	80.63	80.63
PIX backwash	10.45	17.43	FSA	100	100
			SS	625	625
			Cl	80.63	80.63
SIX rinse	1.3	Negligible (Flow<0.02)	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	80.63
CIP	6.38	6.38	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	80.63
PIX NH3 dilution	0.16	Process stream	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	80.63
IX acid dilution	1.38	Process stream	FSA	0.00*	0.00*
			SS	1.38	1.38
			Cl	80.63	80.63
Fermentation	3.99	Process stream	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	80.63
PIX strip rinse	12.43	Process stream	FSA	0.00*	0.00*
			SS	24.9	24.9
			Cl	80.63	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 Linnhoff-March WaterPinch software was used to carry out the optimisation subject to the specified constraints. The configuration of the resulting water-using system is shown in figure 4.4.

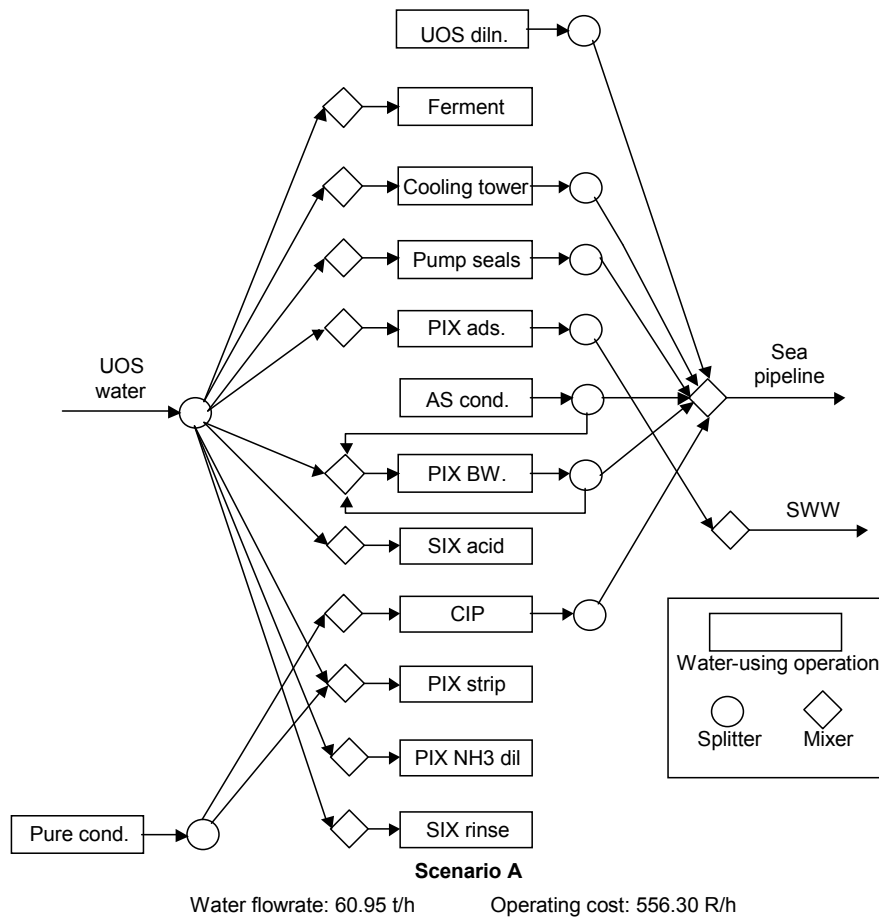


Figure 4.4 : Configuration of the optimised water-using network for Scenario A.

The flowrates for the above configuration are presented in table 4.10. The configuration does not differ substantially from the existing configuration (figure 4.3). The reuse of AS condensate is reduced, some of which is discharged to the sea pipeline.

Table 4.10 : Matrix of inter-operation flows for the configuration of the Scenario A water system; flows in t/h.

From \ To	Ferment	CIP	Pump seals	Cooling tower	PIX strip	PIX NH ₃ dil.	PIX ads.	PIX bw	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 backwash								3.48			16.43	
PIX adsorption												24.97
AS condensate								4.29			2.11	
UOS water	3.99		6.50	29.76	0.90		14.44	2.68	1.30	1.38		

Existing connenction

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 2.32 t/h in this operation, leading to a decrease in the water-using system operating cost of 0.61% or R 29 635 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.

4.6.1.1 Initial sensitivity values

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 4.5 (a)). The potential for further relaxation of the SS constraint to the PIX backwash (as well as other constraints) is explored in section 4.7. Reducing the outlet concentration of SS from the AS evaporator provides the greatest potential for saving by regeneration of this stream.

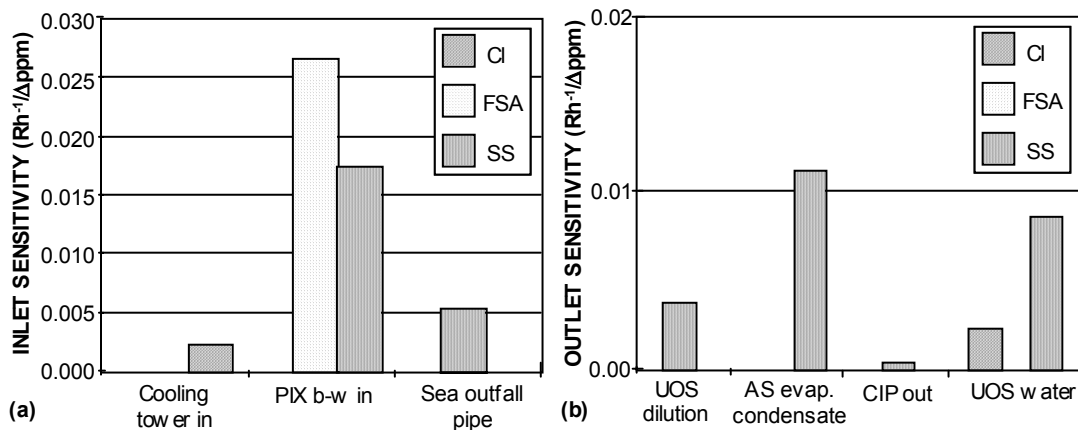


Figure 4.5 : Inlet (a) and outlet (b) sensitivity values for Scenario A.

4.6.2 Scenario B

The system configuration was investigated for the case where the AS condensate is pure (table 4.11), i.e., no contamination of the condensate from the process stream occurs. Mass-loading characteristics (table 4.2) for the operations and inlet concentration constraints (table 4.9) remain the same as for Scenario A.

Table 4.11 : Conditions for the AS evaporator (Scenario B)

Operation	F _{out} (t/h)	Contaminant	C ^{out}
AS Condensate	6.40	SS	0.00
		FSA	0.00
		Cl	0.00

The network configuration generated by the WaterPinch software is presented in figure 4.6. 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 58.84 t/h, which is a total water-using system operating cost saving of 1.56 % or R 75 443 per annum.

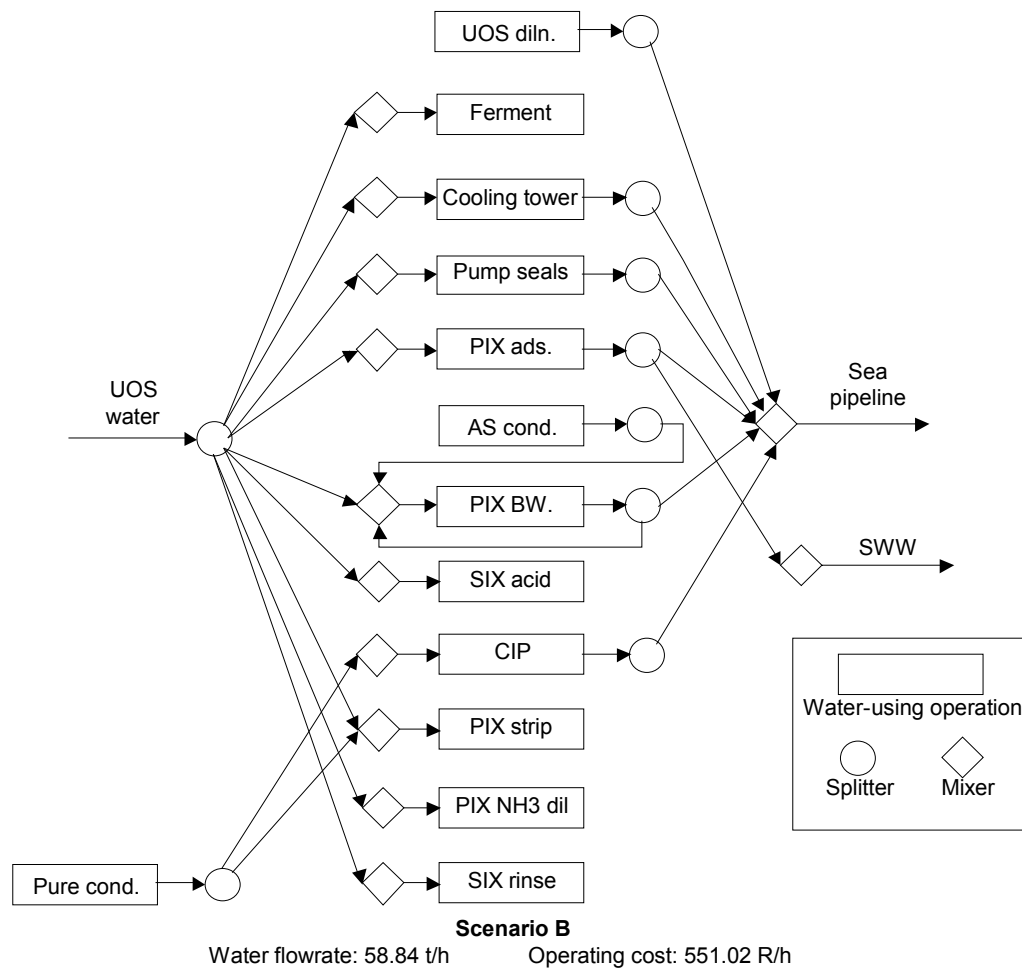


Figure 4.6 : Configuration of the water-using system with pure AS evaporator condensate (Scenario B).

4.6.2.1 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 4.7 (a)). The reported initial sensitivity of the objective cost to changing outlet concentrations is negligible for this scenario (figure 4.7 (b)).

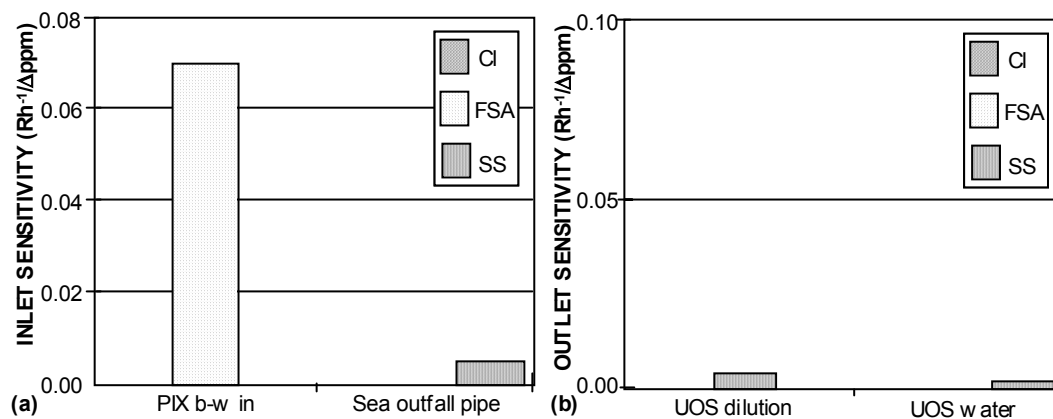


Figure 4.7: Inlet (a) and outlet (b) sensitivity values for Scenario B.

4.6.3 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 4.9). The structural constraints are similar (table 4.6), 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 4.8.

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 567.02 R/h.

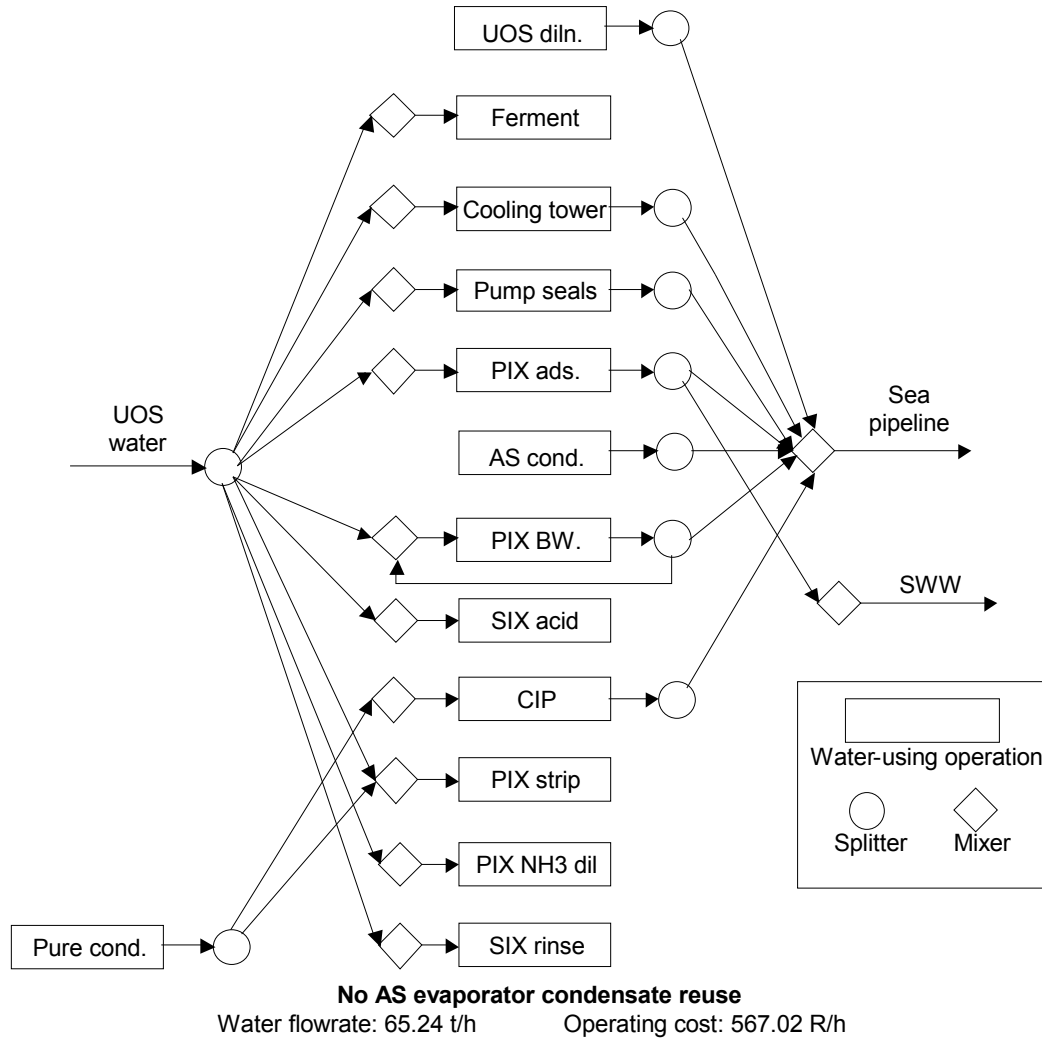


Figure 4.8 : Configuration of the water-using system with the AS evaporator condensate reuse prohibited (Scenario C).

4.6.3.1 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.

4.7 Model sensitivity analysis

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 4.5. 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 above mentioned cost, flowrate, and concentration conditions.

4.7.1 Fresh water

The sensitivity of the objective cost to changes in freshwater cost was explored first. In figure 4.9, a plot of the total objective cost (in R/h) as a function of the freshwater supply (in R/t), is presented.

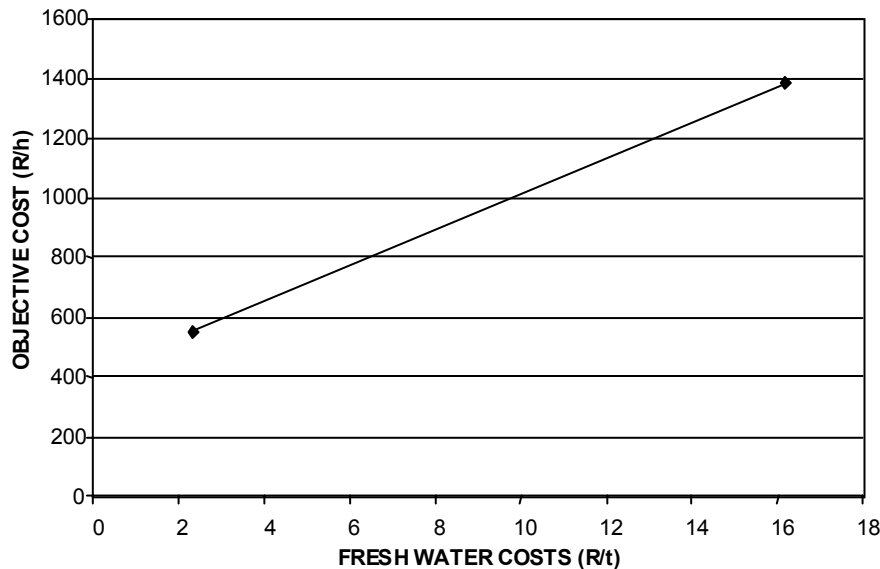


Figure 4.9: Sensitivity of the optimum objective function to freshwater costs.

In this range, the network structure and flow rates did not change as the water cost increased.

4.7.2 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 the changing the inlet constraint for chlorides was found to be negligible for all operations.

4.7.2.1 PIX Backwash sensitivity

In figure 4.10, 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

1 000 ppm) reused in this process may be increased, while simultaneously maintaining a backwash recycle flowrate of 3.48 t/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 630 ppm. 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.

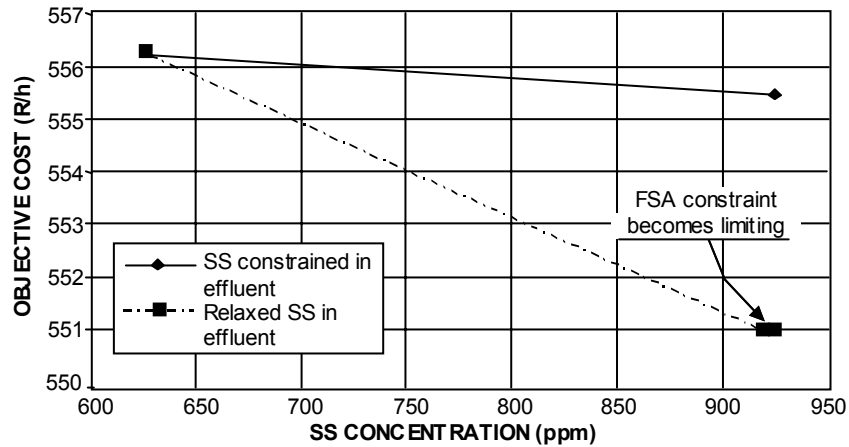


Figure 4.10: Sensitivity of the objective cost to relaxation of the inlet SS constraint to the PIX backwash.

The plot with the steeper negative gradient in figure 4.10 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 925 ppm, 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 4.6) prevented PIX adsorption effluent (broth effluent) from entering the sea pipeline.

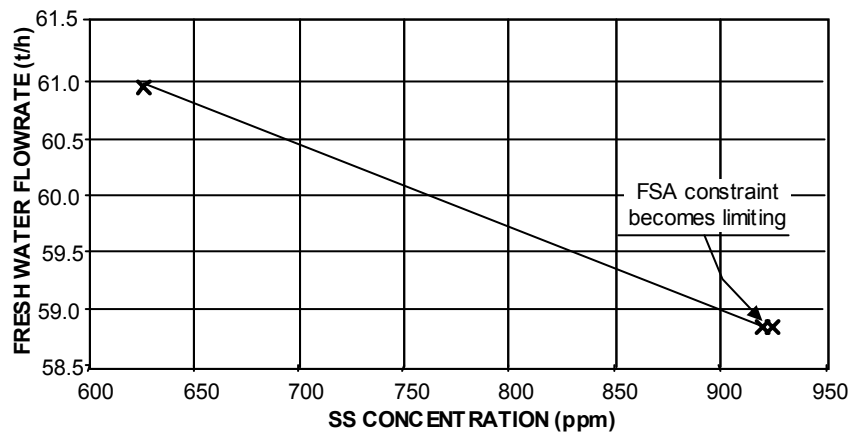


Figure 4.11: Overall freshwater flowrate as a function of SS inlet concentration constraint to the PIX backwash.

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 4.11, 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 an SS concentration of 925 ppm, where the FSA constraint became limiting.

4.7.2.2 Sea Pipeline sensitivity

The sensitivity of the solution to changing the SS and FSA constraints 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 4.12 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 300 ppm and the mass flowrate of suspended solids is approximately 360.6 kg/h. Figure 4.13 shows a linear increase in FSA with relaxation of the SS mass flowrate.

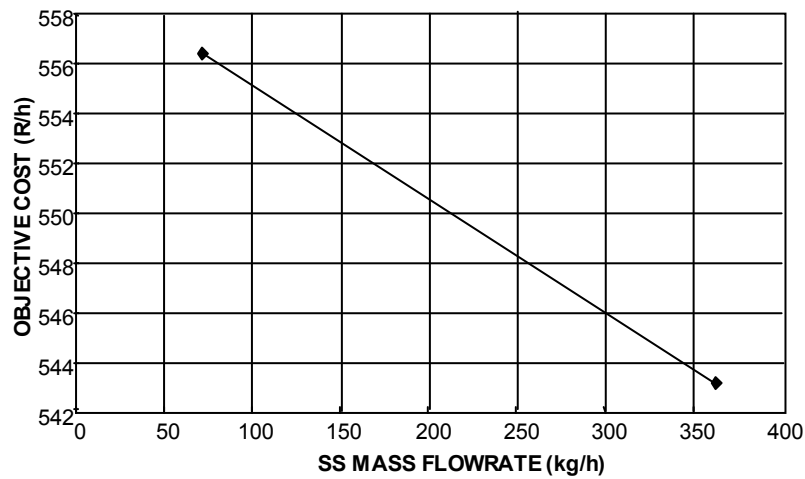


Figure 4.12: Objective cost sensitivity to SS concentration in the sea pipeline.

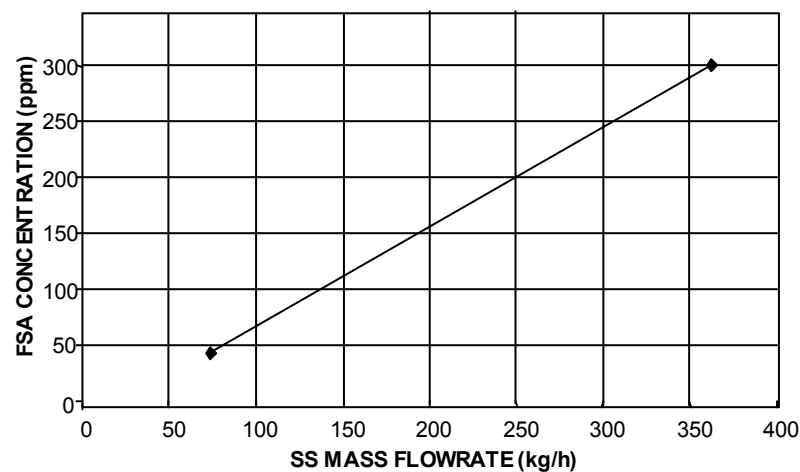


Figure 4.13: FSA concentration in the sea pipeline as a function SS mass-flowrate.

At the point at which FSA became limiting, at a FSA concentration of 300 ppm, 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 4.14. Initially, it can be seen that the objective cost decreases linearly with an increasing FSA concentration constraint. However, after a concentration of 5 000 ppm 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 4.15. After a concentration of 5 000 ppm 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.

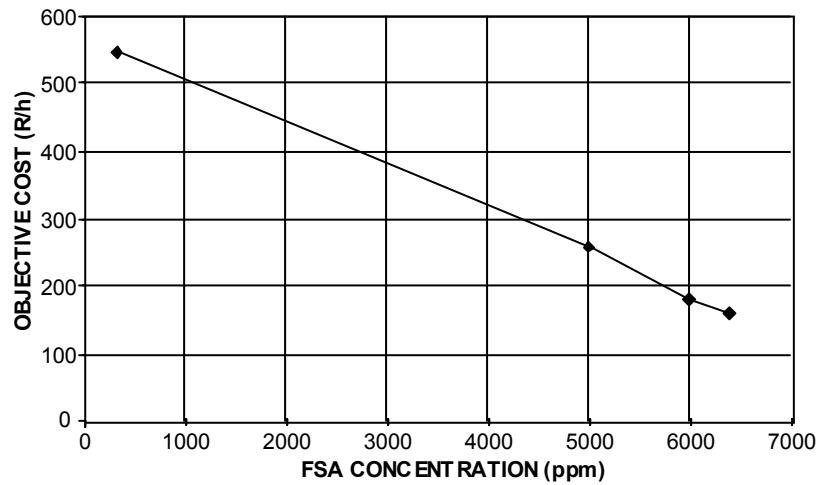


Figure 4.14 : Objective cost sensitivity to FSA concentration in the sea pipeline.

The sensitivity of the configuration to increasing the FSA concentration constraint in sea pipeline was explored in figure 4.15, which shows the plot of sea pipeline effluent flowrate and freshwater flowrate as a function of FSA concentration.

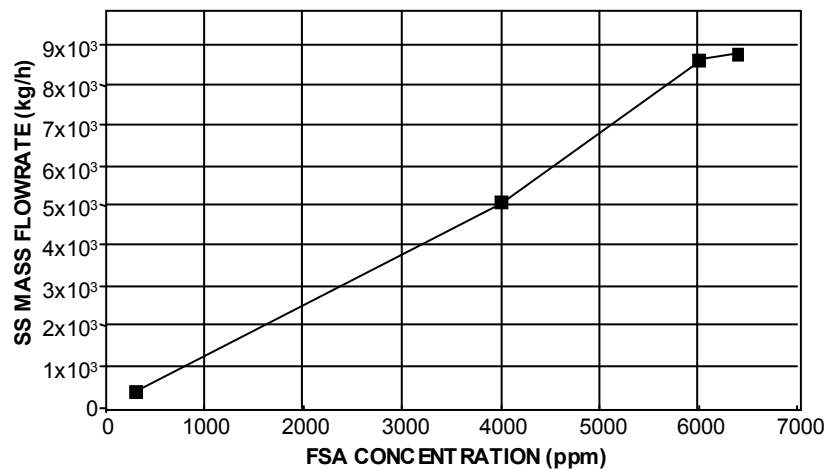


Figure 4.15: SS mass-flowrate as a function of the FSA constraint in the sea pipeline.

The flowrate of effluent discharged to the sea pipeline increased above the rate predicted by a linear relationship. The freshwater flowrate increased from 60.95 t/h to 67.26 t/h in order to produce a more dilute effluent. This flowrate was maintained until the concentration of FSA in the sea pipeline rose above 6 000 ppm. At this point the freshwater flowrate dropped to 62.3 t/h.

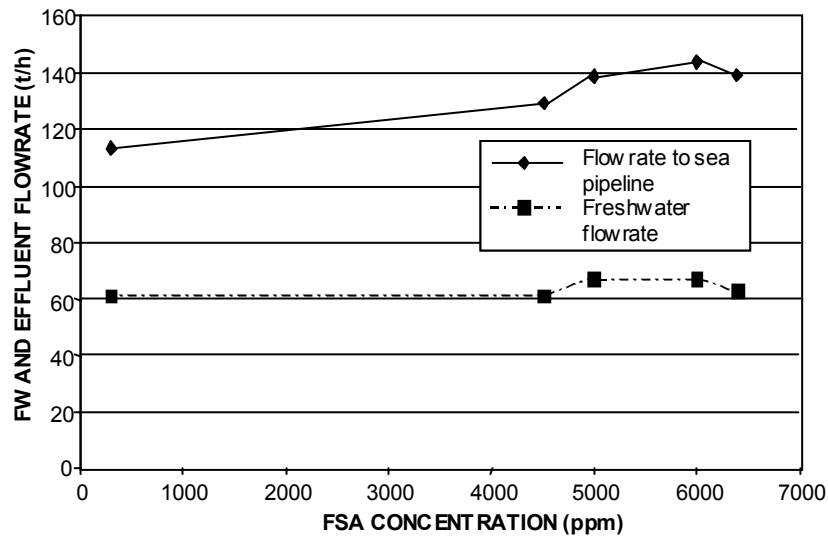


Figure 4.16 : Sensitivity of the design to FSA concentration in the sea pipeline (in terms of freshwater and effluent flowrate).

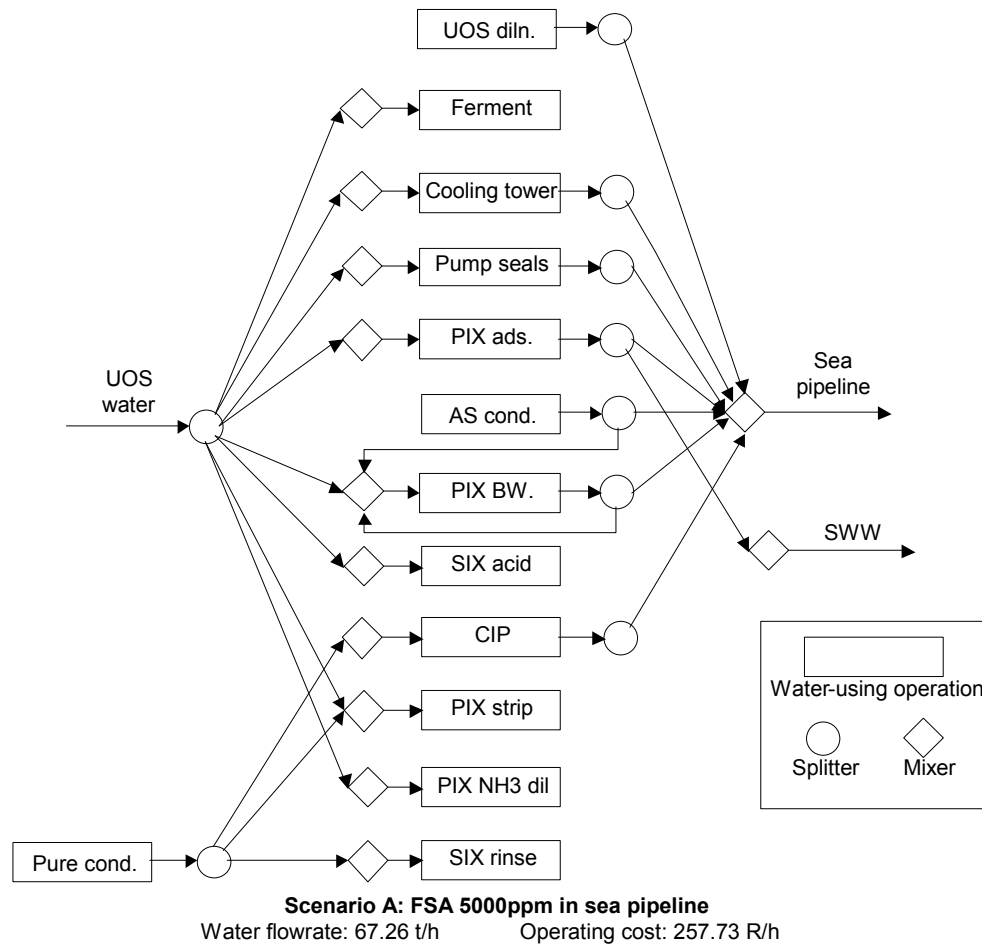


Figure 4.17: Configuration of the water-using system with the FSA concentration constraint in the sea pipeline relaxed to 5 000 ppm and SS unconstrained. (Scenario A).

The configuration of the water-using system with the FSA concentration constraint set to 5 000 ppm in the sea pipeline and SS unconstrained is shown in figure 4.17. 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 4.29 t/h to 0.46 t/h and backwash recycle from 3.48 t/h to 1.00 t/h resulted in an increase of 6.31 t/h in the freshwater feed to this operation.
- ii) PIX NH₃ dilution. Use of 0.16 t/h freshwater in the PIX NH₃ dilution operation in place of condensate.

4.7.2.3 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.

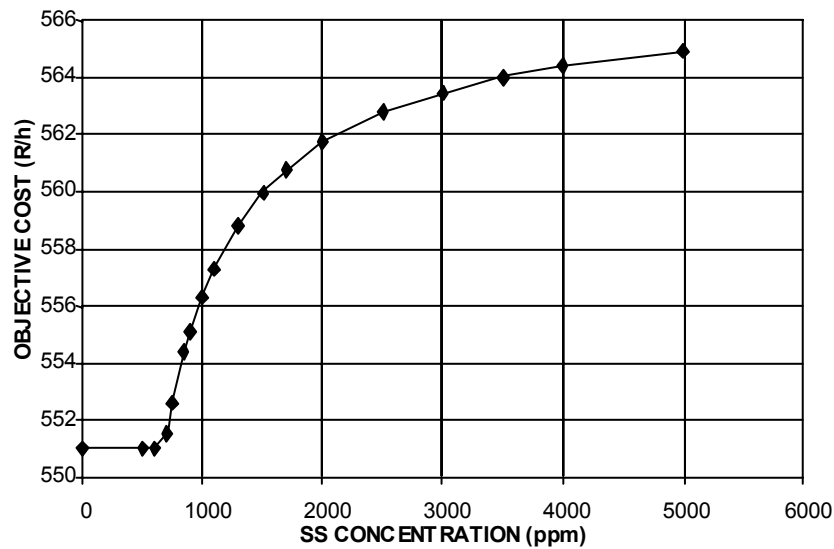


Figure 4.18 : Sensitivity of the objective cost to AS evaporator condensate SS concentration.

In figure 4.18, the objective cost is initially constant at 551.02 R/h as the AS evaporator condensate is completely reused in the PIX backwash process. At a concentration of approximately 700 ppm, the objective cost increases sharply at first with reduced AS condensate reuse, but begins to level-off as the SS concentration increases above 1500 ppm. The asymptotic limit of the objective cost with no AS reuse was identified as 567.02 R/h. This represents the worst-case operating scenario for the AS evaporator, which was presented in Scenario C.

The condensate reuse flowrate is plotted as a function of SS concentration in figure 4.19. At relatively low SS levels (below 2 000 ppm) 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.

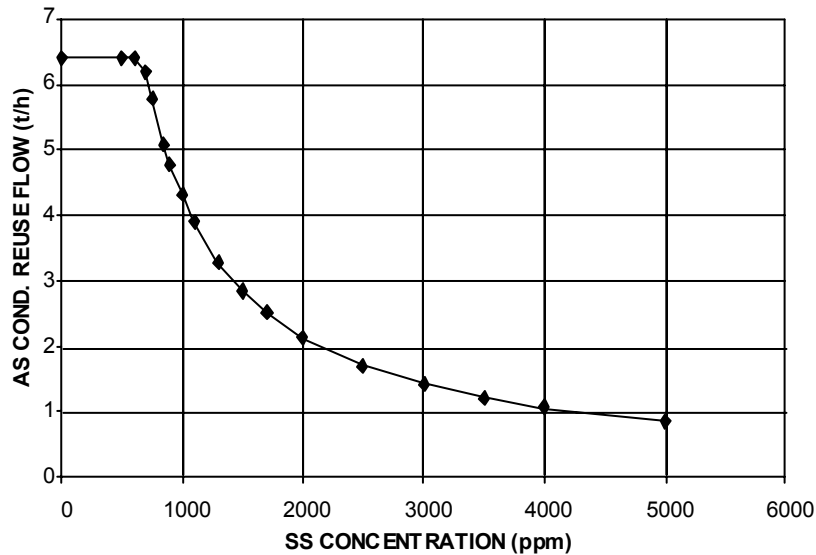


Figure 4.19: Sensitivity of reuse flowrate to AS evaporator condensate SS concentration.

4.8 Evaluation of the results

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.

4.8.1 Scenario A

This scenario examined the case where the AS evaporator condensate at a SS concentration of 1 000 ppm, in which case reuse (to the PIX backwash inlet) is barely allowed. When compared with the base-case operating conditions, the following savings were identified:

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

4.8.1.1 PIX recycle

The solution for Scenario A identified the configuration change of the recycle of PIX backwash effluent back to the inlet. The AS condensate reuse in the PIX backwash was reduced; 4.29 t/h was reused, as opposed to 6.40 t/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 1 000 ppm) as feed to the PIX backwash prevents the backwash recycle, due to the comparatively high SS concentration in the condensate source. Consequentially, 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 would require further investigation.

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.

4.8.2 Scenario B

This scenario 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 following savings were identified:

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

The cost reduction identified in this scenario, less the saving identified in Scenario A, reflects the upper limit for annualised 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 5.28 R/h, or R 45 619 per annum.

4.8.3 Scenario C

This scenario 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. In this case, the AS evaporator condensate is discharged directly to the sea pipeline. When compared with the base-case model, an increase in cost of 1.30 % was identified, although when compared to normal 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.

4.8.4 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 4.7.3). As illustrated in figure 4.20, at concentrations below 700 ppm, 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 2000 ppm 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:

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

where $p = 4284.00 \text{ t/(h}\cdot\text{ppm)} \pm 0.79\%$ 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

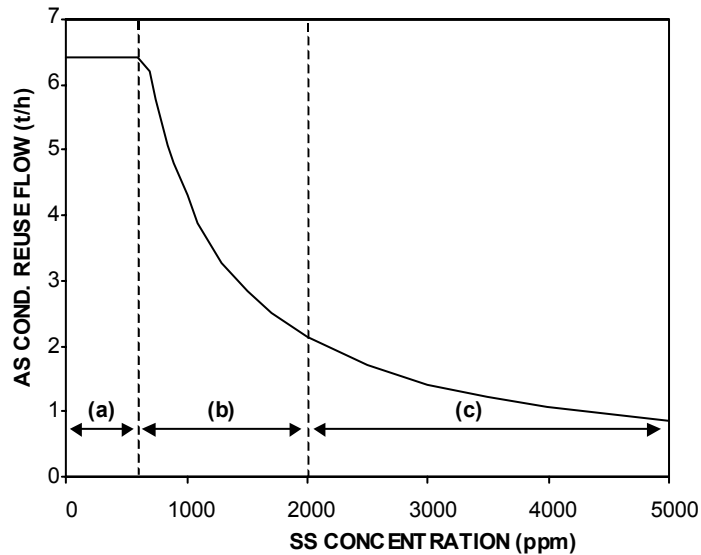


Figure 4.20 : AS evaporator condensate reuse flowrate as a function of outlet concentration of SS.

In the region $C_{out} < 700$ ppm (a), complete reuse of the condensate is allowed. In the region $700 \text{ ppm} = C_{out} < 2\,000$ ppm (b) the reuse flowrate is governed by the inverse relationship of equation 4.1. For outlet concentrations greater than 2 000 ppm reuse is probably prevented due to the 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. At the time 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 1 000 ppm.

4.8.5 Sea pipeline constraints

Relaxation of the constraints associated with the pipeline showed the greatest scope for cost reduction.

4.8.5.1 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 75 kg/h (which corresponds to a concentration of 666 ppm) over a range. At the point at which the FSA concentration constraint became limiting (at a SS mass-flowrate of 360 kg/h), the objective cost had decreased to 543 R/h. This corresponds to a financial saving of 2.9 % 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.

4.8.5.2 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 4 500 ppm 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.

4.8.5.3 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 157 R/h, which corresponds to a saving of 72 %. 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.

4.8.6 Overall saving

The structure of the optimised water-using network is almost invariant 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 3.48 t/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 4.21).

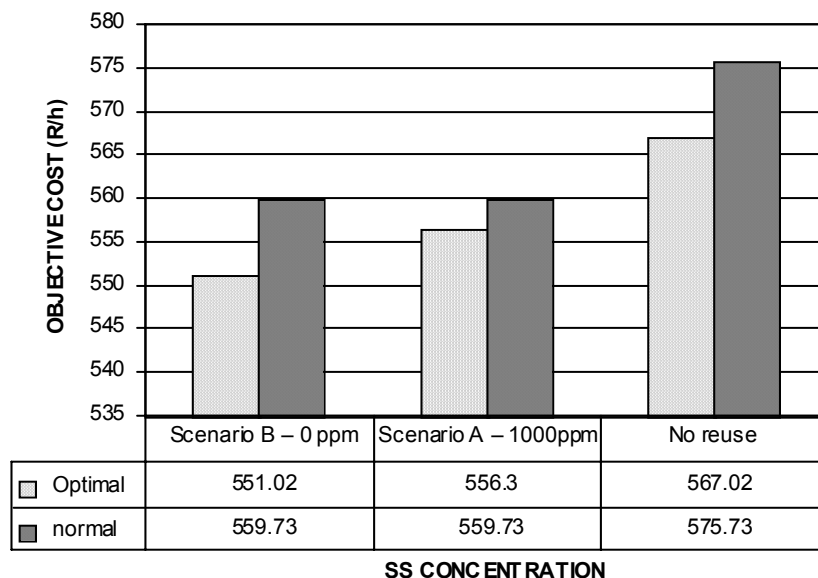


Figure 4.21 : Comparison of the optimal design cost with the current water-using network operating cost.

Figure 4.21 shows that the optimal water-using network hourly operating cost lies between R 551 with complete integration of the AS evaporator condensate, and R 567 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 %.

4.8.7 Barriers to saving

Two kinds of limiting constraints were identified, those due to the process technology, and those due to the environmental regulations.

4.8.7.1 Technical obstacles to process integration

The Scenario A objective function was shown (in figure 4.5, section 4.6.1.1) 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 4.11) that a larger saving could be realised 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 the critical constraint limiting economic saving, as well as limiting improvement of operating conditions through increased process integration.

4.8.7.2 Broth effluent discharge regulations

At the time of the investigation, the regulations 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 400 R/h an amount which is 71 % of the base-case water-using system operating cost, and between 98 % (Scenario B operating conditions) and 99 % (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 and Glatz (1996). 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.

4.8.8 Summary of results

The reductions to the cost of operating the water-using network and freshwater consumption identified in the investigation are summarised in table 4.12.

Table 4.12 : *Summary of economic and freshwater savings at AECI Bioproducts.*

Action	Cost saving		Freshwater saving	
	(R/h)	%	(t/h)	%
PIX backwash recycle.	3.41	0.61	1.37	2.2
Discharge of Broth effluent to sea pipeline.	399.52	71.38	0	0
AS condensate reuse (Scenario B).	5.26	0.94	2.11	3.39
Total	408.19	72.93	3.48	5.58

4.9 Discussion and conclusions

This case study had the following notable features:

- 1) It demonstrated the use of the Linnhoff-March WaterTarget software and the mathematical programming approach to water pinch analysis. It was limited to utility water streams and process effluent, considered multiple contaminants, an economic objective function, and used sensitivity analysis extensively.
- 2) Although it was not able to identify significant *water* savings, it did identify significant *cost* savings, which is in strong contrast to the classical pinch analysis methodology.
- 3) The nature of these cost savings raised some interesting issues. The pinch analysis demonstrated that savings were prevented by the external limit on the concentration of suspended solids (SS) constraint at the sea pipeline. Saving could be achieved by relaxing this constraint and allowing for discharge of broth effluent to the sea. At R16 /t, the hourly cost of disposing the broth effluent at the local wastewater treatment works amounted to R400 /h, approximately 72% of the total water-using network operating cost of R 556 /h. Thus, the DWAF effluent discharge permit concerning the broth effluent, with its SS constraint of 400 mg/L at the sea outfall, was established as the major barrier to further savings. Subsequently to the study, the factory applied to DWAF to allow the discharge of broth effluent to sea, and to increase the 400 mg/L SS limit. The reason for setting this limit had been purely to avoid an unsightly stain of the sea surface, and the scientific basis for the value of 400 mg/L was far from certain. However, DWAF would not consider environmental arguments for relaxing it until the factory had demonstrated that it had reached the limit of what could be achieved by improving its operation. The pinch analysis was accepted as evidence that this was indeed the case, so it was agreed to relax the limits, subject to monitoring the resulting condition of the sea. To date no adverse effects resulting from the discharge have been detected.
- 4) This outcome suggests a useful role for pinch analysis in the interaction between industries and regulatory authorities in establishing the parameters of water use permits. It offers systematic and transparent analysis of the industry's water needs which could provide the basis for trust between the parties. However, it does require a capacity in both parties to understand and question the basis of the analysis.

5 THE MONDI PAPER MILL AT MEREBANK, DURBAN

During the project three studies were started at paper mills, Mondi Merebank, Sappi Tugela and Sappi Ngodwana. All three were undertaken by process engineers at the respective companies, who enrolled part-time for MScEng degrees. Unfortunately only the Mondi Merebank study was complete at the time that this report was compiled. However, because the students involved met regularly to exchange experiences, the others had a significant influence on the success of this one. This chapter is based on the MScEng thesis of Gladys Naylor (née Crampton).

5.1 Process description

The Mondi Paper mill at Merebank in south Durban is an integrated pulp and paper mill, producing three types of pulp, supercalendered magazine paper, uncoated woodfree paper, newsprint, telephone directory and carbonless coated paper. The three types of pulp produced at Mondi Paper are:

- thermomechanical pulp
- groundwood pulp
- recycled fibre pulp

The groundwood and thermomechanical pulps are produced by mechanically separating the fibres from other wood constituents, by means of log grinding in the groundwood process and chip refining in the thermomechanical process.

The fibre sources used in the production of the pulp and paper are:

- logs and chips - pine
- recycled paper - newspapers and magazines
- chemical pulp - hardwood pulp produced from eucalyptus wood and softwood pulp produced from pine

There are five paper machines at Mondi Paper producing the following paper grades:

Paper Machine 1	Supercalendered magazine paper
Paper Machines 2 and 3	Uncoated woodfree paper
Paper Machines 4 and 5	Newsprint and telephone directory

Some of the uncoated woodfree paper produced at the mill is coated with microcapsules, on a separate coating machine, to produce carbonless coated paper.

The steam requirements of the mill are supplied by the power plant which comprises two coal fired boilers, two standby oil boilers and two standby gas boilers. The coal boilers supply the steam required to produce the pulp and dry the paper.

The paper produced is wound into various size reels to meet customers' requirements or cut into sheets and sold as flat sheets.

5.1.1 Pulp mill

The pulp mill consists of the wood yard as well as the three pulping plants, namely the thermo-mechanical pulping plant, the groundwood pulping plant and the recycled fibre pulping plant.

5.1.1.1 Wood yard

The wood used in the thermomechanical and groundwood pulping processes arrives at Mondi in the form of logs and chips. The logs are transported to the mill via rail trucks and road trucks. The production of pulp requires approximately 1 600 t of logs per day.

The logs are debarked in a dry drum debarker and then fed to the saw decks to be cut into smaller logs for the groundwood pulping process or fed to the chipper to be chipped for the thermo-mechanical pulping process.

5.1.1.2 Thermo-mechanical Pulping

Thermo-mechanical pulping produces pulp with high tearing resistance for newsprint and telephone directory paper. The process involves steaming wood chips under pressure for a short period of time prior to and during refining. The steaming, which happens in the digester, softens the chips and the result is a greater percentage of long fibres in the pulp produced and fewer shives. The heating and first stage refining are carried out under pressure, while the second stage refining is carried out at atmospheric pressure.

The refiner consists of two revolving discs driven in opposite directions by two electric motors. The chips are fed in between the discs at the centre of the discs and the centrifugal force forces the chips along the discs and over the edges. Consistency control of the stock is very important as it plays a large part in the retention time of the stock between the plates.

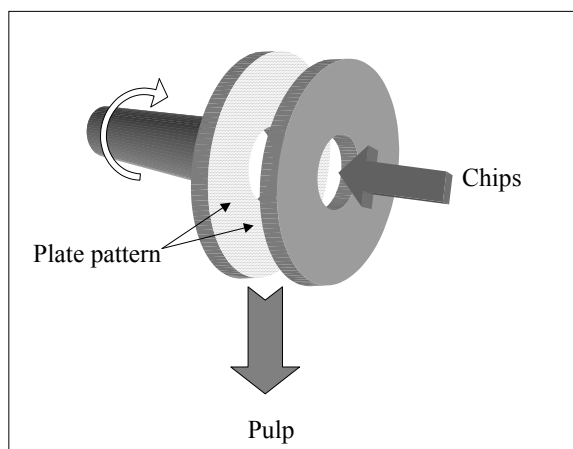


Figure 5.1: *Principle of refining*

After refining, the stock is screened and cleaned and finally thickened, before being fed to the paper machines. The purpose of screening and cleaning is to remove unseparated fibre bundles, shives, and other undesirable components (e.g. dirt particles) from the pulp stream. The objective of thickening is to remove water containing impurities dissolved during pulping and to raise the consistency of the stock before it is pumped to the paper machines.

5.1.1.3 Groundwood pulping

In the stone groundwood process, pulp is produced by pressing logs against an abrasive rotating stone surface. The logs are oriented parallel to the axis of the stone so that the grinding action removes intact fibres.

Temperature control by showering is an important aspect of the grinding operation since virtually all the grinding energy is dissipated as heat in the grinding zone. Too much cooling water will impede the softening action, while insufficient cooling water will allow the wood to become charred.

5.1.1.4 Recycled fibre pulping

The raw material for this process is newspapers and magazines. The recycled fibre process removes contaminants, including ink, from the waste paper and produces clean fibre for paper making.

Ink is separated from the fibres by chemical and mechanical action and removed from the stock by flotation. Other contaminants are removed by sorting, screening and cleaning. The process comprises of the following stages:

5.1.1.5 Waste paper repulping

Bales of waste paper are slushed in a high consistency batch pulper at about 14 %. Set amounts of water and chemicals are added at the start of the repulping cycle. A combination of chemical and mechanical action separates the fibres and loosens the ink particles from the fibres.

After repulping the stock is diluted to 4-5 % consistency and dumped through a coarse screen, where the largest contaminants are removed. Accepted stock is pumped to a tank where chemical reaction continues. Water for repulping is heated to 50 °C with direct steam injection. The chemicals added to the pulper are: caustic soda, sodium stearate, sodium silicate and hydrogen peroxide.

5.1.1.6 High density cleaning and screening

After the pulper the process becomes continuous. Contaminants with a high density are removed in the high density cleaners and other large contaminants are removed in the coarse screens. The consistency of the stock is controlled to approximately 3 % by the addition of cloudy filtrate.

5.1.1.7 Flotation

Once the larger contaminants have been removed from the stock, it is fed to the flotation cell. Here the ink is removed from the process using air bubbles and calcium ions. Calcium soaps form in the hard water conditions. These act as collectors for the ink particles by attaching to the ink particles and also attaching to the air bubbles. The air bubbles carry the ink to the surface and are removed by overflows. Stock in the flotation feed tank is diluted to 1.2 % by the addition of cloudy filtrate dilution water. The pH of the stock flowing to the flotation cell is controlled to a preset value, normally 8.5, by the addition of sulphuric acid. The pH is adjusted to this level to prevent precipitation of calcium salts in the flotation cells. Calcium chloride solution is added to give the required amount of water hardness.

5.1.1.8 Cleaning for removal of lightweight rejects

After the flotation cell, the next sections of the plant are designed to remove the smaller contaminants by centrifugal cleaning and fine screening. Stock is first pumped through rotary, horizontal hydrocyclones, which efficiently remove the light weight contaminants, those with specific gravity of less than one.

5.1.1.9 Cleaning for removal of heavy rejects

Fine sand, grit and heavy clay particles with specific gravity of greater than one are removed by a four stage, cascade cleaner plant.

5.1.1.10 Screening with pressure screens

Final cleaning of the stock is achieved by pressure screens. A three stage cascade arrangement is used. These screens have slotted baskets with a slot width of 0.25 mm and remove any fibre clumps which are still held together.

5.1.1.11 Thickening and washing

In this section of the plant the chemicals from the de-inking process are removed from the stock by thickening it to remove the alkaline, de-inking process water. Accepted stock from the fine screens is thickened to about 10 % consistency and then diluted to approximately 5 % consistency with cleaner water. The stock is then thickened to approximately 30 % in a wire pulp press to prevent water from being carried over from the pulp mill to the paper machines. The pH is adjusted to the level used on the paper machines. This is so that extra stickies which precipitate at low pH can be dispersed in the disperser. A displacement washing section of the press uses paper machine water to replace up to 30 % of the process water.

5.1.1.12 Dispersion

Other chemical contaminants and remaining ink particles are made less troublesome by dispersing them evenly throughout the stock. Stock from the wire pulp press is heated to soften *stickies* such as hot melt adhesives and other similar contaminants. The disperser also removes any ink particles still attached to the fibres and breaks them up into smaller particles so that they are less noticeable. The dispersing section consists of a heating screw and a disperser. The stock is pushed through the screw and heated by direct injection of steam. The temperature is normally controlled to about 90 °C to melt the stickies and adhesives. After the disperser the stock is diluted to 10 to 12 % consistency using water from the paper machines.

5.1.2 Paper mill

The paper mill consists of the stock preparation plant, the additives plant and five paper machines.

5.1.2.1 Additives plant

Additives is the term used to describe a wide range of chemicals and other substances used in the manufacture of paper. The additives plant is where these substances are mixed and stored before they are dosed to the paper machines.

5.1.2.2 Stock preparation plant

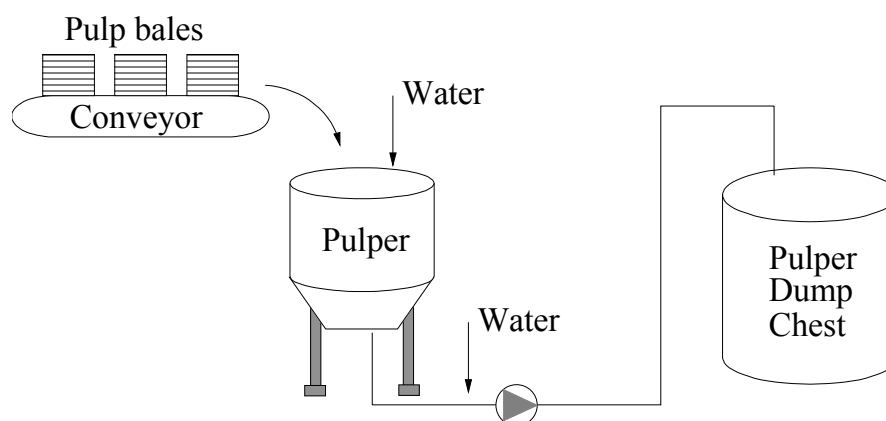


Figure 5.2 : *Slushing of baled pulp*

The chemical pulp purchased primarily for the production of uncoated woodfree grades, as well as for strength properties in the other paper grades, is delivered to Mondi Paper in bales of dry pulp. Water and dry pulp bales are fed into a pulper vat and a rotor disintegrates the bales to form the fibre slurry. The objectives of slushing are to disintegrate:

- the bales into a pumpable slurry by releasing fibre bonds created in the pulp dewatering and drying processes
- the fibre slurry so that there are no visible fibre flakes or bundles
- the fibre slurry so that fibres are separated, wetted, and flexible before entering the refining stage.

The stock preparation plant has nine vertical pulpers, with the rotor located at the bottom of the pulper vats. The pulp bales are fed onto conveyors, which feed the bales into the pulper vats. The operation of the pulpers is batch wise and at 5 to 6 % consistency. The fibre slurry is diluted to 4 to 5 % during discharging. Figure 5.2 shows the slushing sequence.

The pulper vat is filled with a given amount of water and a given amount of pulp. The bales are dropped into the pulper, which has been filled with water. Water temperature and pH influence the pulper operation. A higher water temperature reduces slushing time and energy requirement. A low pH means slower water penetration into the fibres and higher energy requirements in pulping.

5.1.3 Paper machines

The production conditions and parameters on the five paper machines are quite different according to the different paper grades produced. Process conditions have to be stable to ensure the required product quality and a high production efficiency. Variation in any of the following can cause problems on the paper machines:

- Flow rate
- Pressure
- Temperature
- Turbulence
- Consistency
- Furnish composition and inorganic solids content
- Specific surface of fibres, content of fines, freeness
- Charge content, cationic demand, pH
- Content and distribution of chemicals and additives
- Undesired substances and contaminants, including air

The properties of the different paper grades produced on the paper machines are determined by the properties of the stock components used. The stock is a blend of the different components in order to achieve the desired paper properties in the most economical way. Figure 5.3 is a schematic diagram of the operations taking place in a paper machine.

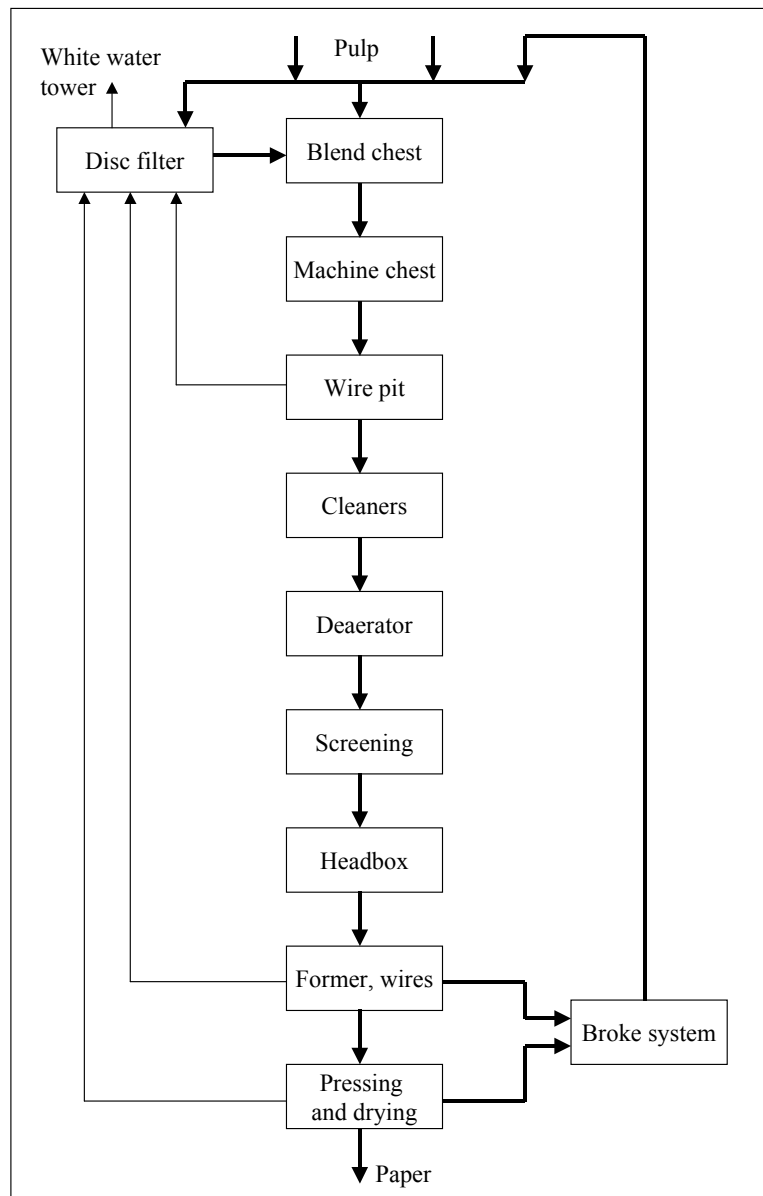


Figure 5.3 : Block diagram of a paper machine

5.2 Development of a of water pinch model for Mondi Paper

In order to perform a Water Pinch analysis on a site which is as complicated as the Merebank mill, the operation was divided into manageable sections (see Figure 5.4). A flow sheet model of the sections was then developed and a water and contaminant balance was developed, accurate to within 10 % of the metered amounts of the larger streams. Once a sufficiently accurate water and contaminant balance was achieved, the streams which were not variable, and therefore did not form part of the water pinch analysis (e.g. product streams), were not considered further. In order to perform a water pinch analysis a relationship between streams into and out of the unit operations which make up the sections was required. In this study the balance produced using the Water Tracker software was used to determine these relationships. Once the streams which did not form part of the water pinch analysis had been removed and the water pinch model of the plant had been developed, this model was tested by forcing the streams to represent the actual plant situation as closely as possible by introducing flow constraints into the model. The next step involved removing those constraints which appeared not to be absolutely required in terms of process

considerations, and allowing the model to re-route streams in order to achieve a minimum fresh water consumption.

5.2.1 Division of the mill into sections

The Merebank mill can be divided into three main sections based on the paper grades produced.

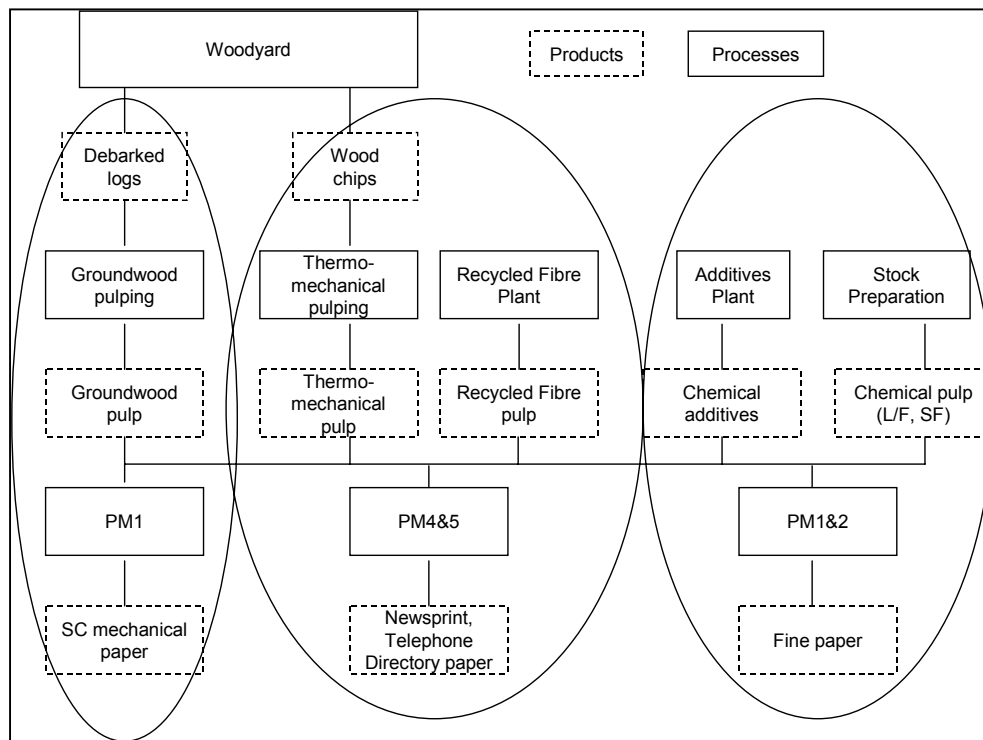


Figure 5.4 : Division of the mill into sections

The paper machine number one, producing supercalendered magazine paper, along with the groundwood pulp mill forms the first section. The second section of the mill consists of paper machines numbers two and three which produce fine paper, the additives plant and the stock preparation plant. The third section of the mill consists of the two newsprint paper machines, machines numbers four and five, as well as the woodyard, the thermo-mechanical pulp mill and the recycled fibre plant. The utility plants which service the production plant include are the power plant and the waterworks. These utility sections were not included in this study.

5.2.2 Choice of key contaminant

In order to perform a pinch analysis at the Merebank mill it was necessary to select key contaminants which would limit the recycling and reuse of water streams. The key contaminants which could be considered are as follows:

- i) Dissolved solids
- ii) Suspended solids
- iii) COD

In order to perform this water pinch analysis with the information available, the assumption was made that in the Merebank mill fibre is the main contaminant in the streams which form part of the analysis. Data on dissolved solids, COD and temperature of all the streams was not readily available. Suspended solids, i.e.. fibre, was therefore selected as the key

contaminant that would prevent recycling and reuse of streams in this analysis and dissolved solids and COD were not included as contaminants.

There were areas in the process where other contaminants were the limiting factors, for example: if suspended solids (fibre) is the only contaminant limiting the use of water in all areas in the plant, clean cold water could be used in the showers in the head box of the paper machine. In reality this is not the case, since the water used in the head box needs to be hot. In this study, flow constraints were used to prevent streams from being used in certain areas where suspended solids was not the only factor limiting the use of water as in the example above.

5.2.3 Data gathering

The Merebank mill was built in 1969 and consisted of only one paper machine. The mill has grown over the years to its current size, now comprising of five paper machines and three pulp mills. Water consumption has become increasingly important over the years, however when the mill was constructed, water consumption was not a primary concern and as a result there are very few water meters throughout the mill. Similarly, contaminant concentration data was limited and in order to evaluate contaminant concentration in the various streams throughout the mill a large number of measurements would have been required. The approach taken in this study was to use the data readily available to determine a water balance accurate to within 10 % of the measured major flow rates.

The fresh water flows which were measured on a routine basis were:

- i) Total flow to the Newsprint Circuit
- ii) Total flow to the Recycled Fibre Plant
- iii) Total flow to the Thermo-mechanical Pulp Mill
- iv) Cold fresh water to Paper Machine No. 4

These streams make up the larger fresh water flows in the Newsprint circuit and a year's data was averaged for use in the water balances.

The amount of fibre in the various streams which formed part of the water and fibre balances was based on average operating conditions. The data used in the balances was based on measured consistencies averaged over a period of a year as well as target consistencies in certain streams. An average dryness of the paper produced was used to calculate the evaporation from the paper machine.

The flow rate of shower water on the paper machines was based on the specification from the nozzle suppliers and the number of showers in use during the study.

The reject rates from cleaners and screens was based on design reject rates.

Chemical additives flow rates were based on one year's consumption data.

Where data was missing information provided by experienced engineers in the plant was used, with appropriate uncertainty factors in the Water Tracker software. For example, in the thermo-mechanical pulp mill no data was available for the amount of plug wiper water or sealing water used, and the estimates of experienced plant engineers was used as approximations in the model. The Water Tracker software allows the user to enter a *trust category* which represents the reliability of the estimate. Where estimated data was used, the trust category was larger, for example a trust category of $\pm 25\%$ was used for data that was estimated by plant engineers, and data which came from flow measurements taken over the period of one year had a much lower trust category of $\pm 2\%$.

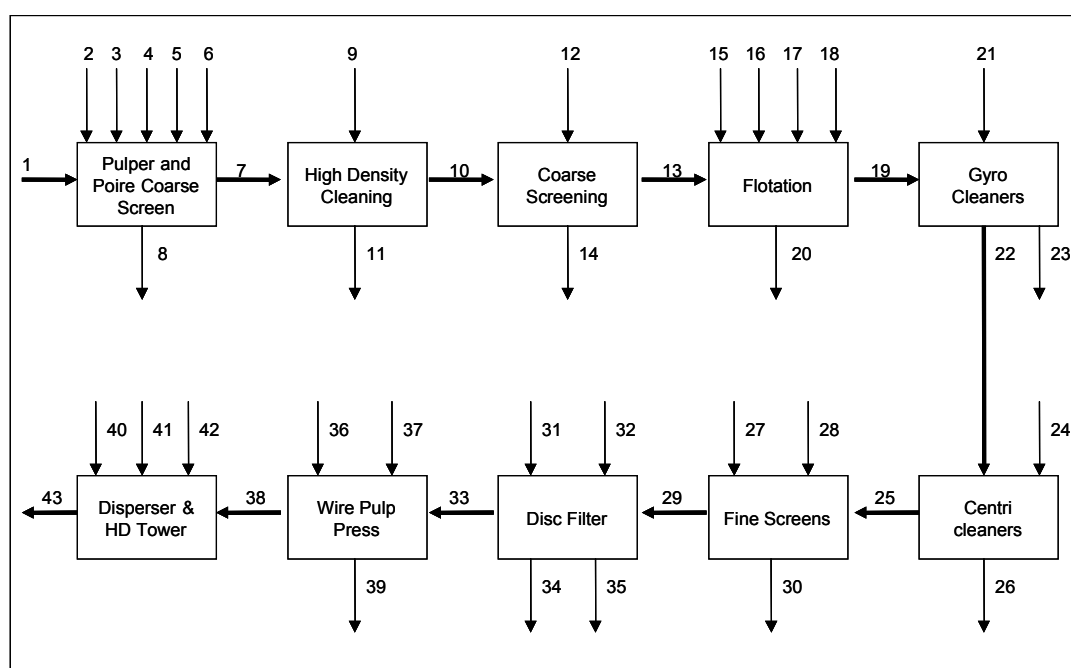
Another type of data which was used in the mass balances was plant data - for example, pressure readings from pumps were recorded and the corresponding flow rates, from the pump curves, were used to estimate the flows for certain streams. This type of information was used where there were no flow measurements available, however the trust category for these streams was also set to $\pm 25\%$.

5.2.4 Water balances

Water balances for each of the sections were performed using the Linnhoff March *Water Tracker* software, which performs the water and contaminant balance simultaneously. In what follows, only the model of the recycled fibre plant will be presented in detail, as the models for the other sections followed very much the same pattern.

5.2.4.1 Recycled fibre plant

The Recycled Fibre Plant was divided into functional units and each unit / block analysed. Figure 5.5 shows the breakdown of this section of the plant.



1 Waste Paper	2 Sodium Silicate	3 H ₂ O ₂	4 Caustic Soda
5 Cloudy Filtrate	6 Steam	7 Pulp	8 Rejects
9 Cloudy Filtrate	10 Pulp	11 Rejects	12 Cloudy Filtrate
13 Pulp	14 Rejects	15 Cloudy Filtrate	16 Soap
17 CaCl ₂	18 H ₂ SO ₄	19 Pulp	20 Ink Sludge
21 Clear Filtrate	22 Pulp	23 Rejects	24 Clear Filtrate
25 Pulp	26 Rejects	27 Clear Filtrate	28 Cloudy Filtrate
29 Pulp	30 Rejects	31 Clear Filtrate	32 Tempered Water
33 Pulp	34 Cloudy Filtrate	35 Clear Filtrate	36 White Water
37 H ₂ SO ₄	38 Pulp	39 Cloudy Filtrate	40 White Water
41 Steam	42 Hydrosulphite	43 Pulp	

Figure 5.5 : Recycled fibre plant functional units. The bold arrows represent process streams which were excluded from the pinch analysis.

The function of each unit shown in Figure 5.5 is described in Table 5.1.

Table 5.1: *Function of each process unit in the Recycled Fibre Plant*

Pulper and Poire Screen	Waste paper repulping and coarse screening to remove largest contaminants
High density cleaning	Removal of high density contaminants from pulp
Coarse screening	Removal of remaining large contaminants
Flotation	Removal of ink
Gyro cleaners	Removal of smaller, lightweight contaminants (specific gravity <1)
Centri cleaners	Removal of fine sand, grit and heavy clay particles with specific gravity > 1
Fine screens	Removal of fibre clumps
Disc filter	Thickening pulp
Wire pulp press	Pulp is thickened from 5 % to 30 % consistency to remove alkaline de-inking process water
Disperser and HD tower	Pulp is heated to soften stickies, hot melt adhesives and other similar contaminants. These contaminants are then dispersed evenly throughout the stock. Any ink particles still attached to the fibres are broken up into smaller particles so that they are less noticeable.

A mass and water balance was performed over these functional units using the Water Tracker software. The water flow rates were based on design conditions for the recycled fibre plant as well as the total flow rate of fresh water to this plant, which is metered. The fibre content of the streams was based on design conditions and on-line consistency measurements in the plant.

5.2.4.2 Thermo-mechanical plant and paper machine sections

The water and contaminant balances for these sections followed the same pattern as for the recycled fibre plant, and are not presented here.

5.3 Water pinch models of the individual sections of the plant

The individual sections of the plant, as described in sections 5.2, were analysed separately to determine the minimum fresh water consumption in each of these sections of the plant. This section describes the methodology used to perform the analysis on the individual plant sections, before considering the analysis of the combined system.

5.3.1 Recycled fibre plant (RFP)

Following the standard methodology of water pinch analysis, the plant was divided into component functional units, as shown in figure 5.6. These are shown without any interconnections, since the purpose of the analysis is to find the best set of connections.

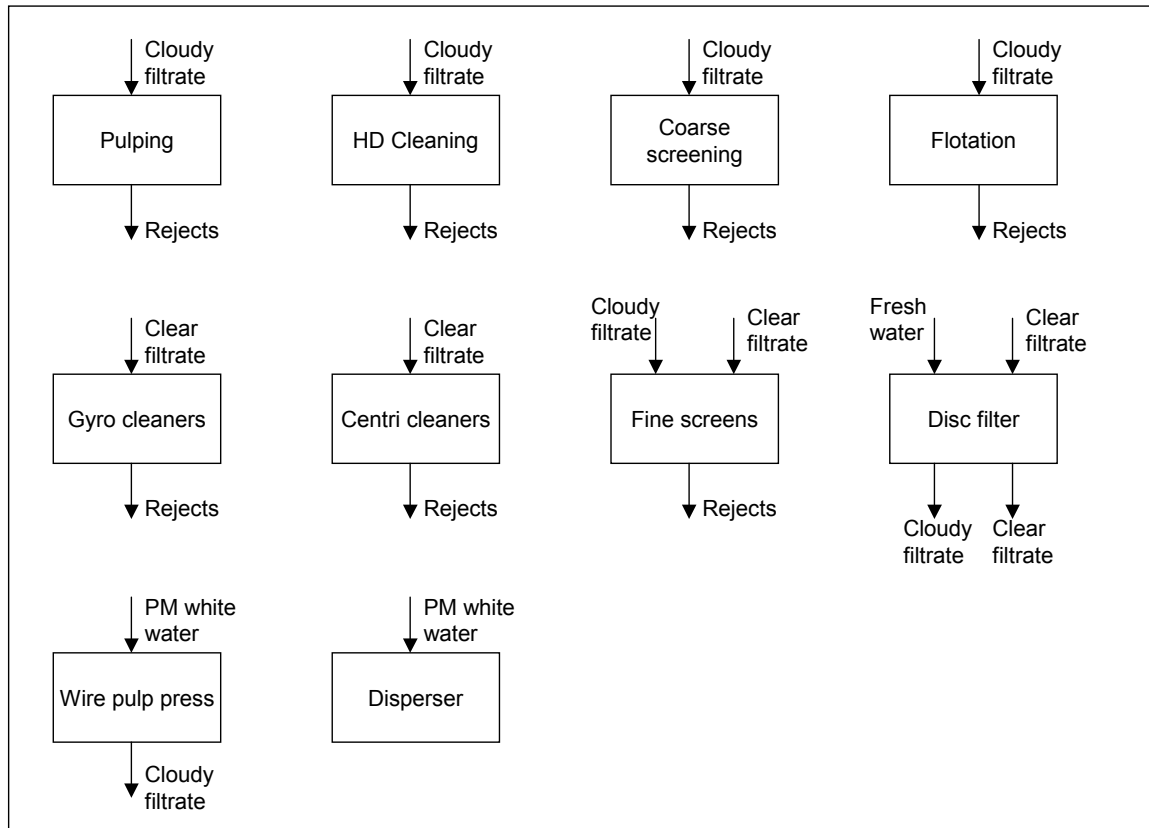


Figure 5.6 : Representation of the Recycled Fibre Plant for the water pinch analysis

The **process sources** in the recycled fibre plant were:

- Cloudy filtrate
- Clear filtrate
- Paper machine white water

The **process unit operations** were:

- Pulping
- High density cleaning
- Coarse screening
- Flotation
- Gyro-cleaning
- Centri-cleaning
- Fine screening
- Filtering
- Pressing

The **utility source and sink** were fresh water and effluent.

The flowrates and fibre content of each source are given in Table 5.2 and 5.3.

Table 5.2 : Utility source flowrates and fibre content in the Recycled Fibre Plant

Source	Flowrate [t/h]	Fibre Content [ppm]
Cloudy filtrate	Variable	1 000
Clear filtrate	Variable	600
Paper machine white water	Variable	100
Fresh water	Variable	0

Table 5.3 : Flow and fibre constraints for process sinks in the Recycled Fibre Plant

Operation	Stream	Flow [t/h]	Max Fibre [ppm]
RFP Pulping	Cloudy filtrate	288	1 800
RFP High Density Cleaning	Cloudy filtrate	87	1 800
RFP Coarse Screening	Cloudy filtrate	3.7	1 800
RFP Flotation	Cloudy filtrate	251.7	1 800
RFP Gyrocleaners	Clear filtrate	96.7	1 000
RFP Centricleaners	Clear filtrate	224.4	1 000
RFP Fine screens	Clear filtrate	50.7	1 000
	Cloudy filtrate	0	1 800
RFP Disc filter	Clear filtrate	103.7	1 000
RFP Wire pulp press	Paper machine white water	43.2	600
RFP Disperser	Paper machine white water	125.6	600

* RFP: Recycled fibre plant

The model represented by the above figures was analysed using the Linnhoff-March WaterPinch software. This water pinch analysis of the recycled fibre plant in isolation was unable to identify a significant reduction in fresh water consumption. The minimum fresh water consumption determined by the water pinch analysis was 45 t/h while in reality the process consumes 44 t/h, based on a production of 150 t/day. The routing of the streams in the water pinch solution differed in some detail from the actual plant configuration, however this could be expected since multiple optimal solutions often occur for simple objective functions. These are referred to in optimisation theory as *degenerate solutions*. It is possible for the flows to be split in different ways between various units and still give rise to the same optimum objective function value. The difference in the amount of fresh water consumption determined by the water pinch model and the actual plant consumption was negligible, and could be attributed to the accuracy of the data available for producing this model.

5.3.2 Thermo-mechanical pulp mill (TMP)

The thermo-mechanical pulp mill was broken down into functional units for the pinch analysis as shown in Figure 5.7.

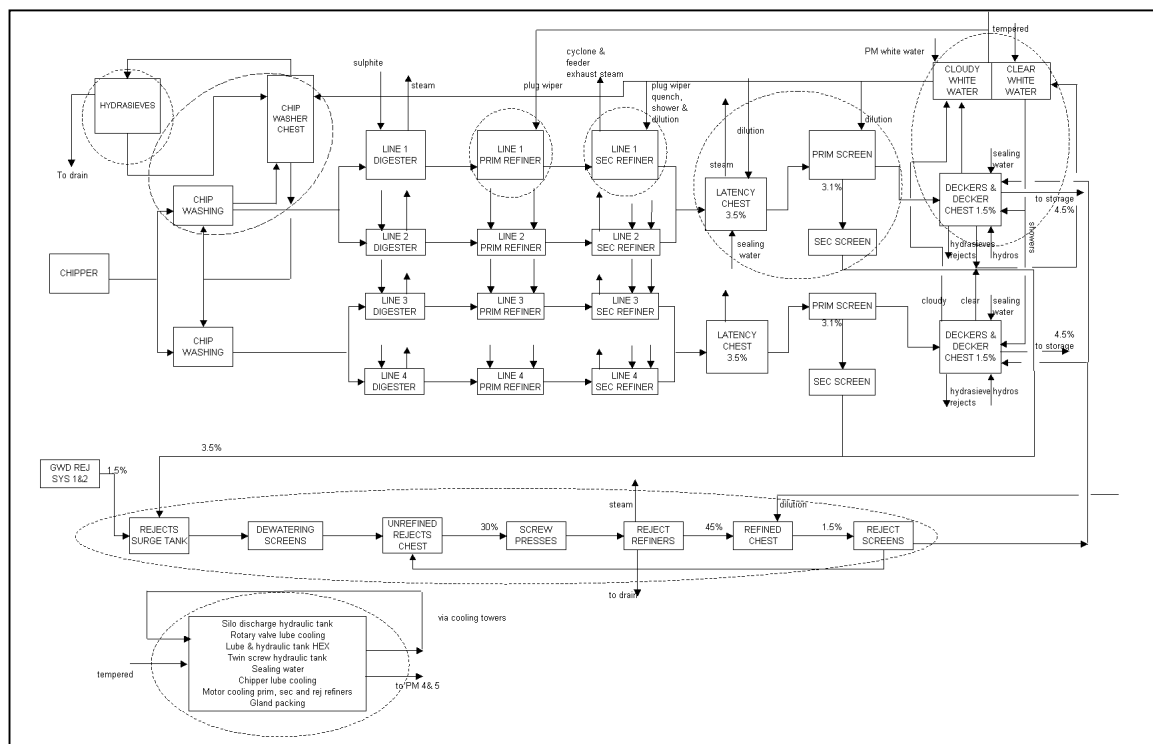


Figure 5.7 : Grouping of equipment in the TMP mill. The dotted lines indicate the plant equipment that were grouped together for the water pinch analysis.

The resulting set of functional units representing the thermo-mechanical pulp mill are shown in figure 5.8.

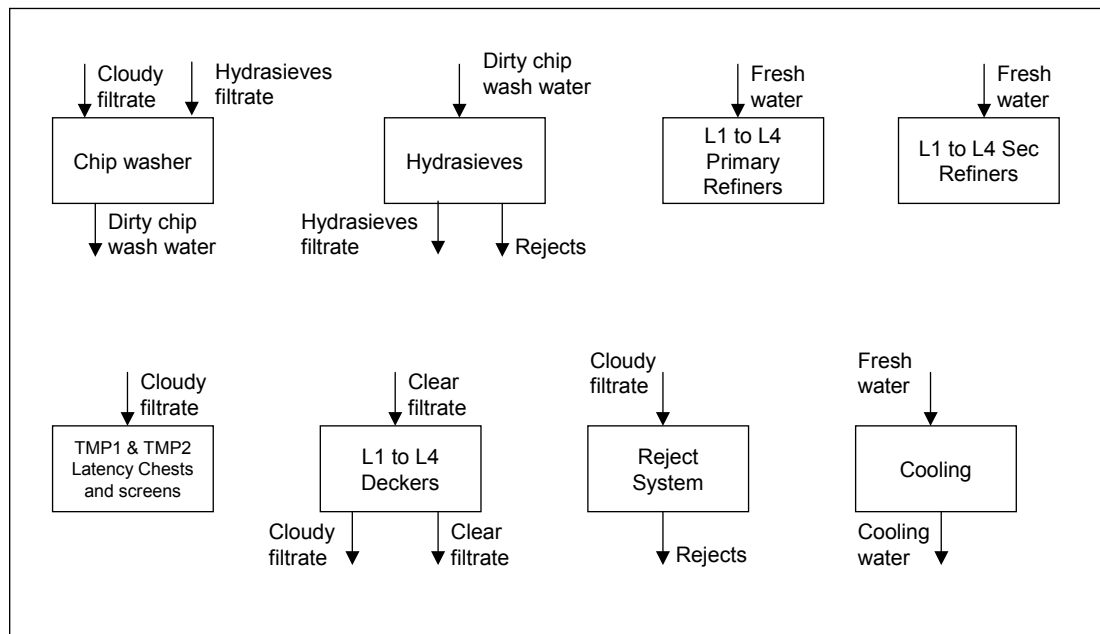


Figure 5.8 : Representation of the TMP mill for the water pinch analysis

The flowrates and fibre content of each source are given in Table 5.4 and 5.5.

Table 5.4 : Process source flowrates and fibre content in the TMP mill.

Source	Flowrate [t/h]	Fibre Content [ppm]
Cloudy filtrate	Variable	1000
Clear filtrate	Variable	600
Paper machine white water	Variable	100
Fresh water	Variable	0

Table 5.5 : Flow and fibre constraints for process sinks in the TMP plant.

Operation	Stream	Flow[t/h]	Max Fibre
Chip washer	Cloudy filtrate	22.27	3000
	Hydrasieves filtrate	376.15	3000
Hydrasieves	Dirty chip wash water	395.7	4000
Line 1 Primary Refiner	Fresh water	0.01	0
Line 2 Primary Refiner	Fresh water	0.01	0
Line 3 Primary Refiner	Fresh water	0.01	0
Line 4 Primary Refiner	Fresh water	0.01	0
Line 1 Secondary Refiner	Fresh water	126.35	0
Line 2 Secondary Refiner	Fresh water	126.35	0
Line 3 Secondary Refiner	Fresh water	126.35	0
Line 4 Secondary Refiner	Fresh water	126.35	0
TMP1 Latency and screens	Cloudy filtrate	398.65	1000
TMP1 Latency and screens	Cloudy filtrate	398.65	1000
Line 1 Decker	Clear filtrate	120	1000
Line 2 Decker	Clear filtrate	120	1000
Line 3 Decker	Clear filtrate	120	1000
Line 4 Decker	Clear filtrate	120	1000
Reject system	Cloudy filtrate	277.2	2000
Cooling	Fresh water	20	0

The **process sources** in the thermo-mechanical pulp mill were:

- Cloudy filtrate •Clear filtrate •Paper machine white water

The **utility source and sink** were fresh water and effluent.

The **process unit operations** were:

- Chip washer •Hydrasieves •Cooling
- Reject System •Line 1 to Line 4 Deckers •Sealing water

The **process sinks** were:

- Line 1 to Line 4 Primary refiners
- Line 1 to Line 4 Secondary refiners
- TMP1 and TMP2 Latency and screens

The model represented by the above figures was analysed using the Linnhoff-March WaterPinch software. This water pinch analysis of the thermo-mechanical pulp plant in isolation was unable to identify a significant reduction in fresh water consumption. The minimum fresh water consumption determined by the water pinch analysis was 182 t/h while in reality the process consumes 185 t/h, based on a production of 150 t/day of paper per line. As was the case in the water pinch analysis of the recycled fibre plant, the routing of the streams within the water pinch solution differed from the actual plant configuration. This solution is once again an example of a degenerate solution, as was the case in the recycled fibre plant, where difference routings of the streams gave rise to the same objective function value. The difference between the actual consumption of fresh water in the thermo-mechanical pulp mill and the modelled minimum fresh water consumption is simply a reflection of the accuracy of the data used to develop the model and does not represent an real opportunity for fresh water saving.

5.3.3 Paper machines

In view of the results for the other two sections, an individual water pinch analysis of the paper machines was not carried out when it was realised how limited opportunity there was for re-routing streams, since the paper machines were already effectively countercurrent systems. However, the units making up the paper machines (figure 5.9) were subsequently incorporated in the combined pinch analysis of the entire newsprint circuit (see section 5.4)

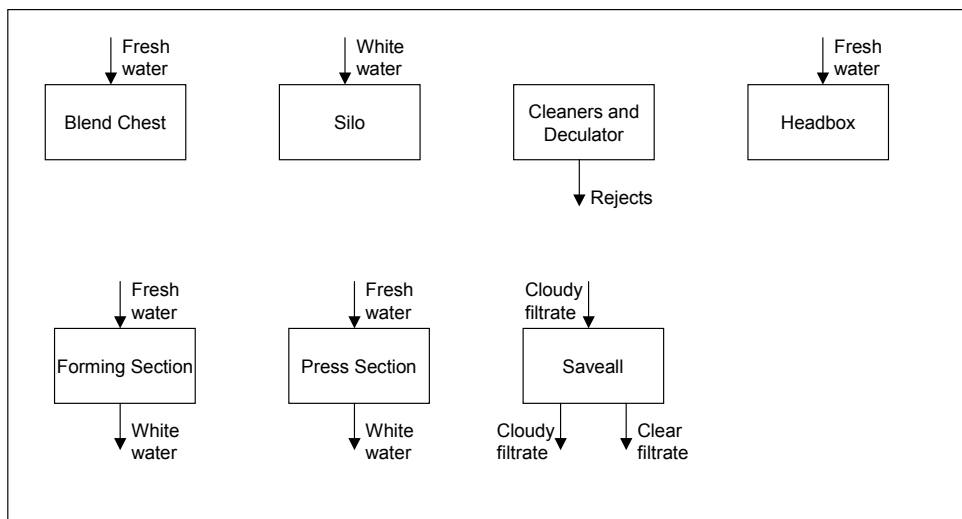


Figure 5.9 : Representation of a paper machine for the water pinch analysis

5.4 Water pinch analysis of the newsprint circuit

The Newsprint circuit, as described earlier, is the combination of the individual sections considered earlier: recycled fibre plant, the thermo-mechanical pulp mill and the paper machines.

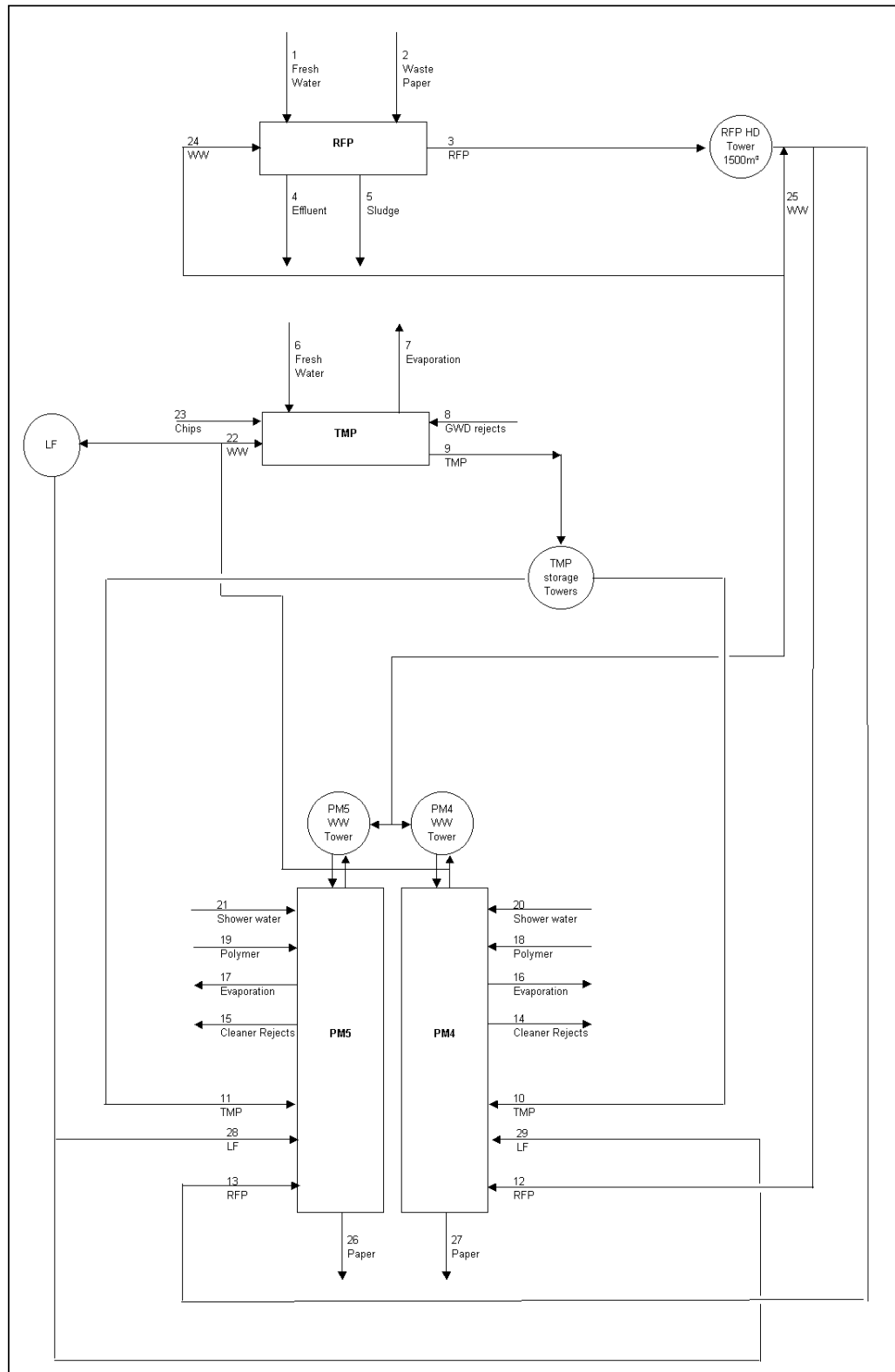


Figure 5.10 : Newsprint circuit

Stream key for figure 5.10 :

1	Fresh water	2	Waste Paper	3	RF Pulp	4	Effluent
5	Sludge	6	Fresh water	7	Evaporation	8	Groundwood rejects
9	TM pulp	10	TM pulp	11	TM pulp	12	RF Pulp
13	RF Pulp	14	Cleaner rejects	15	Cleaner rejects	16	Evaporation
17	Evaporation	18	Polymer	19	Polymer	20	Shower water
21	Shower water	22	White water	23	Chips	24	White water
25	White water	26	Paper	27	Paper	28	Long Fibre
29	Long Fibre						

* RF : recycled fibre TM : thermo-mechanical

Figure 5.10 above represents the newsprint circuit without showing the details of the individual plants. In order to identify opportunities for re-routing streams and minimising fresh water consumption it is necessary to include the details of each of the sections of the newsprint circuit and the model used for the water pinch analysis is shown in Figure 5.11 with the dotted line indicating the various sections that were combined to form the newsprint circuit.

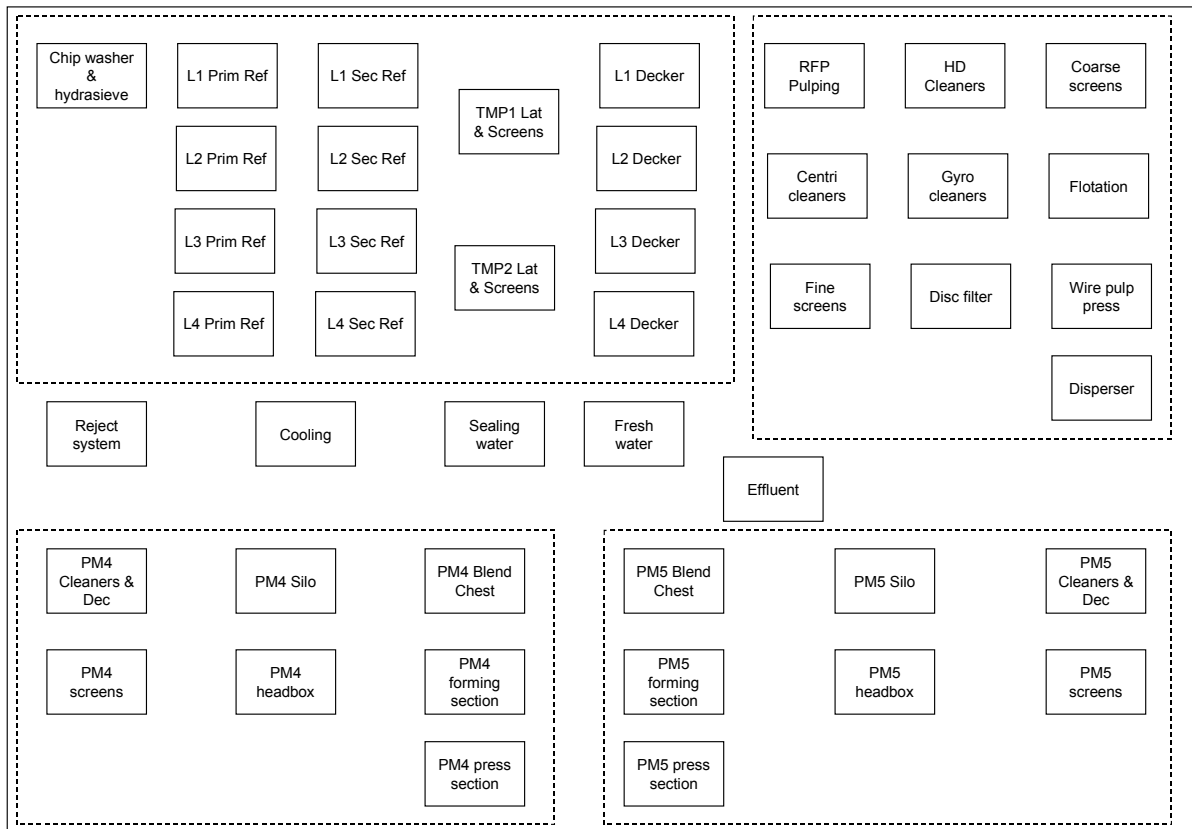


Figure 5.11 : The newsprint circuit as represented in the water pinch analysis

The water pinch model elements for the newsprint circuit were:

Utility source and sink: Fresh water and effluent

Process unit operations:

- | | | |
|----------------------|-----------------------------|------------------------|
| • Chip washer | • Hydrasieves | • Reject system |
| • Cooling | • Line 2 Decker | • Line 3 Decker |
| • Line 1 Decker | • Line 4 Decker | • RFP Pulping |
| • Sealing water | • RFP High density cleaning | • RFP Coarse screening |
| • RFP Flotation | • RFP Gyro-cleaning | • RFP Centri-cleaning |
| • RFP Fine screening | • RFP Filtering | • RFP Pressing |
| • PM4 blend chest | • PM4 Forming section | • PM4 Press section |
| • PM4 Saveall | • PM5 Forming section | • PM5 blend chest |
| • PM5 Press section | • PM5 Saveall | |

Process sources :

- | | |
|------------------------------|---------------|
| • PM4 Cleaners and deculator | • PM4 Screens |
| • PM5 Cleaners and deculator | • PM4 Screens |

Process sinks :

- | | |
|--------------------------------------|------------------------------------|
| • RFP Disperser | • TMP Lines 1 - 4 Primary refiners |
| • TMP Lines 1 - 2 Secondary refiners | • TMP1 & TMP2 Latency and screens |
| • PM4 Silo | • PM4 Head box |
| • PM5 Silo | • PM5 Head box |

The relationships between the inlet and the outlet streams in the unit operations were determined using the results from the water balance performed using the Water Tracker software and a mass pickup equation with the constant A (see equation 2.1, section 2.3.3.2) determined by the relationship between the inlet and outlet stream in the water balance.

Table 5.6 contains the flow and concentration constraints that were applied to the process sinks.

Table 5.6 : Constraints for process sinks

Operation	Stream	Flow [t/h]	Max Fibre [ppm]
RFP Pulping	Cloudy filtrate	288	1 800
RFP High Density Cleaning	Cloudy filtrate	87	1 800
RFP Coarse Screening	Cloudy filtrate	3.7	1 800
RFP Flotation	Cloudy filtrate	251.7	1 800
RFP Gyrocleaners	Clear filtrate	96.7	1 000
RFP Centricleaners	Clear filtrate	224.4	1 000
RFP Fine screens	Clear filtrate	50.7	1 000
RFP Disc filter	Cloudy filtrate	0	1 800
	Clear filtrate	103.7	1 000
RFP Wire pulp press	Paper machine white water	43.2	600
RFP Disperser	Paper machine white water	125.6	600
Chip washer	Cloudy filtrate	22.3	3 000
	Hydrasieves filtrate	376.2	3 000
Hydrasieves	Dirty chip wash water	395.7	4 000
L1 Primary Refiner	Fresh water	0.01	0
L2 Primary Refiner	Fresh water	0.01	0
L3 Primary Refiner	Fresh water	0.01	0
L4 Primary Refiner	Fresh water	0.01	0
L1 Secondary Refiner	Fresh water	126.4	0
L2 Secondary Refiner	Fresh water	126.4	0
L3 Secondary Refiner	Fresh water	126.4	0
L4 Secondary Refiner	Fresh water	126.4	0
TMP1 Latency and screens	Cloudy filtrate	398.7	1 000
TMP1 Latency and screens	Cloudy filtrate	398.7	1 000
L1 Decker	Clear filtrate	120	1 000
L2 Decker	Clear filtrate	120	1 000
L3 Decker	Clear filtrate	120	1 000
L4 Decker	Clear filtrate	120	1 000
Reject system	Cloudy filtrate	277.2	2 000
Cooling	Fresh water	20	0
Sealing	Fresh water	19	50
PM4 Blend Chest	Fresh water	4.5	0
PM4 Silo	Cloudy white water	2 181	3 600
PM4 Head box	Fresh water	20	0
PM4 Forming section	Fresh water	21	0
	Clear white water	122	300
PM4 Press section	Fresh water	88	0
PM4 Saveall	Cloudy white water	1428	700
PM5 Blend Chest	Fresh water	4.5	0
PM5 Silo	Cloudy white water	2 179	3 600
PM5 Head box	Fresh water	20	0
PM5 Forming section	Fresh water	21	0
	Clear white water	166	300
PM5 Press section	Fresh water	88	0
PM5 Saveall	Cloudy white water	1 428	700

The newsprint circuit, which is a combination of the recycled fibre plant, the thermo-mechanical pulp mill and the two newsprint paper machines provided greater opportunity for optimising the amount of fresh water consumed by re-routing existing water streams between the individual sections of the circuit.

The analysis was carried out in three stages. In the first step (**A**), the model was forced to correspond to the then current operating state of the plant by introducing flow constraints which fixed the flow rates of all streams to the operating values. For this scenario, the total fresh water consumption for the plant was 636.3 t/h and the total effluent generated 954.4 t/h. This initial step served three purposes:

- i) Comparing the model output to available plant data, in terms of flow rates and fibre contents of streams, provided a check on the validity of the model's representation of the plant.
- ii) The objective function calculated by the model, representing the operating cost associated with the water system, served as a reference for comparing the results obtained subsequently.
- iii) The optimiser calculates *sensitivities* of the objective function to all imposed constraints. Looking at the values of the sensitivities for the flow constraints which were imposed to force the model to match the plant configuration, it was possible to identify where relaxing particular constraints would have the greatest benefit.

The second step (**B**) involved removing all the flow constraints that were specifically imposed to match the actual plant configuration (constraints that reflected process requirements were retained). This optimised result from this step was taken to represent the best water utilisation that could be achieved with the given process technology. However, this solution was considered impractical due to the large number of small-flowrate new connections that it required. A total of 32 new connections were used in the solution, and the overall fresh water consumption and effluent generation were reduced by 51.54 t/h to 584.5 t/h and 902.9 t/h respectively. These values were taken to represent the best water usage that could possibly be achieved - effectively the equivalents of the water use *targets* in the classical pinch analysis methodology.

The final step (**C**) involved removing the constraints one at a time (instead of all together as in step B) from those connections which were identified as having the greatest cost sensitivity in step A. After only 3 new connections, the fresh water consumption and effluent generation were reduced to same values as obtained in step B. These figures amount to 8.1 % reduction in fresh water consumption and 5.4 % effluent generation.

The identical overall performance of the scenario B and scenario C solutions provides another illustration of the *degeneracy* phenomenon.

To present the various solutions in detail would be ineffective due to the number of streams involved. Since the pinch analysis was unable to identify significant savings *within* the three individual sections of the plant, it follows that the most significant changes must involve flows *between* the sections. These can be seen by comparing figures 5.11 (step A) and 5.12 (step C), which show only the flows which go between the three sections of the factory. The bold lines in Figure 5.12 represent the new connections identified by the pinch analysis.

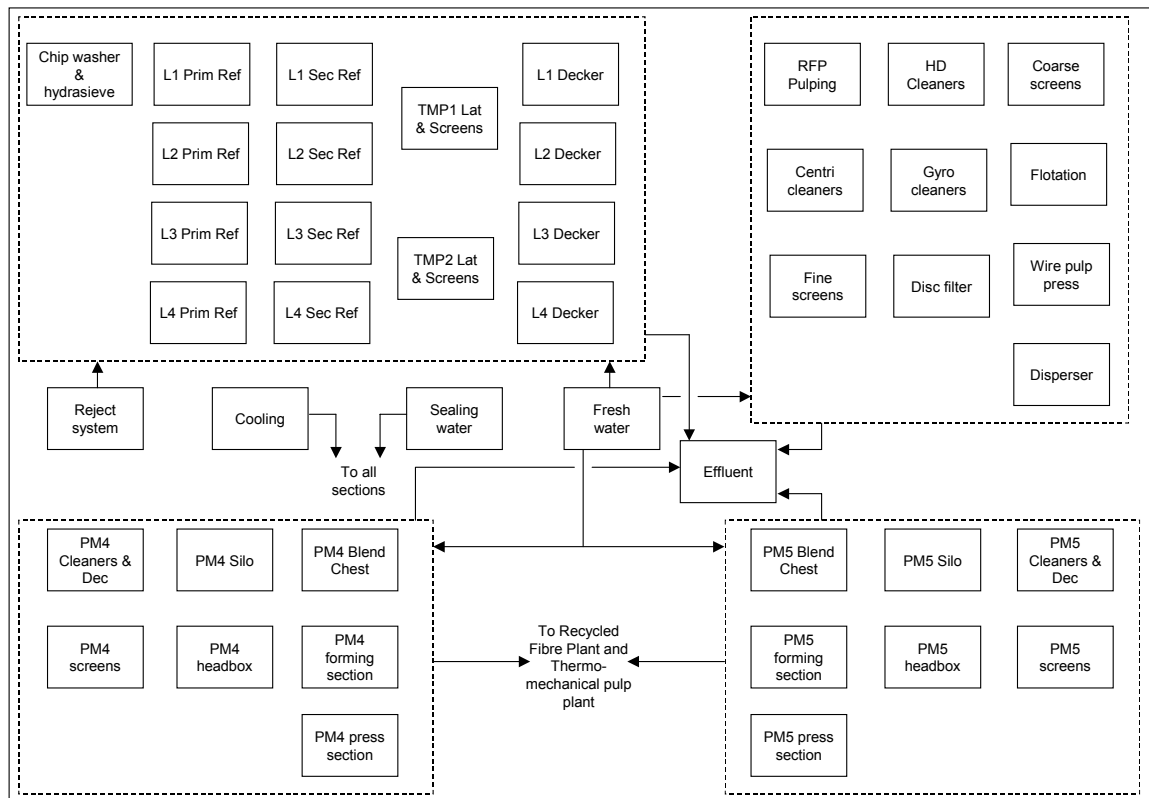


Figure 5.12 : Flow of water streams between sections of the newsprint circuit in the current plant configuration (corresponding to step A of the analysis).

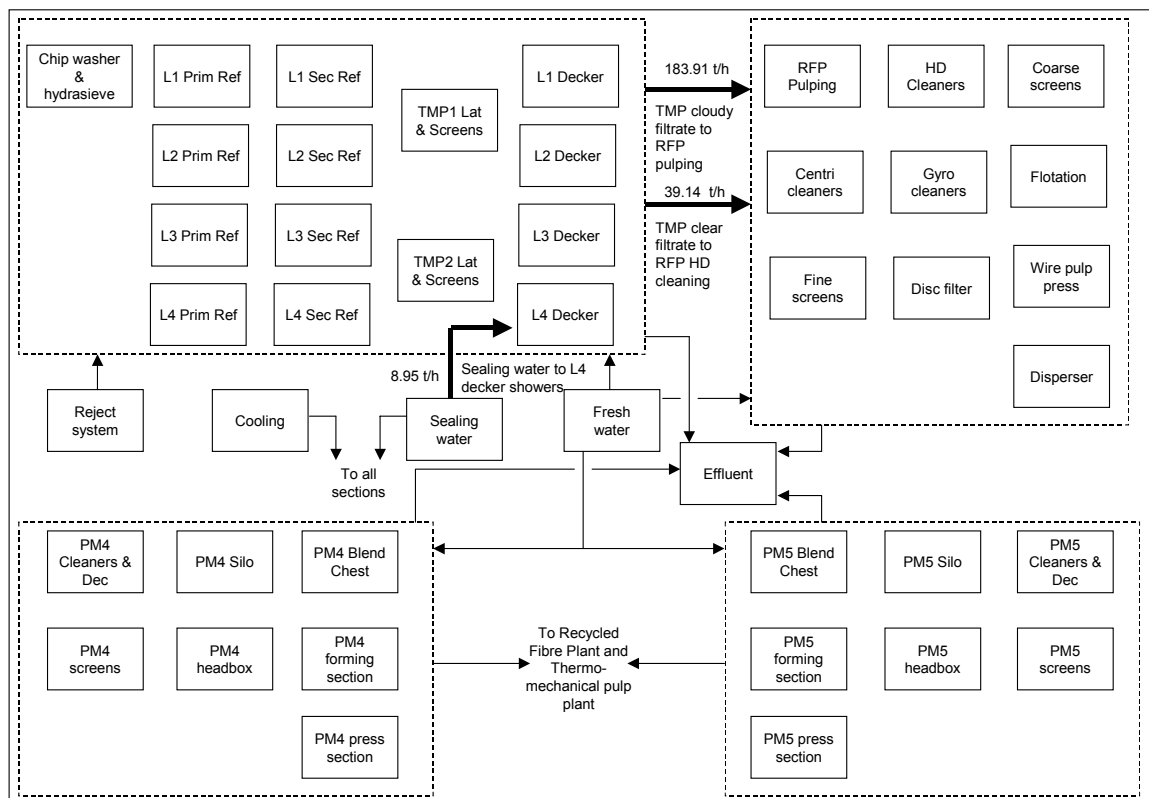


Figure 5.13 : Flow of water streams between sections of the newsprint circuit in the optimised model (corresponding to step C of the analysis)

5.5 Discussion and conclusions

From this investigation of the application of water pinch analysis in an integrated pulp and paper mill, the following can be concluded:

- i) Scope for optimisation and water savings within individual sections of the mill was insignificant. There were a number of reasons for this namely:
 - only utility water was considered in this analysis;
 - There has been a considerable amount of effort already put into reducing water consumption at the mill over a number of years;
 - water is already recycled and reused within the process.
- ii) By application of single contaminant analysis to a larger section of the mill it was possible to reduce the fresh water requirement by 51.54 t/h (8.1 %) and effluent generated by the same amount (5.4 %).
- iii) These reductions translated into a saving of R1 548 593 /annum. The savings was calculated by the objective function which included fresh water costs and effluent costs, but did not include engineering costs or piping costs. In addition, the objective function did not take geographical costs into account, the distance between the sections in the plant was not included in the analysis.
- iv) There are operability constraints which could prevent these savings from being achieved, since they involve the transfer of water from two batch processes which are not always in operation at the same time. The thermo-mechanical pulp plant is operated at full capacity during periods when the electricity charges are the lowest, which is during the night. The recycled fibre plant is operated according the paper machines' demand for recycled fibre. As a result there are times when the thermo-mechanical plant is in operation and the recycled fibre plant is not in operation or vice versa. The transfer of water between these two sections of the plant is therefore not ideal.
- v) Thirty two new connections were generated in the optimised model, however, only however the same savings could be achieved with just three. These three streams were identified using a novel approach to implementing water pinch analysis which involved the evaluation of sensitivity coefficients of the flow constraints in combination with the magnitude of the streams involved. The top three new connections identified in this manner corresponded to the three streams which were responsible for the fresh water savings in the optimised model generated by the water pinch analysis.

This study did not consider the use of treatment options to reduce the fibre content in the existing streams and thereby reduce the fresh water consumption further. Removal of fibre from streams will allow further reuse and recycling within the process and thus a further reduction in the amount of fresh water required.

During the course of the study, the water supply situation for the mill was changed substantially with the commissioning of the Durban Water Recycling Plant. This treats recovered domestic and industrial wastewater to a standard which makes it suitable for industrial use. Mondi is the scheme's main customer, and is supplied recycled water in terms of a "take or pay" agreement. The mill uses the recycled water for all the process requirements and in terms of the agreement with the Recycling Plant the mill pays for a minimum amount of water per day, whether this amount of water is used or not. Currently the mill consumption of water is slightly below the "take or pay" minimum specification, so the commercial incentive to implement water saving measures has disappeared.

From a theoretical point of view, the method of first introducing and then selectively relaxing flow constraints to find an optimal solution which involves the minimum installation of new piping is a novelty, and constitutes a small but possibly significant contribution to the theory and practice of water pinch analysis. To put it into perspective, in the past water pinch analysis has largely focussed on concentration constraints, and has developed various elegant techniques for handling them. This is particular true of the graphical pinch analysis techniques, and it is notable that, in the current water pinch analysis literature, the ‘pinch’ itself refers to a concentration limit. This emphasis on concentration limits has been carried over into the versions of pinch analysis which are based on the use of general purpose optimisation algorithms, such as the version of the Linnhoff-March WaterPinch software used for this study. Although facilities for applying flow constraints were provided, the facilities for interpreting their effects on the system had not been developed, in contrast with the facilities for interpreting concentration constraints.

At the level of the optimisation algorithm, all constraints are treated in exactly the same way, and exactly the same kind of information is available for flow constraints as for concentration constraints, however the user interface selected only the concentration limit sensitivities to present to the user. (Fortunately it was possible to extract the missing flow constraint sensitivities from the temporary files used by the GAMS solver to communicate the optimised solution to the WaterPinch software user interface.)

In the Linnhoff-March framework, these concentration sensitivities take the place of the pinch concentration in the simple graphical approach. The results of this study point to the usefulness of the flow rate sensitivities, and suggest a further extension of the pinch concept to include the **entire** set of constraints which prevent further optimisation of the system (the set of *active* constraints at the constrained optimum point).

6 THE SASOL POLYMERS CHLOR-ALKALI COMPLEX AT UMBOGINTWINI

The application of Pinch Analysis to water and wastewater management at the Sasol Polymers chlor-alkali complex was first addressed as part of WRC Project K5/851 (Brouckaert and Buckley (2003). As part of that project, a Water Pinch Analysis study at the chlor-alkali complex was conducted by Gardner, starting in 1997 (Gardner, 2000). Motivated by the results from this study and with a number of process changes that had been made to the chlor-alkali complex, the follow-up study reported here was undertaken by Paolo Gianadda and began in 1999. This chapter is based on his PhD thesis.

The Sasol Polymers chlor-alkali complex, formerly operated by Polifin Limited and previously by AECI Chlor-Alkali and Plastics Limited, was located within the Umbogintwini Industrial Site some 25 km south of Durban, South Africa. During its period of operation, which extended from 1955 to 2001, the complex produced chlorine and caustic soda, together with a range of other derived products. It was also in this period that the complex underwent a number of changes as processes were upgraded and decommissioned. As it stood at the time of its closure, the complex produced caustic soda, chlorine, hydrogen, hydrochloric acid and sodium hypochlorite. Unless otherwise indicated, references to the plant describe its configuration as it stood at the point of closure.

6.1 Description of the complex

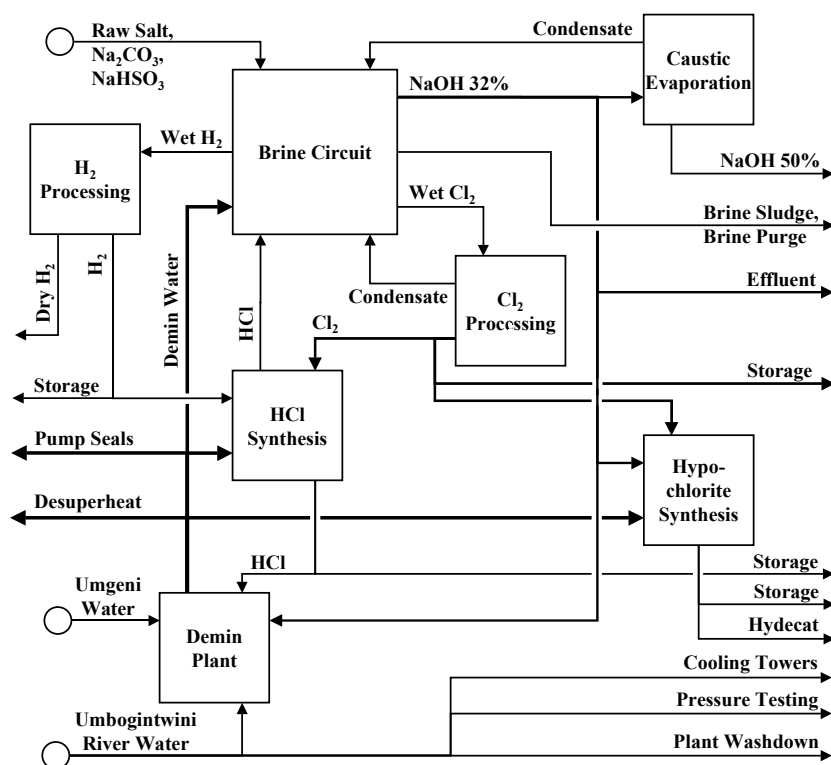


Figure 6.1 : Schematic diagram of the Sasol Polymers chlor-alkali complex

Figure 6.1 presents a schematic diagram of the various plants which made up the Sasol Polymers chlor-alkali plant at Umbogintwini. Central to the activities of the complex was the brine circuit which converts raw salt to caustic soda, chlorine and hydrogen. Part of the chlorine and hydrogen generated from the circuit was used for the production of hydrochloric acid in the hydrochloric acid synthesis plant. Chlorine was further used, along with caustic soda, in the manufacture of sodium hypochlorite in the sodium hypochlorite synthesis plant. Two other plants located within the complex were the demineralisation plant, which produced a high quality water for use within the complex, and the Hydecat destruction plant which destroyed surplus or below-specification sodium hypochlorite along with other chlorine-containing effluents.

6.1.1 The Brine circuit

Figure 6.2 presents a simplified process flow diagram of the brine circuit. The electrolyser was the core process of the circuit and the operation in which sodium chloride was converted to chlorine gas and caustic soda, with hydrogen gas being generated simultaneously. The electrolyser was preceded by a series of raw material purification operations (precipitation, clarification, filtration and ion-exchange) which condition the brine solution to a standard acceptable to the electrolyser. The electrolyser was followed by various product processing operations (chlorine processing, hydrogen processing and caustic evaporation) and brine recycle conditioning operations (physical and chemical dechlorination and resaturation).

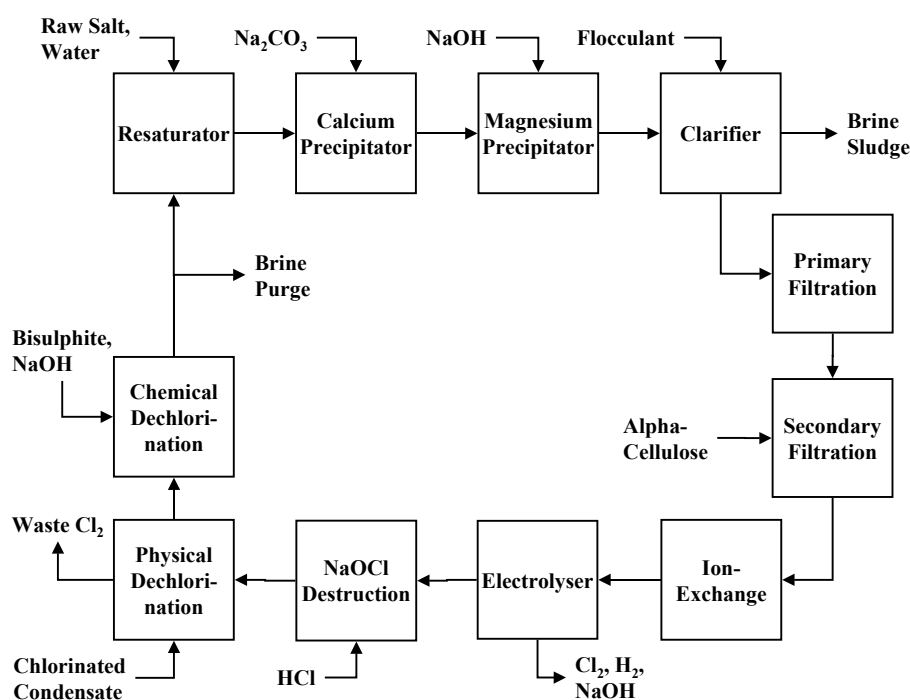


Figure 6.2 : Schematic diagram of the brine circuit.

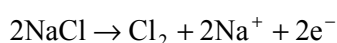
6.1.1.1 Raw material purification

Raw salt was dissolved in a solution made up of recycled brine and demineralised water in the resaturator. The salt contained predominantly sodium chloride but also some trace impurities, amongst which were calcium and magnesium cations. Brine from the resaturator (~25% m/m NaCl) passed through the calcium precipitator, where dilute sodium carbonate (~16% m/m Na₂CO₃) was added to precipitate the calcium as calcium carbonate, and the magnesium precipitator, where dilute caustic soda (18% m/m NaOH) was added to precipitate the magnesium as magnesium hydroxide. A flocculant was added ahead of the clarifier where the precipitated material was removed from the brine stream as brine sludge.

The clarified brine passed through the anthracite filters (primary filtration stage) where residual insoluble matter and precipitate (not removed by the clarifier) and a small quantity of the remaining calcium and magnesium were removed. This filter was back washed periodically with polished brine and the backwash stream returned to the precipitation stage. The filtered brine passed through the brine polishing filters (secondary filtration stage) where small residual quantities of calcium and magnesium were removed. The polished brine was heated before it entered the ion-exchanger where the calcium and magnesium concentrations were reduced to levels acceptable to the electrolyser. The ion-exchanger consisted of two cation-exchange resin beds arranged in series. Regeneration of each cation-exchange resin bed occurred every 72 h.

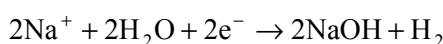
6.1.1.2 The electrolyser

The electrolyser consisted of three banks of membrane cells arranged in parallel. The conversion of sodium chloride to chlorine proceeds at the anode as follows:



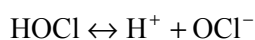
and the anolyte (brine solution) decreased in strength as the reaction proceeded. The chlorine evolved at the anode was sent to chlorine processing.

The anode was separated from the cathode by a selectively permeable membrane which allowed the migration of sodium cations from the anode to the cathode. At the cathode, the following reaction occurred:

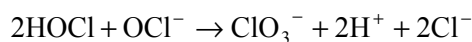


and the catholyte (caustic soda solution) increased in strength as the reaction proceeded. The caustic soda produced at the cathode (~32% m/m NaOH) was either sent to caustic evaporation, used within the plant, or diluted and recycled to the membrane cells. The hydrogen evolved at the cathode was sent to the hydrogen processing operations.

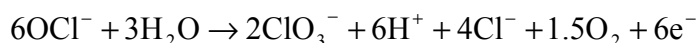
Alongside the reaction which produces chlorine, chlorates and hypochlorites were generated by side-reactions. Hypochlorites were generated within the electrolyser by:



Chlorates were generated via:



and to a lesser extent, electrochemically at the anode:

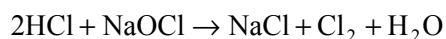


The level of chlorate in the circuit was controlled by a purge stream while the level of hypochlorite was controlled by the dechlorination operations.

6.1.1.3 Raw material conditioning

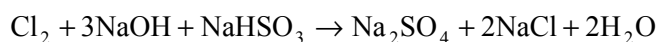
The depleted brine solution (~20% m/m NaCl) leaving the electrolyser was saturated with dissolved chlorine and chlorine-releasing species (hypochlorites), and was mixed with chlorine-containing condensate from the chlorine processing operations. The cation-exchange resin is extremely sensitive to oxidising species and all chlorine and chlorine-releasing species must be eliminated before the brine is recycled to the ion-exchanger.

Dechlorination was carried out in two stages. In the primary stage, concentrated hydrochloric acid (31% m/m HCl) was dosed to the brine such that chlorine was liberated from the chlorine-releasing species:



Following acid dosing, the brine was passed through three dechlorinators in which the dissolved chlorine was displaced by an air stream blown through the dechlorinators (physical dechlorination). The displaced chlorine gas was routed to the sodium hypochlorite synthesis plant. The pH of the brine leaving the primary dechlorination stage was corrected through the addition of caustic soda (18% m/m NaOH).

A residual quantity of dissolved chlorine remained in the brine stream following physical dechlorination. This was removed by chemical (secondary) dechlorination. Chemical dechlorination involved the addition of excess sodium bisulphite (10% m/m NaHSO₃) to the brine. The chlorine was destroyed via the following reaction:



The build-up of sulphate in the circuit was controlled via the brine purge. The depleted brine was cooled and returned to the resaturator.

6.1.1.4 Cation-exchange regeneration

The cation-exchange regeneration sequence comprised seven stages: Brine Displacement, Backwash, Acid Regeneration, Acid Rinse, Caustic Regeneration, Caustic Rinse and Brine Replacement. During the Brine Displacement stage, brine was displaced from the cation-exchange resin bed using demineralised water. The Backwash stage saw the resin bed being flushed with demineralised water in the opposite direction to the brine flow. A weak hydrochloric acid solution (7% m/m HCl) was used for the Acid Regeneration stage. During this stage, the cation-exchange resin was converted from the divalent cation form to the hydrogen form.

The hydrochloric acid hold-up from the Acid Regeneration stage was displaced from the resin bed using demineralised water (Acid Displacement stage). A weak caustic soda solution (4% m/m NaOH) was used in the Caustic Regeneration stage to convert the cation-exchange resin back to the sodium form.

The caustic soda hold-up from the Caustic Regeneration stage is displaced from the resin bed using demineralised water (Caustic Displacement). The regeneration sequence is completed by the replacement of brine in the resin bed (Brine Replacement). Effluent from the cation-exchange regeneration sequence is sent to an acid pit where partial neutralisation of the hydrochloric acid effluent by the caustic soda effluent occurs, prior to the effluent being discharged to the effluent treatment facility.

6.1.1.5 Chlorine processing

The chlorine gas stream emerging from the electrolyser was saturated with water at an elevated temperature (~87 °C). The majority of this water condensed out of the chlorine gas

stream in the chlorine cooler; the residual water was removed by concentrated sulphuric acid drying. The condensate from the chlorine cooler, which contained a quantity of dissolved chlorine, was blended with the depleted brine stream prior to the primary dechlorination stage while the dry chlorine was either used within the complex or sent to storage.

6.1.1.6 Hydrogen processing

The hydrogen gas stream left the electrolyser at an elevated temperature (~89 °C) and in a saturated state. Most of the water was removed via condensation, as the hydrogen stream was cooled in the hydrogen cooler. Hydrogen gas leaving the cooler was either used internally within the complex, bottled for sale or cooled further in the hydrogen chiller for export to the hydrogen peroxide plant located on the Umbogintwini Industrial Site.

6.1.1.7 Caustic evaporation

Caustic soda left the electrolyser at a strength of approximately 32 % m/m NaOH. The concentration was increased to saleable strength (50 % m/m NaOH) in the dual-effect caustic evaporation plant. Steam condensate and process condensate from the evaporators were recycled to the brine resaturator.

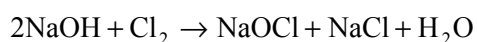
6.1.2 The hydrochloric acid synthesis plant

The hydrochloric acid synthesis plant comprised two hydrochloric acid synthesis units, each consisting of a burner and an absorption section. Chlorine gas was burnt in excess hydrogen gas in the burner to produce hydrogen chloride gas.

The hydrogen chloride gas and unreacted gases rose into the absorption section of the unit where the hydrogen chloride was absorbed in demineralised water to produce hydrochloric acid. This was drawn off from the unit. The remaining gas stream was passed to a scrubber where a weak caustic soda solution removed any residual hydrogen chloride and chlorine gas prior to the gas stream being vented to the atmosphere.

6.1.3 The sodium hypochlorite synthesis plant

While sodium hypochlorite was produced for sale, the sodium hypochlorite synthesis plant had the added function of being a reliable sink for any excess chlorine present within the various process systems of the complex. All waste chlorine from the brine circuit and the chlorine processing system was sent to the sodium hypochlorite synthesis plant where it is reacted, together with a make-up chlorine stream, with dilute caustic soda (22 % m/m NaOH) according to:



The sodium hypochlorite synthesis plant consisted of five primary absorption towers, three of which were on-line at any given time. The dilute caustic soda was circulated over the absorption towers where it reacted with the chlorine. The batch was withdrawn from the towers when the sodium hypochlorite has reached the required strength (~17.5 % m/m NaOCl).

6.1.4 The Hydecats destruction plant

With some of the sodium hypochlorite production being forced to absorb excess chlorine from the various process systems of the complex, the quantity of sodium hypochlorite produced sometimes exceeded the saleable demand. In such situations, or when the quality of sodium hypochlorite was off-specification, the waste sodium hypochlorite had to be disposed of through the effluent treatment facility. Before disposal however, chlorine-releasing species had to be destroyed so as to prevent downstream releases. This was done by processing the waste sodium hypochlorite in the Hydecats destruction plant.

Waste sodium hypochlorite was diluted with Umbogintwini River water and preheated by direct steam injection. The dilute sodium hypochlorite (4 % m/m NaOCl) was passed over a nickel-based catalyst which destroys the hypochlorite species.

The effluent produced by the Hydecatt destruction plant, a weak brine solution with trace quantities of dissolved chlorine and nickel, was sent to the effluent treatment facility.

6.1.5 The demineralisation plant

The demineralisation plant provided a steady supply of high purity water to the various process systems within the chlor-alkali complex. The plant consisted of a cation-exchange resin bed and an anion-exchange resin bed arranged in series. The raw water feed to the plant comprised an equal-ratio blend of Umgeni Water (municipal supply) and water from the Umbogintwini River.

During the normal ion-exchange cycle of operation, cations were removed from the influent water in the cation-exchange bed and the cation-exchange resin is converted from the hydrogen form to the cation form. Anions were removed from the influent water in the anion-exchange bed, and the anion-exchange resin was converted from the hydroxide form to the anion form. These reactions proceeded until the exchange capacities of the ion-exchange resins had been reached. Regeneration of the demineralisation plant took place every 16 h.

The regeneration sequence had five stages: *Pre-Inject*, *Regenerant Inject*, *Regenerant Displacement*, *Fast Rinse* and *Quality Rinse*. The *Pre-Inject* stage established a flow of demineralised water through the elution ducts. During the *Regenerant Inject* stage, dilute caustic soda (~4 % m/m NaOH) was used to convert the anion-exchange resin from the anion form to the hydroxide form, and dilute hydrochloric acid (~4 % m/m HCl) was used to convert the cation-exchange resin from the cation form to the hydrogen form. Demineralised water was used to displace the hydrochloric acid and caustic soda hold-ups from the cation-exchange and anion-exchange beds respectively during the *Regenerant Displacement* stage. Two rinse stages completed the regeneration sequence: a *Fast Rinse* stage, using raw water, and a *Quality Rinse* stage, using demineralised water. All effluents from the various stages, except that of the *Quality Rinse* stage, which was recycled, were sent to the effluent treatment facility.

6.1.6 Miscellaneous operations

Miscellaneous operations includes those activities within the chlor-alkali complex that did not necessarily fall into the process systems described previously. These activities included: cooling circuits, pump seals, plant wash down, cylinder and drum pressure testing and cleaning, effluent pH correction and steam desuperheating.

6.1.6.1 Cooling circuits

The complex had four cooling circuits: the Linde, the Sulzer, the Liquid Chlorine (LC) and the Membrane Cell (MBC). The Linde and Sulzer cooling circuits were associated with the liquefaction of chlorine, while the LC cooling circuit met the cooling requirements associated with the use of the liquefied chlorine. The MBC cooling circuit satisfied the cooling requirements of the brine circuit. All the cooling towers used water from the Umbogintwini River as make-up; the blow downs were sent to the effluent treatment facility.

6.1.6.2 Pump seals

Demineralised water was used to maintain the seal on several pumps within the complex. After use, this water was sent to the effluent treatment facility.

6.1.6.3 Plant wash down

The plant was washed down once a week using Umbogintwini River water. This water was drained to the effluent treatment facility.

6.1.6.4 Cylinder and drum pressure testing and cleaning

The empty gas cylinders and drums were cleaned using steam and pressure tested using Umbogintwini River water. Effluent from these activities was sent to the effluent treatment facility.

6.1.6.5 Effluent pH correction

The effluent treatment facility is owned and managed by Umbogintwini Operational Services (UOS) which serves the industrial site as a whole. Excess hydrochloric acid present in the effluent had to be neutralised prior to the effluent leaving the Sasol Polymers site, and this was done through the addition of concentrated caustic soda (~32% m/m NaOH) at a point near the boundary of the complex.

6.1.6.6 Steam desuperheating

Steam was supplied to the Sasol Polymers site by UOS in a superheated form. This steam was desuperheated by direct injection of demineralised water.

6.2 Theoretical considerations

Results from the initial study (presented in WRC report 851/1/03) showed that there was significant potential for savings to be effected on the chlor-alkali complex through the reuse and recovery of **both** water and reagents. However, the approach adopted at the time resulted in the problem being considered from a *single contaminant* perspective; as such the optimality and even the feasibility of the proposed network configurations could not be guaranteed from the *multiple contaminant* perspective. Thus, with a number of changes also having taken place on the complex in terms of the closure of certain plants, the follow-up study was proposed with the intention of optimising water-use from the multiple contaminant perspective.

As seen in the previous study, the chlor-alkali complex did not correspond to the typical situation associated with the application of water pinch analysis. Existing water pinch analysis tools, and the theory from which they developed, rely on the assumption that a clear distinction can be made between so-called *water streams* and *process streams*. With this distinction in place, only the water side of the problem is considered in the pinch analysis: the process-side is not represented explicitly. As will however be illustrated by the following discussion, it is not easy to distinguish between process streams and water streams in the chlor-alkali complex.

Consider the brine circuit presented in Figure 6.2. The most sensitive region of this circuit is the electrolyser for which there exists a range of strict concentration limits on the various species in the brine stream, in particular calcium and magnesium cations. Calcium and magnesium cations enter the brine circuit alongside the sodium chloride in the raw salt and are removed from the circuit via the series of operations which precede the electrolyser. The major portion of the calcium and magnesium load is removed via the precipitation stage. During this stage, sodium carbonate is used to precipitate the calcium as calcium carbonate and caustic soda is used to precipitate magnesium as magnesium hydroxide, both of which are subsequently removed via clarification. Precipitation of calcium carbonate and magnesium hydroxide are controlled by their associated solubility products. Thus, using the precipitation of calcium carbonate for the purposes of discussion, to achieve a desired residual calcium cation concentration in the stream leaving the precipitator requires an adjustment to the dose of sodium carbonate. The amount of sodium carbonate required is

further dependent on the concentration of calcium cations entering the precipitator. Hence, if the calcium cation load entering the precipitator was to increase through the reuse of water or the recovery of reagent, an additional amount of sodium carbonate would be needed to produce the required residual concentration in the outlet stream. Thus a balance must be struck between the savings achieved through increased reuse of water and reagents and the penalties incurred through the need to remove additional contaminant loads from the system. Similar situations occur in a number of other operations within the brine circuit.

A further aspect of the above operations is the transformation of species via chemical reaction. Individual species are not independently conserved, as is the case with the non-reacting systems considered by standard water pinch analysis theory. Chemical reactions do not only occur between reagent species and external contaminant species either. A range of by-products are generated via chemical reaction in the electrolyser alongside the caustic soda, chlorine and hydrogen products. These species are contaminants which must have their concentration controlled within the system. Further operations in which chemical reactions take place include the hydrochloric acid synthesis plant, the sodium hypochlorite synthesis plant, the Hydecats destruction plant, the demineralisation plant and the effluent pH correction stage. In addition, the operating cost of the demineralisation plant and the effluent pH correction stage is dependent on the contaminant load entering the operation.

Thus, there were three key aspects to the problem presented by the chlor-alkali complex which make the application of current water pinch analysis theory to the situation difficult. These were:

- The lack of distinction between process streams and water streams;
- The presence of multiple resources, in this case reagents and raw materials, in addition to water. These resources carried species which had an economic value to the system, and could not be treated in the same way as contaminants; and
- The chemical reactions taking place between the various species in the system.

An extension of the theory was needed to address these issues, and the term *Combined Water and Materials Pinch Analysis* was coined to describe the new methodology.

6.2.1 Problem statement for *Combined Water and Materials Pinch Analysis*

A general statement of the problem is:

The system is characterised by a set of *process operations* which convert the raw materials to the desired products at the desired production level. Within this process system, a number of *demands* for *water*, *reagents* and *raw materials* are present, each of which may be characterised by specific quantity and/or quality requirements which are established by the process operations. These demands must be satisfied using *sources* of water, reagent or raw material which are either internal to the process system or supplied externally. Each *external source*, whether it be water, reagent or raw material, is characterised by a composition profile of contaminants and other species, a cost associated with its supply and possibly a finite availability limit. Each *internal source* is similarly characterised by a composition profile of contaminants and other species and a finite availability limit, both of which are dependent on the functioning of the various process operations within the process system; these sources may also have a cost associated with their use. The process operations do not conform to any one particular model and may have any number of associated sources and demands. In addition, the various species present in the system may or may not be *chemically reactive*. Finally, the process system is characterised by certain *effluent discharge limits*, whether they be flowrate or composition based, which must be satisfied. As such, a number of different

treatment operations, each with an associated cost which may be volume and/or load dependent, are available such that these discharge limits are satisfied. The task at hand is then to *satisfy the various demands within the process system together with the effluent discharge requirements at the lowest overall cost*.

The problem statement may be extended to include other considerations such as imposed and forbidden matches, safety, controllability and plant geography. The overall cost may comprise only operating costs or the total annualised investment cost. The assumption is made that energy and pressure effects are not significant. The assumption is also made that the individual process operations are functioning optimally for the current water allocation. As usual for design, this problem considers the system at steady-state.

6.2.2 Model formulation for combined water and materials pinch analysis

This section presents a general mathematical model for Combined Water and Materials Pinch Analysis. This model involves the representation of the various options as a *superstructure*, as is the usual approach with this type of problem.

The superstructure for the water and materials minimisation problem represents the set of all potential inter-process flows between the various process operations within the process system and the flows to and from the external sinks and sources respectively. The typical superstructure encountered in the literature on water minimisation considers only a single type of process operation (Takama et al., 1980a,b; Doyle and Smith, 1997; Alva-Argáez et al., 1998b; Alva-Argáez, 1999; Mann and Liu, 1999; Benkő et al., 2000; Dericks et al., 2001; Bagajewicz and Savelski, 2001), that is, the fixed contaminant mass-load addition model considered by Wang and Smith (1994). The majority of operations encountered on the chlor-alkali complex however did not conform to one particular type of unit model. Apart from not being able to describe the different operations according to a single performance characteristic such as mass transfer, the operations did not have a common topological structure in terms of the number of associated inlets and outlets. In formulating the superstructure for the model, it was desirable that the model framework be sufficiently general for all process operations to be integrated efficiently and easily. As such, the overall framework of the superstructure needed to be independent of the types of process operations considered. This was accomplished by formulating the superstructure in such a way that it represented the set of all possible flows from any source to any sink. The models for the individual process operations are then incorporated as modules within this framework. The superstructure is thus described as follows:

- Every sink is preceded by a mixer.
- Every source is followed by a splitter.
- Process units are incorporated as modules connected between sinks and sources.

Figure 6.3 uses a simple example with three process modules to illustrate the superstructure framework.

The question of reagents and raw materials in the system was simply a matter of the kinds of concentration limits that could be applied. For contaminants, the only kind of limit that is appropriate is a maximum value that can be tolerated by the equipment. For reagents and raw materials, the constraint might be a minimum value, or a required value (an *equality constraint*).

Chemical reactions were accommodated by providing for stoichiometric transformations within the process unit modules.

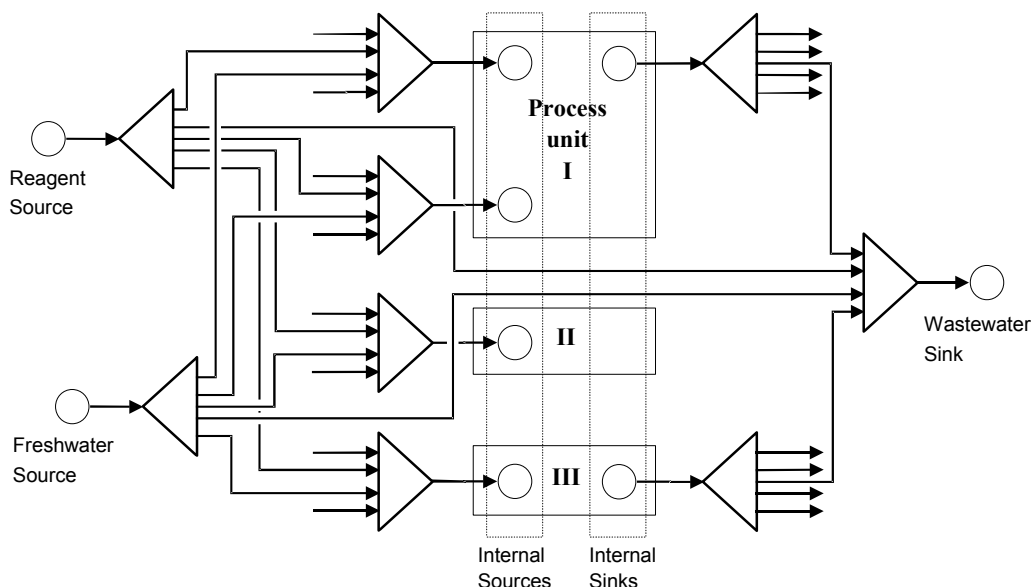


Figure 6.3 : *An example of a superstructure for a simple process with three units.*

The pinch model was formulated from the mass balance equations for the water and materials flows in the superstructure, together with the input-output relationships for all the process modules. To these were added all the concentration and flow rate constraints that applied at each node of the superstructure. The result is a standard non-linear programming (NLP) problem, which can be solved using a general-purpose NLP algorithm. The software platform used in this study was GAMS (General Algebraic Modelling System) (GAMS Development Corporation, 2001). GAMS is a high-level language for the compact representation of large and complex optimisation problems (Brooke et al., 1998). A key feature of the language is that the model may be described independently of the required solution algorithm. Thus, models are formulated using a consistent notation and within a common development environment, termed the Integrated Development Environment.

6.2.3 Species selection

Table 6.1 presents a listing of the species of significance to the chlor-alkali system considered in this investigation. Included within this table is both a justification for the selection of the species and a categorisation of the species in terms of its associated desirability or undesirability. Some of these species were neither desirable nor undesirable, but were included since they were involved in some of the chemical reactions taking place in the complex. The inclusion of these species in the Pinch Analysis was not essential since they did not constrain the reuse of materials; their inclusion did however provide a more realistic representation of what was occurring in the system from a mass-balance perspective.

Table 6.1: *Species considered in the combined water and materials pinch analysis*

Species	Status	Justification for Selection
Ca ²⁺	Undesirable	Precipitates as hydroxide in electrolyser membranes
CaCO ₃	Undesirable	A precipitate which can foul electrolyser membranes
Cl ₂	Desirable Undesirable	Product produced and raw material used by the complex Destroys cation-exchange resin in brine circuit
H ₂	Desirable	Product produced and raw material used by the complex
HCl	Desirable Undesirable	Product produced and reagent/raw material used by the complex Contaminant where caustic soda is required
H ₂ O	-	Involved in chemical reactions
Mg ²⁺	Undesirable	Precipitates as hydroxide in electrolyser membranes
Mg(OH) ₂	Undesirable	A precipitate which can foul electrolyser membranes
NaCl	Desirable Undesirable	Raw material used in the complex Contaminant in demineralised water production
NaClO ₃	Undesirable	Damages cation-exchange resin in brine circuit
Na ₂ CO ₃	Desirable Undesirable	Used as a reagent to precipitate calcium in brine circuit Affects electrolyser membranes at high concentrations
NaHSO ₃	Desirable Undesirable	Destroys Cl ₂ in brine stream Converts to sulphate which is undesirable
NaOCl	Desirable Undesirable	Product produced by the complex Cl ₂ releasing species - problematic in brine circuit and effluent
NaOH	Desirable Undesirable	Product produced and reagent/raw material used by the complex Contaminant where hydrochloric acid is required
Na ₂ SO ₄	Undesirable	Diffuses through electrolyser membranes with some precipitation taking place
O ₂	-	Product of chemical reactions
Insolubles	Undesirable	Fouling of equipment
TDS	Undesirable	Of significance in the cooling towers

6.2.4 Division of the complex into sections

The complexity of the system made the problem difficult to solve. The application of a decomposition strategy to a process system results in a number of smaller problems rather than one large problem. Decomposition strategies which divide the process system into a number of different zones have been proposed by Oleson and Polley (1996) as a means of dealing with plant geography in the design of water-reuse networks, and by Amidpour and Polley (1997) in the context of producing simpler designs for heat integration. In this investigation, the chlor-alkali complex was divided into three subsystems. Reuse opportunities for water are maximised within each subsystem before reuse opportunities are investigated in other subsystems. The subsystems were:

- the demineralisation plant subsystem;
- the chemical production subsystem, which is made up of the brine circuit, the hydrogen and chlorine processing plants, the caustic evaporators, the

hydrochloric acid synthesis plant, the sodium hypochlorite synthesis plant and the Hydecats destruction plant; and,

- the cooling circuit subsystem, which is made up of the various cooling towers and their associated cooling circuits located within the complex.

Aside from making it easier to handle the problem from the perspective of optimisation, these divisions were justified to some extent on practical grounds. Water from the cooling circuit subsystem, which may have biological contaminants associated with it, could not be used the demineralisation plant subsystem or the chemical production subsystem. Similarly, effluent from the regeneration cycle of the demineralisation plant subsystem could not be reused in the chemical production subsystem or the cooling circuit subsystem.

Nevertheless, interactions between these divisions did exist. In particular, demineralised water from the demineralisation plant subsystem was required by the chemical production subsystem. Similarly, caustic soda and hydrochloric acid from the chemical production subsystem were required by the demineralisation plant subsystem. Thus in modelling the subsystems, it was necessary to account these interactions.

With the subsystem approach to dealing with the chlor-alkali complex, water not reused internally within a subsystem was available for reuse in other subsystems. This interaction between the subsystems was handled by assigning a hierarchy to each subsystem with respect to the allocation of water resources from other subsystems. As has already been noted, water from the cooling circuit subsystem could not be reused in either of the other subsystems. Demineralised water from the demineralisation plant subsystem could be used in either of the other subsystems, though it may not have been economic to use the water in the cooling circuit subsystem. The chemical production subsystem however took priority with regard to the use of demineralised water. Excess water from the chemical production subsystem may similarly be reused in either of the other subsystems. However, since the quality of the water entering the demineralisation plant subsystem had a greater impact on cost than that for the cooling circuit subsystem, priority was assigned to reusing excess water from the chemical production subsystem in the demineralisation plant subsystem. Any of the water not accepted by the demineralisation plant subsystem was made available for use in the cooling circuit subsystem.

Figure 6.4 provides a schematic representation of the interactions between the various subsystems of the chlor-alkali complex. The strategy for dealing with them was to first optimise the water use **within** each subsystem, regarding the streams flowing between them as fixed, and then to consider the opportunities for reuse **between** the subsystems.

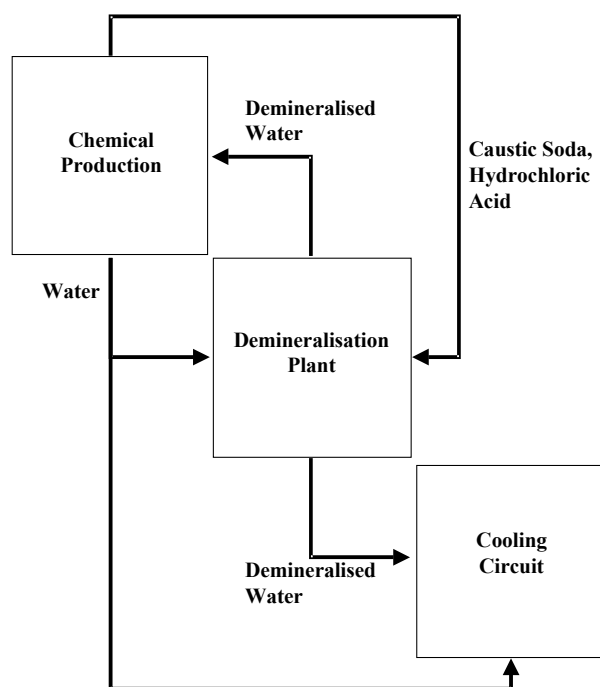


Figure 6.4 : *The interactions between the three subsystems of the complex.*

6.2.5 Subsystem modelling

The following sections consider the modelling of each of the individual subsystems in isolation from each other. The different process modules which constitute the various subsystems are presented together with their integration into the superstructure framework. As a general strategy for the optimisation of the different subsystems, the initial set of concentration constraints imposed on the subsystem superstructures were derived from plant records. Relaxation of constraints was considered only in subsequent optimisation runs and only where appropriate.

6.2.5.1 The demineralisation plant

The demineralisation plant subsystem had only one process module, which was used to describe both the normal cycle of operation and the regeneration cycle of operation of the demineralisation plant. This section considers the optimisation of the demineralisation plant subsystem in isolation from the other subsystems. The demand for demineralised water within the chlor-alkali complex was therefore assumed to remain at the level determined from the plant data; this assumption was relaxed when the different subsystems were integrated.

Figure 6.5 shows the different stages of the regeneration sequence, together with the effluents produced by each stage and the hold-up volumes at the conclusion of each stage. The positioning of the regeneration cycle relative to the normal cycle of operation is also indicated. The normal cycle of operation is represented in Figure 6.5a and 6.5h while the regeneration sequence is represented in Figure 6.5c to 6.5g. Figure 6.5b represents the changeover from the normal cycle of operation to the regeneration cycle.

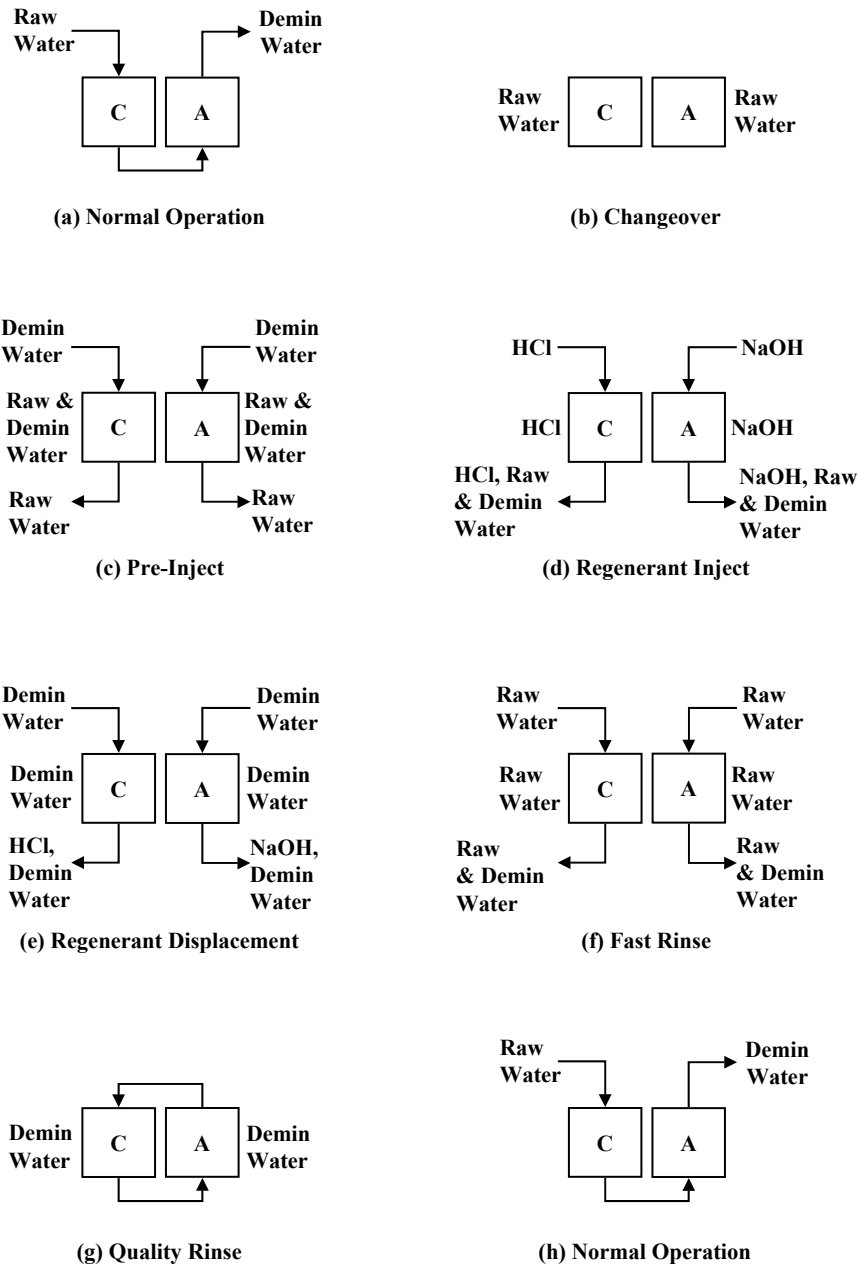


Figure 6.5 : The various stages of operation of the demineralisation plant

The progress of fluid through the demineralisation plant during the regeneration sequence may be described as follows:

- **Changeover** (Figure 6.5b): When the changeover from the normal cycle of operation to the regeneration cycle is made, both the anion-exchange (A) and cation-exchange (C) resin beds contain raw water.
- **Pre-Inject Stage** (Figure 6.5c): The Pre-Inject stage introduces a small volume of demineralised water into each resin bed. This demineralised water displaces an equal volume of raw water from the bed. At the end of this stage, the resin bed contains raw water and the small volume of demineralised water introduced during the stage.

•**Regenerant Inject Stage** (Figure 6.5d): During the Regenerant Inject stage, hydrochloric acid, at the required concentration, is injected into the cation-exchange bed and caustic soda, at the required concentration, is injected into the anion-exchange bed. As the stage proceeds, water presently in the resin beds is displaced by the regenerants. Simultaneously, the cations are stripped from the cation-exchange resin and replaced by H^+ cations while the anions are stripped from the anion-exchange resin and replaced by OH^- anions. At the end of the stage, the resin bed volumes are occupied by the regenerants at the concentrations at which they were supplied to the stage. The effluent from this stage comprises a mixture of the raw water displaced from the resin beds, the regenerants that have passed through the resin beds and the ions eluted from the ion-exchange resins.

•**Regenerant Displacement Stage** (Figure 6.5e): During the Regenerant Displacement stage, demineralised water is used to displace the regenerant hold-ups from the Regenerant Inject stage. At the end of this stage, the resin beds are filled with demineralised water. The effluent from this stage is a weak hydrochloric acid solution from the cation-exchange bed and a weak caustic soda solution from the anion-exchange bed.

The regeneration sequence is completed by two rinse stages, the Fast Rinse and the Quality Rinse:

•**Fast Rinse Stage** (Figure 6.5f): The Fast Rinse stage uses raw water. The demineralised water hold-up in the resin bed from the previous stage is displaced by this raw water and at the end of the stage the resin bed is filled with raw water. The effluent from the Fast Rinse stage is a mixture of the raw water that has passed through the resin beds and the demineralised water hold-up from the Regenerant Displacement stage.

•**Quality Rinse Stage** (Figure 6.5g): The Quality Rinse stage uses demineralised water. This water is recycled through the resin beds and after a period of time, the demineralisation plant returns to the normal cycle of operation (Figure 6.2h). No effluent is produced during this stage.

From the preceding description, four demands associated with the regeneration sequence of the demineralisation plant may be identified. These demands are for demineralised water, raw water, caustic soda and hydrochloric acid. Raw water is also required by the normal cycle of operation of the demineralisation plant. From a survey of the effluents arising from the regeneration cycle, the following potential reuse opportunities are identified:

While the effluents from the Regenerant Inject stage were considered too contaminated for reuse, the effluents from the Displacement stage may be reused in subsequent regeneration cycles. From the cation-exchange bed, the effluent is a weak solution of hydrochloric acid and this could be used when the hydrochloric acid supply for the subsequent cycle is prepared. From the anion-exchange bed, the effluent is a weak solution of caustic soda and this could be used when the caustic soda supply for the subsequent cycle is prepared. Both reuse opportunities would result in savings in demineralised water, concentrated regenerant (reagent) and effluent treatment costs.

Effluents from the Fast Rinse stage may be reused during the normal cycle of operation of the demineralisation plant. This effluent is a mixture of demineralised water and raw water. Its reuse would result in savings in raw water and effluent treatment costs.

Both of the above opportunities, if feasible, would further result in small reductions in the frequency of regeneration of the demineralisation plant. The reuse of the effluent (raw water)

from the Pre-Inject stage is not considered a viable possibility since the quantity involved is small.

From a modelling perspective, the superstructure concept implies that all flow emerging from a source in the superstructure must flow to a sink in the superstructure. Thus, all effluents not reused directly within the demineralisation plant process module must be sent elsewhere, and two terminal sinks were provided for this purpose. The first sink was used for the storage of the demineralised water produced by the demineralisation plant while the second sink represented the effluent treatment facility. The connectivity matrix representing the logical possibility of connections between process sources and sinks for the demineralisation plant thus appears as shown in Table 6.2. All process sources may be sent to the effluent treatment facility.

Demands associated with the demineralisation plant process module not satisfied by the associated process sources must be satisfied by an external source. Two sources of raw water were available, namely Umgeni Water (municipal supply), for which an availability limit existed, and Umbogintwini River water, for which no availability limit existed. A single source of hydrochloric acid was available to meet the demands requiring hydrochloric acid, while three sources of caustic soda, each of differing strength, were available to meet the demands requiring caustic soda. These three sources correspond to the caustic soda produced by the electrolyser, and the caustic soda withdrawn after the first and second effects of the dual-effect caustic evaporators. The connectivity matrix representing the possible connections between external sources and sinks for the demineralisation plant is shown in Table 6.3

Table 6.2 : The connectivity matrix between process sources and sinks for the demineralisation plant subsystem. Shaded squares show disallowed connections.

Sinks Sources	Effluent Treatment Facility	Demineralised Water Storage	Raw Water Demand - Normal Operation	Raw Water Demand - Regeneration	Demineralised Water Demand - Regeneration	Caustic Soda Demand - Regeneration	Hydrochloric Acid Demand - Regeneration
Effluent - Cation Regeneration - Pre-Inject & Regenerant Inject Stage							
Effluent - Cation Regeneration - Regenerant Displacement Stage							
Effluent - Cation Regeneration - Fast Rinse Stage							
Effluent - Anion Regeneration - Pre-inject & Regenerant Inject Stage							
Effluent - Anion Regeneration - Regenerant Displacement Stage							
Effluent - Anion Regeneration - Fast Rinse Stage							
Demineralised Water							

Table 6.3 : *The connectivity matrix between external sources and sinks for the demineralisation plant subsystem. Shaded squares show disallowed connections.*

Sources \ Sinks	Effluent Treatment Facility	Demineralised Water Storage	Raw Water Demand - Normal Operation	Raw Water Demand - Regeneration	Demineralised Water Demand - Regeneration	Caustic Soda Demand - Regeneration	Hydrochloric Acid Demand - Regeneration
Umgeni Water (Municipal Supply)							
Umbogintwini River Water							
Hydrochloric Acid (31% m/m HCl)							
Caustic Soda (32% m/m NaOH)							
Caustic Soda (38% m/m NaOH)							
Caustic Soda (50% m/m NaOH)							

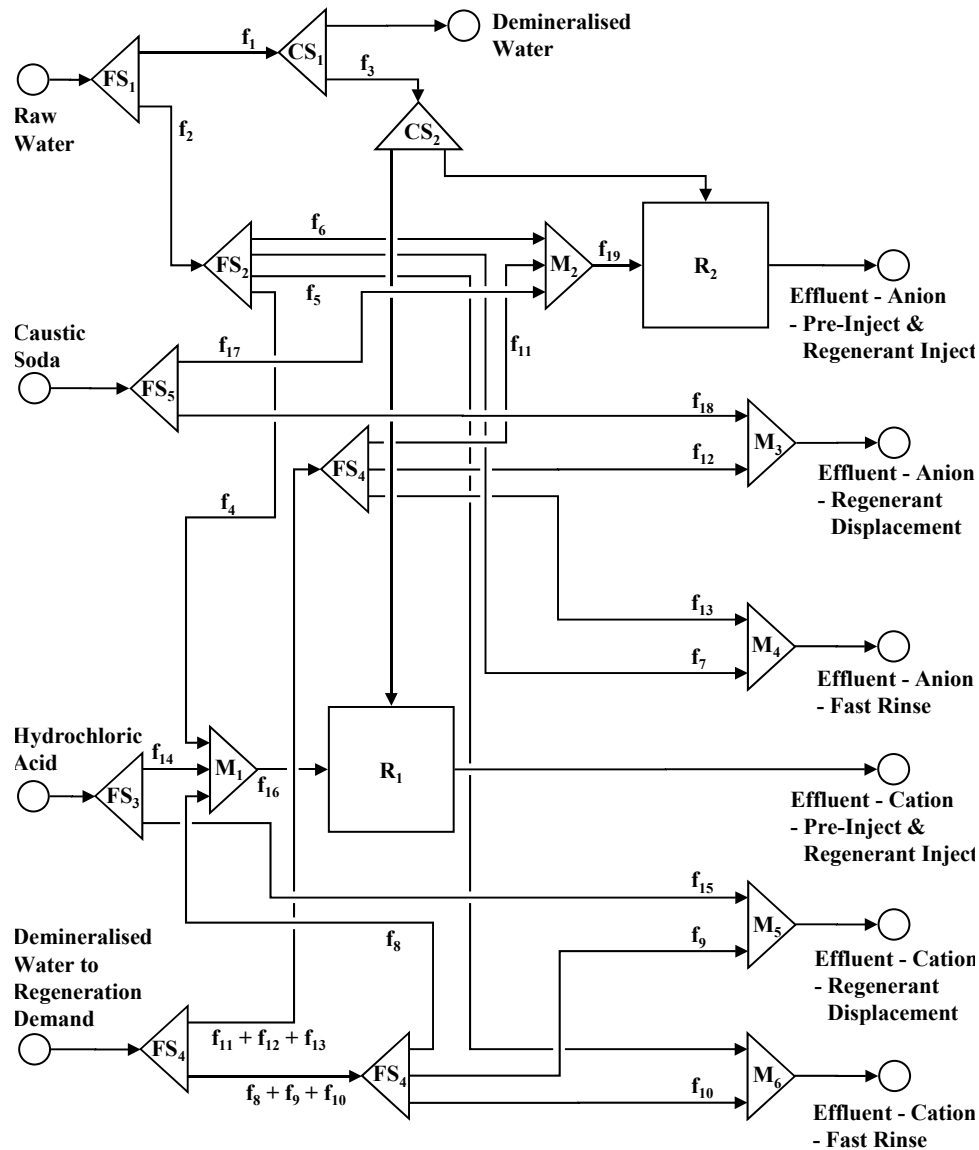
The unshaded squares in Table 6.2 and Table 6.3 represent the total set of possible network configurations included in the optimisation problem for the demineralisation plant subsystem. It is from this set of configurations that the optimal network configuration was selected.

Figure 6.6 illustrates the model for the demineralisation plant process module. The functions of the various building blocks associated with the normal cycle of operation and the various stages of the regeneration sequence are described in Table 6.4.

The objective function for this problem may be stated verbally as follows:

Given two different sources of raw water, together with sources of hydrochloric acid and caustic soda, the task is to identify an optimal network configuration which achieves the required rate of production of demineralised water at the lowest cost. This cost includes the costs associated with the replacement of the cation-exchange and anion-exchange resins, the purchase of external sources and the disposal of the effluents produced by the system.

The objective function did not include capital costs. Given that this was a *retrofit* problem, capital costs require of new piping rather than the purchase of costly equipment. Additional storage capacity may also be required. It was assumed that the savings in operating costs through the more efficient use of water and materials would be sufficient to offset the costs associated with effecting these minor changes to the process system, so capital costs were not considered explicitly.



f_1 Raw water to normal operation	f_{11} Demin water to anion regen Pre-Inject & Regen Inject
f_2 Raw water to regeneration	f_{12} Demin water to anion regen Regen Displacement
f_3 Salts from demin to regen	f_{13} Demin water hold-up from anion regen Regen Displacement to anion regen Fast Rinse
f_4 Raw water to cation regen Pre-Inject & Regen Inject	f_{14} Mass flow of HCl cation regen Pre-Inject & Regen Inject
f_5 Raw water to cation regen Fast Rinse	f_{15} HCl hold-up from cation regen Pre-Inject & Regen Inject to Regen Displacement
f_6 anion regen Pre-Inject & Regen Inject	f_{16} Raw water, demin water and HCl to cation regen Pre-Inject & Regen Inject reaction
f_7 Raw water to anion regen Fast Rinse	f_{17} NaOH to anion regen Pre-Inject & Regen Inject
f_8 Demin water to cation regen Pre-Inject & Regen Inject	f_{18} NaOH hold-up from anion regen Pre-Inject & Regen Inject to Regen Displacement
f_9 Demin water to cation regen Regen Displacement	f_{19} Raw water, demin water and NaOH to anion regen Pre-Inject & Regen Inject reaction
f_{10} Demin water hold-up from cation regen Regen Displacement to Fast Rinse	

Figure 6.6 : The model for the demineralisation plant module.

Table 6.4 : *The building blocks of the demineralisation plant module.*

Building Block	Function
FS ₁	Divides the flow of raw water between the normal cycle of operation (f_1) and the regeneration sequence (f_2) of the demineralisation plant.
FS ₂	Divides the flow of raw water between the cation-exchange regeneration part of the model and the anion-exchange regeneration part of the model. Two streams are sent to the cation-exchange regeneration part of the model (f_4 and f_5) and two streams are sent to the anion-exchange regeneration part of the model (f_6 and f_7).
FS ₃	Associated with the cation-exchange regeneration part of the model. Divides the flow of hydrochloric acid between the Pre-Inject & Regenerant Inject stage (f_{i4}) and the Regenerant Displacement stage (f_{i5}). The Pre-Inject stage and the Regenerant Inject stage are represented as a single stage in the model.
FS ₄	Divides the flow of demineralised water amongst the various stages of the regeneration sequence. f_8 , f_9 and f_{10} are sent to the cation-exchange regeneration part of the model while f_{11} , f_{12} and f_{13} are sent to the anion-exchange part of the model. These streams are associated with the Pre-Inject & Regenerant Inject stage (f_8 and f_{11}), the Regenerant Displacement stage (f_9 and f_{12}) and the Fast Rinse stage (f_{10} and f_{13}).
FS ₅	Associated with the anion-exchange regeneration part of the model. Divides the flow of caustic soda between the Pre-Inject & Regenerant Inject stage (f_{i7}) and the Regenerant Displacement stage (f_{i8}).
CS ₁	Effects the removal of species (f_3) from the raw water being treated by the demineralisation plant (f_1) such that demineralised water is produced.
CS ₂	Divides the species removed by CS ₁ into ions which are sent to the cation-exchange and anion-exchange parts of the model.
M ₁	Associated with the cation-exchange regeneration part of the model. Represents the combination of the raw water (f_4), demineralised water (f_8) and hydrochloric acid (f_{i4}) for the Pre-Inject & Regenerant Inject stage. Stream f_{i6} is produced.
M ₂	Associated with the anion-exchange regeneration part of the model. Represents the combination of the raw water (f_6), demineralised water (f_{i1}) and caustic soda (f_{i7}) for the Pre-Inject & Regenerant Inject stage. Stream f_{i9} is produced.
M ₃	Associated with the anion-exchange regeneration part of the model. Represents the combination of the caustic soda hold-up from the Pre-Inject & Regenerant Inject stage (f_{i8}) and the demineralised water effluent from the Regenerant Displacement stage (f_{i2}).
M ₄	Associated with the anion-exchange regeneration part of the model. Represents the combination of demineralised water hold-up from the Regenerant Displacement stage (f_{i3}) and the raw water effluent from the Fast Rinse stage (f_7).
M ₅	Associated with the cation-exchange regeneration part of the model. Represents the combination of the hydrochloric acid hold-up from the Pre-Inject & Regenerant Inject stage (f_{i5}) and the demineralised water effluent from the Regenerant Displacement stage (f_9).
M ₆	Associated with the cation-exchange regeneration part of the model. Represents the combination of demineralised water hold-up from the Regenerant Displacement stage (f_5) and the raw water effluent from the Fast Rinse stage (f_{i0}).
R ₁	Associated with the cation-exchange regeneration part of the model. Represents the removal of cations from the cation-exchange resin by the regenerant.
R ₂	Associated with the anion-exchange regeneration part of the model. Represents the removal of anions from the anion-exchange resin by the regenerant.

The regeneration frequency is dependent on the quantity and quality of the water treated by the plant. As the solver alters the flow configuration in search of the optimum, these might change, requiring in turn a change in the regeneration frequency. This will affect the quantities of regenerant chemicals required and the amount of effluent generated by the demineralisation plant subsystem. While the quantities of these materials and the effluent generated will be the same per regeneration cycle, the time-average quantities will be different. In addition, a change in the regeneration frequency will affect on the rate of production of demineralised water.

A cost factor associated with the replacement of the ion-exchange resins was included in the objective function. In practice, a portion of the ion-exchange resin had to be replaced annually due to resin losses and resin fracture. This portion was related to the number of regeneration cycles taking place annually, and is thus to the total ionic load removed from the influent water.

The model considered the production of an amount of demineralised water over one total cycle of operation at the current regeneration frequency, that is, the amount of water produced between two successive regenerations over a period of 16 h. A demineralised water production rate of 16 m³/h is assumed over the normal cycle of operation. The regeneration procedure lasts 191 min which means that the average rate of production over the total cycle of operation is 13.3 m³/h.

Figure 6.7 shows the demineralisation plant process module integrated with the external sources and terminal sinks present in the superstructure as a representation of the overall optimisation problem for the demineralisation plant subsystem.

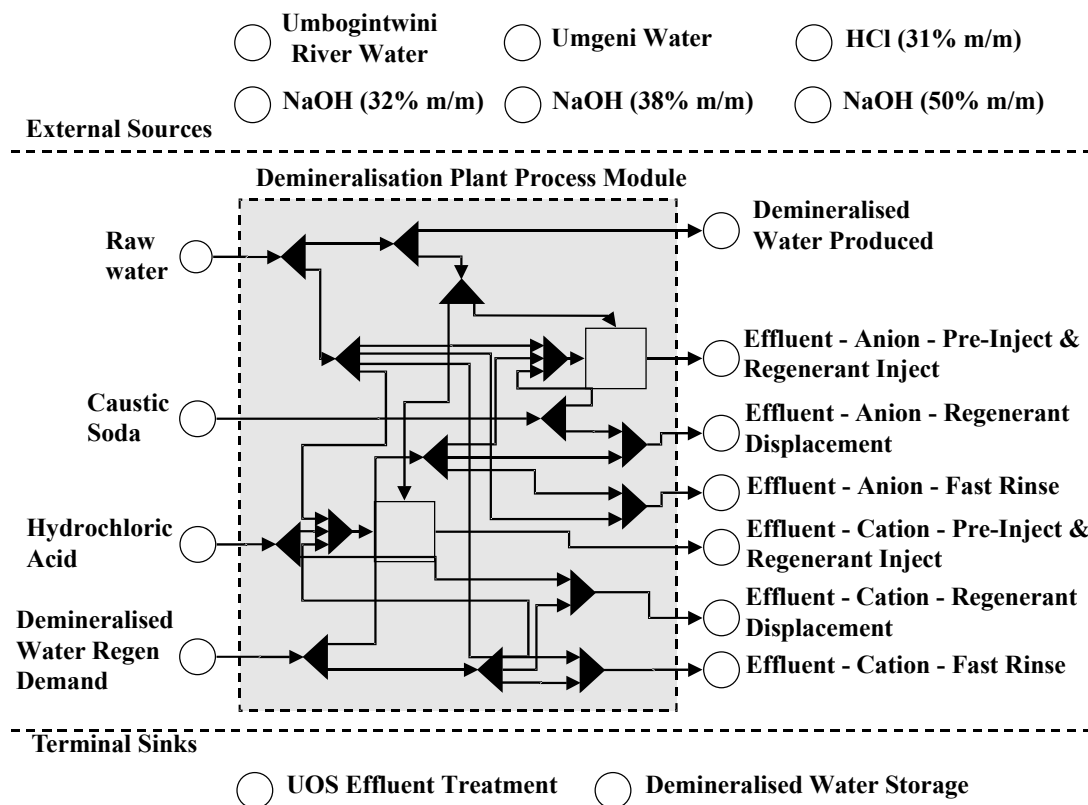


Figure 6.7 : Diagram showing the integration of the demineralisation plant process module with the external sources and terminal sinks present in the superstructure as a representation of the overall optimisation problem for the demineralisation plant subsystem.

Table 6.5 : Comparison of water and material requirements and effluent production associated with the existing network configuration and the optimised network configuration.

	Unit	Existing Configuration	Optimised Configuration
Demineralised Water Produced	[t]	254.87	254.87
Number of Regeneration Cycles	[]	1	1.22
Umbogintwini River Water	[t]	130.45	254.93
Umgeni Water	[t]	130.45	0
Total Water	[t]	260.90	254.93
Hydrochloric Acid (31% m/m HCl)	[kg]	350.00	366.42
Caustic Soda (32% m/m NaOH)	[kg]	390.00	407.70
Caustic Soda (38% m/m NaOH)	[kg]	0	0
Caustic Soda (50% m/m NaOH)	[kg]	0	0
Demineralised Water Available to Other Subsystems	[t]	239.20	241.18
Effluent	[t]	22.42	14.51
NaCl Load to Effluent	[kg]	195.13	202.64

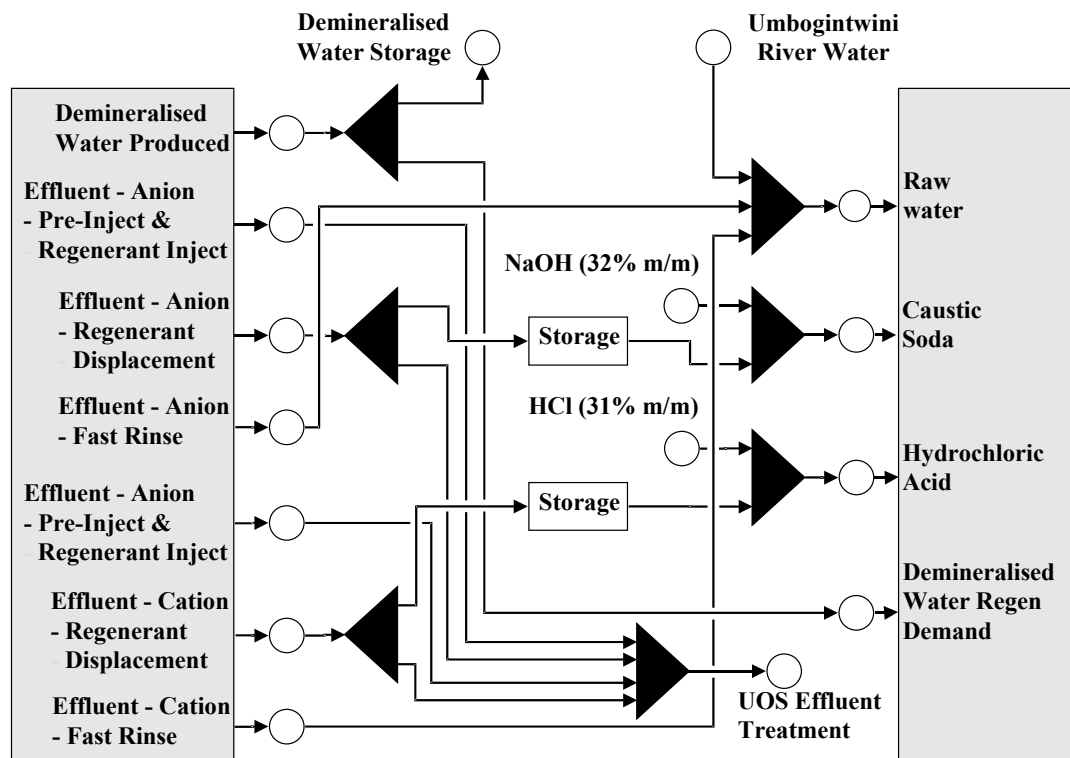


Figure 6.8 : Diagram showing the optimal network configuration for the demineralisation plant subsystem

The results of the optimisation are summarised in table 6.5 and figure 6.8

The notable features of the solution from the optimisation of the demineralisation plant subsystem are:

- Only Umbogintwini River water is used in the production of demineralised water
- A portion of the NaOH containing effluent from the Regenerant Displacement stage of the anion regeneration is used in the preparation of the dilute caustic soda required for the subsequent regeneration cycle. HCl containing effluent from the Regenerant Displacement stage of the cation regeneration is reused in a similar way.
- Effluent from the Fast Rinse stages of the cation and anion regenerations is recovered completely and used in the production of demineralised water.
- There is an increase in the frequency of regeneration of the demineralisation plant. This increase is due to the exclusive use of the Umbogintwini River water rather than the blend of Umgeni Water and Umbogintwini River water. This indicates that the costs associated with the increased regeneration frequency are offset by the savings accrued through the use of the less expensive, but lower quality, water source.
- There are increases in the amounts of caustic soda and hydrochloric acid required in the production of the fixed quantity of demineralised water. However, the quantity of water required for this production and the effluent associated with this production are reduced. The NaCl load associated with the effluent does however show a slight increase.
- The proportion of the total demineralised water production available to the rest of the plant has increased in the optimal configuration; a smaller proportion of the water treated by the demineralisation plant is used for regeneration purposes, despite the increase in regeneration frequency.
- There is a 36 % reduction in the quantity of effluent produced by the optimal configuration, and an 18 % reduction in the overall operating cost. This reduction sees a decrease in the unit cost associated with demineralised water from R 4.71 per ton to R 3.88 per ton.

The implementation of the proposed reuse strategy would have involved only minor process changes.

6.2.5.2 The Chemical Production subsystem

The chemical production subsystem included the brine circuit, the hydrogen and chlorine processing plants, the caustic evaporators, the hydrochloric acid synthesis plant, the sodium hypochlorite synthesis plant, the Hydecats destruction plant, and a number of other associated demands and sources of water located within the chlor-alkali complex. This subsection considers the optimisation of the chemical production subsystem in isolation from the other subsystems. Allowance was made for the various interdependencies that existed between the chemical production subsystem and the demineralisation plant subsystem.

Figure 6.9 shows the chemical production subsystem in terms of its constituent plants. Each of these divisions in turn may consist of a number of process modules.

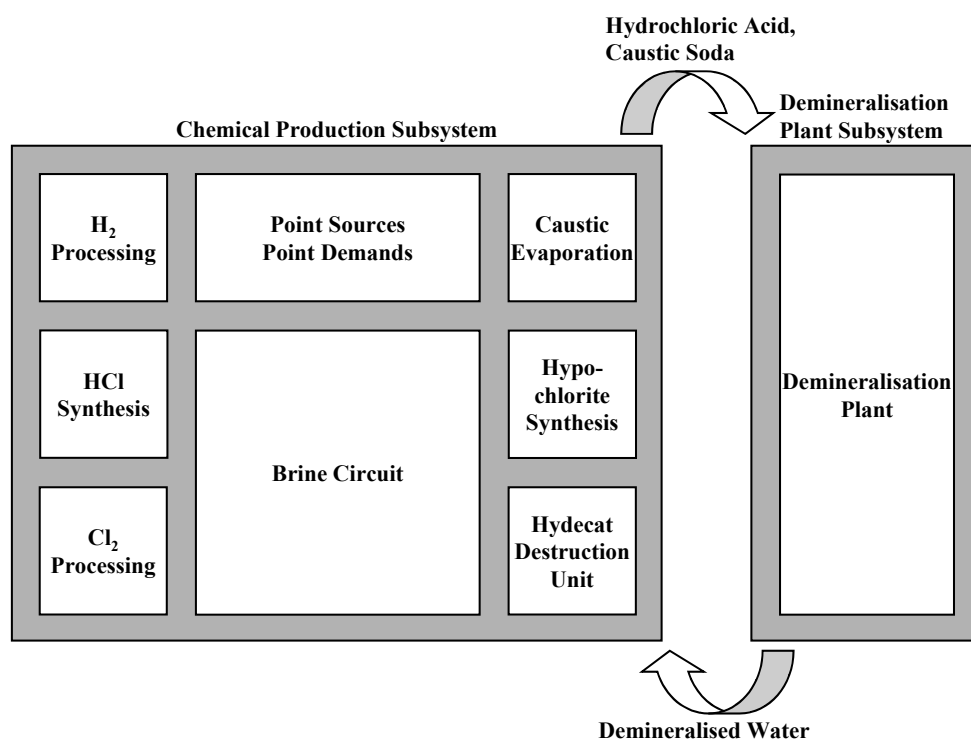


Figure 6.9 : The chemical production subsystem and its existing interactions with the demineralisation plant subsystem.

The **brine circuit** was the major component of the chemical production subsystem, and the various operations making up the circuit were modelled as a number of process modules (refer to figure 6.2). A series of raw material purification steps preceded the electrolyser and conditioned the brine to a standard acceptable to the electrolyser. The chief contaminants that these operations removed were calcium and magnesium, which were impurities in the raw salt introduced at the resaturator. This purification sequence was considered to be fixed, and not subject to the optimisation.

Figure 6.10 presents the brine circuit model as a collection of process modules. These process modules include the electrolyser, primary dechlorination, secondary dechlorination, precipitation, clarification, primary filtration, secondary filtration and cation-exchange. It should be noted that while the brine circuit is modelled as a collection of process modules, the required sequence of the raw material purification steps is established by the incorporation of the necessary logic into the connectivity matrix.

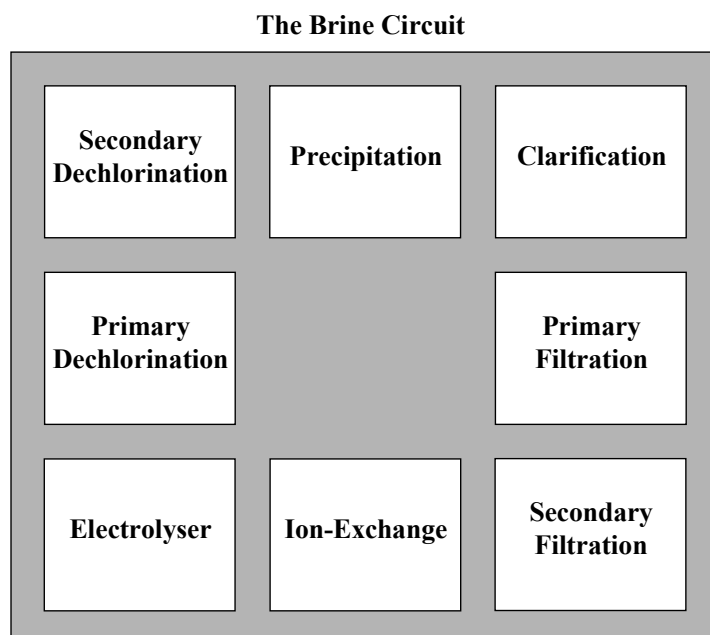


Figure 6.10 : *The brine circuit model process modules.*

The electrolyser module

The electrolyser module contained elements which model the conversion of NaCl to products and by-products, the transfer of species across the membrane into the caustic soda solution and the processing of the chlorine and hydrogen gases produced by the electrolyser. In addition, the process module included an element for the dosing of hydrochloric acid to the lean brine emerging from the electrolyser.

Three demands and five sources were associated with the electrolyser process module. The demands are for brine, demineralised water (a process requirement) and hydrochloric acid, while the sources produced by the process module were treated brine, caustic soda and condensate from the chlorine and hydrogen coolers and hydrogen chiller. The treated brine was routed to the primary dechlorination process module as a process requirement. The caustic soda could be used within the complex or sent to the caustic evaporators. The condensate from the chlorine cooler could be sent to either of the dechlorination stages or to the sodium hypochlorite synthesis module. No restrictions were placed on the routing of the condensate from the hydrogen cooler and chiller.

The primary dechlorination process module

The primary dechlorinator was used air to strip chlorine from the brine stream. Alongside the removal of chlorine, water was also removed from the brine. The quantity of water removed from the brine was assumed to be the same as that currently removed by the dechlorinators, while the removal of chlorine was represented by a removal ratio. The primary dechlorination process module had a single brine inlet and produces two sources of material, that is, a dechlorinated brine stream and a waste chlorine stream. The dechlorinated brine was sent to the secondary dechlorination stage as a process requirement, while the waste chlorine stream was sent to the sodium hypochlorite synthesis module.

The secondary dechlorination process module

The secondary dechlorination module had three demands associated with it, that is, brine, caustic soda and sodium bisulphite. Caustic soda was used for the neutralisation of any

hydrochloric acid remaining in the brine coming from the primary dechlorination stage, while sodium bisulphite was added to destroy residual chlorine present in the brine.

The precipitation process module

The precipitation of calcium as calcium carbonate and the precipitation of magnesium as magnesium hydroxide were represented together in the precipitation process module. The module had associated with it three demands and one source. The demands were for brine, caustic soda and sodium carbonate. The source was the brine stream emerging from the module, and was routed to the clarification process module.

The clarification process module

This module removed insoluble matter from the brine stream as brine sludge. Two demands and two sources were associated with the module. The demands were for brine and flocculant, while the sources produced by the process module were a brine sludge stream and a clarified brine stream. The dose of flocculant was assumed to be proportional to the amount of solid material removed from the brine stream. The flocculant itself was not represented in the model since the assumption is made that it is completely removed by the clarification process; only the dilution water accompanying the flocculant was represented in the model. The removal of solids was modelled in terms of a removal ratio and the total solids fraction associated with the brine sludge was assumed constant. The brine sludge stream emerging from the process module was routed to the terminal effluent sink, while the clarified brine was routed to the primary filtration process module.

The primary filtration process module

Both the normal cycle of operation and the backwash cycle, on a time-average basis, were represented in the model for the primary filtration process module. Correspondingly, there were two demands and two sources associated with this module. The demands were for brine by the normal cycle of operation and by the backwash cycle of operation. The demand by the backwash cycle was assumed proportional to the amount of material removed by the filter. A removal ratio was used to represent the removal of insoluble matter from the brine stream, while removal ratios were also used to represent the concentration differences of calcium and magnesium observed across the filter. The brine stream emerging from the normal cycle of operation could be routed to the backwash cycle of the primary filtration process module if deemed appropriate by the optimisation. Brine from the backwash cycle was routed to the clarification module.

The secondary filtration process module

The secondary filtration process module had two demands and two sources associated with it. These demands are for brine and for alpha-cellulose. The secondary filtration stage uses candle filters, and alpha-cellulose is used as the filter aid. The amount of alpha-cellulose dosed to the brine was assumed proportional to the material removed by the filter. The alpha-cellulose itself was not represented in the model since it was completely removed during the filtration stage and only the water accompanying its addition was represented. A suitable cost factor was however attached to the alpha-cellulose inlet to account for the purchase cost associated with the alpha-cellulose. The removal of material was modelled using a removal ratio for insoluble material; removal ratios were also used to represent the calcium and magnesium concentration differences observed across the filter. The brine stream emerging from the process module was routed to the cation-exchange process module and possibly to the backwash cycle of the primary filtration process module. The solids removed by the filtration process (excluding the spent filter medium) were routed to the

terminal effluent treatment sink. An appropriate cost factor was applied to the material removed by the filter to represent the cost associated with the disposal of this solid waste.

The cation-exchange process module

The cation-exchange module was similar to the demineralisation plant module and both the normal cycle of operation and the regeneration cycle of operation were considered. The module had two demands for brine, one by the normal cycle of operation and one by the regeneration cycle of operation, and demands for hydrochloric acid, caustic soda and water. Eight sources were associated with the module. Apart from the brine stream emerging from the normal cycle of operation which was routed to the electrolyser module, there were seven sources associated with the regeneration cycle of operation. These sources corresponded to the seven stages of the regeneration procedure, that is, Brine Displacement, Backwash, Acid Regeneration, Acid Displacement, Caustic Regeneration, Caustic Displacement and Brine Replacement. The possible reuse opportunities for these effluents were as follows:

- The effluents from the Brine Displacement and Brine Replacement stages were mixtures of demineralised water and polished brine. These effluents could be recycled to the brine circuit.
- Effluent from the Backwash stage was assumed to be of demineralised water quality but may have some filterable material present in it. This effluent could be recycled to the brine circuit, possibly at some point before the filtration stage.
- The effluents from the Caustic Regeneration and Caustic Rinse stages were both mixtures of demineralised water and caustic soda. These effluents could be reused directly in the preparation of the caustic soda requirement for the succeeding regeneration cycle or elsewhere in the chemical production subsystem.
- Effluent from the Acid Rinse stage was a mixture of hydrochloric acid and demineralised water. This effluent could be reused when the hydrochloric acid requirement for the succeeding regeneration cycle is prepared.
- Effluent from the Acid Regeneration stage was a mixture of hydrochloric acid, demineralised water and cations eluted from the cation-exchange resin. This effluent is thus a mixture of desirable species (HCl) and undesirable species (CaCl_2 and MgCl_2).
- In practice, ion-exchange is typically a final polishing step in a series of purification steps. Much of the cation load entering the brine circuit will thus have been removed by this stage and the cation load associated with the effluent is therefore not large. Clearly, with some hydrochloric acid being present in the effluent, there is a certain inherent value associated with this effluent. Conceivably, the effluent could be used in the hydrochloric acid dosing of the brine in the electrolyser process module. The question is however raised as to whether the cost associated with the removal of an additional load of cations from the circuit is offset by the savings accrued from the recovery of HCl.

The above possibilities were included in the connectivity matrix of the chemical production subsystem.

The caustic evaporation plant process module

This module had two demands and four sources associated with it. The demands corresponded to the inlets for caustic soda to the first and second effects, while two of the

sources corresponded to the concentrated caustic soda produced by the first and second effects. The remaining sources corresponded to the steam condensate produced by the first effect and the process condensate removed from the caustic soda during the evaporation process. The steam required by the first effect was assumed to be proportional to the caustic soda throughput.

Two terminal storage sinks were included in the superstructure to accept any concentrated caustic soda from either the first or second effect of the caustic evaporator. Both of these sinks had an appropriate cost factor associated with them which provided an incentive for caustic soda to be sent to these sinks as opposed to the effluent sink.

The hydrochloric acid synthesis process module

The raw materials used in the production of hydrochloric acid are hydrogen gas, chlorine gas and demineralised water. As there were no other acceptable sources of raw materials present in the complex except those currently used, the hydrochloric acid synthesis plant was not considered in the optimisation. The hydrochloric acid product was however available for use in the rest of the complex.

The hydrogen chloride scrubber associated with the elimination of gaseous hydrogen chloride released from the hydrochloric acid product storage vessels was however represented in the module. This scrubber had a single caustic soda demand and produced a single caustic soda source. With the amount of hydrochloric acid produced by the complex constant, the mass-load of gaseous hydrogen chloride entering the scrubber was considered fixed. The caustic soda effluent was available for reuse. NaOH was modelled as a desirable species at the inlet of the scrubber.

The sodium hypochlorite plant process module

Unlike the case of the hydrochloric acid synthesis plant, raw materials for the production of sodium hypochlorite could be drawn from a number of sources within the complex. The sodium hypochlorite plant was thus included in the optimisation model and was represented by a demand requiring a specific flowrate of material. Here, Cl_2 and NaOH were modelled as desirable species. The amount of waste sodium hypochlorite sent to the Hydecats destruction process module was considered fixed.

The Hydecats destruction process module

The function of this module was the destruction of the excess or off-specification sodium hypochlorite. It has a single demand associated with it and produced a single source. Waste sodium hypochlorite and steam were sent to this demand as enforced matches; dilution water was added to this mixture such that the resulting concentration of NaOCl was below the maximum permitted by the operation. Umbogintwini River water was used for this purpose in the existing network configuration. The effluent produced by the process module has a relatively high concentration of NaCl and the recovery of this effluent was a possibility. Alternatively, this effluent was routed to the effluent terminal sink.

Point sources and demands

A number of point sources and demands were present on the complex. The point sources included effluent from the chlorine filter, pump seals and condensate from a number of different sources such as the brine and catholyte heat-exchangers, intercondensators and other steam traps. With the exception of the effluent from the chlorine filter, which has a concentration of chlorine associated with it, these sources were assumed to have a quality close to that of demineralised water. While other point sources did exist, such as the effluents from plant washing, pressure testing and cylinder steaming, these effluents were considered to be either too contaminated for reuse or too difficult to recover and were not

considered in the Pinch Analysis. Point demands associated with these operations were also not considered due to variability in these demands; the quantities involved were however small. The desuperheater and the pump seals represented further point demands; these operations could only use demineralised water and were excluded from the analysis.

The chemical production subsystem objective function

The objective function for the optimisation of the chemical production subsystem may be stated verbally as follows:

The system under consideration comprises the brine circuit and its associated process modules, the caustic evaporation process module, the hydrochloric acid synthesis process module, the sodium hypochlorite synthesis process module, the Hydecats destruction process module, and a number of point sources and demands. Given different material resources, which include water, caustic soda, hydrochloric acid, raw salt, sodium carbonate and sodium bisulphite and other materials such as the flocculant and alpha-cellulose, the task is to identify an optimal network configuration which achieves the required rates of production of chlorine gas, hydrochloric acid and sodium hypochlorite at the lowest cost. This cost includes the costs associated with the replacement of the cation-exchange resin, the purchase of external sources and the disposal of wastes and effluents produced by the system.

Table 6.6 presents the results obtained from the optimisation using GAMS CONOPT.

Table 6.6 : Comparison of the water and material requirements and effluent production associated with the existing network configuration and the optimal network configuration for the chemical production subsystem.

	Unit	Existing Configuration	Optimised Configuration
Demineralised Water	[t/d]	198.09	98.64
Umbogintwini River Water	[t/d]	34.62	0
Total Water	[t/d]	232.71	98.64
Raw Salt	[t/d]	142.96	142.71
Hydrochloric Acid (31% m/m HCl)	[t/d]	7.18	6.73
Caustic Soda (32% m/m NaOH)	[t/d]	67.21	66.82
Caustic Soda (38% m/m NaOH)	[t/d]	0	0
Caustic Soda (50% m/m NaOH)	[t/d]	0	0
Sodium Carbonate	[t/d]	1.055	1.061
Sodium Bisulphite	[kg/d]	359.5	353.7
Flocculant	[kg/d]	7.77	8.03
Alpha-Cellulose	[kg/d]	31.08	29.01
Chlorine	[t/d]	14.73	14.72
Steam	[t/d]	70.80	71.67
Effluent	[t/d]	235.19	104.20
Solid Waste	[kg/d]	39.86	37.63
NaCl Load to Effluent	[t/d]	14.2	13.73
NaOH Load to Effluent	[kg/d]	39.9	84.0
Duration of Normal Cycle of Operation of Cat ion-Exchanger	[h]	72	72.56

The saving in running costs that would be obtained by implementing the optimised solution was calculated at R 730 313 per annum, (rand values for the year 2000).

The optimised solution involved 74 connections, of which 39 were new. Presenting this as a diagram would be ineffective. The most significant features of the solution were:

- The optimal network configuration shows a reduction of 58 % in the amount of water used and a reduction of 56 % in the amount of effluent produced by those elements of the subsystem included in the optimisation model.
- There are slight improvements in the consumption of raw salt, hydrochloric acid, caustic soda, sodium bisulphite, alpha-cellulose and chlorine gas. The proposed network configuration however uses more sodium carbonate, flocculant and steam.
- The salt load associated with the effluent has decreased slightly from the existing configuration but there is a slight increase in the NaOH load.
- The optimal configuration shows a slight decrease in the regeneration frequency for the ion-exchange plant.

6.2.6 The cooling circuit subsystem

The cooling circuit subsystem comprised the four cooling towers and their associated cooling circuits located on the chlor-alkali complex, that is, the Linde, Sulzer, LC and MBC cooling circuits. The Linde and Sulzer cooling circuits were associated with the liquefaction of chlorine while the LC and MBC cooling circuits met the cooling requirements associated with the use of liquefied chlorine and the brine circuit respectively. In optimising this subsystem, thermal effects were not considered and the assumption was made that the necessary cooling requirements of the complex could be met if the flowrates to the various cooling towers were maintained at their current levels.

The model subsystem comprised four modules representing each of the cooling towers and their associated cooling circuits. With the mathematical models being identical for all the cooling towers, the module is considered generally in the following discussion.

With regard to the formulation of a model to represent the operation of the cooling towers, two effects are noted. Firstly, there is the evaporation of water from the cooling tower which concentrates the dissolved species present in the water. The second effect is the absorption of carbon dioxide from the atmosphere which increases the carbonate concentration in the water. With plant data collected for the cooling circuit subsystem not being conclusive on its own, simulation was required in conjunction with this data in deriving models for the various cooling towers. Here, the assumption was made that no dissolved solids are removed by the evaporation process. The absorption of carbon dioxide from the atmosphere by the water was then approximated by the addition of a mass-load of Na_2CO_3 . This quantity was derived from the equilibrium concentration of carbonate in the water (following evaporation) in contact with the atmosphere, as determined using the aquatic speciation software package MINTEQA2 (Allison et al., 1991). It was assumed that this mass-load addition was independent of concentration in the concentration range considered by the optimisation.

The process module for each cooling tower had a single water demand and a single water source associated with it. The blowdown flows were not specified in the models, since these were determined during the course of the optimisation and subject to the inlet concentration limits of the cooling towers (which are maintained at their existing concentrations initially). With the cooling towers only using water, it was not necessary to represent all species in the model. The species included in the model was the total dissolved solids (TDS).

In considering the optimisation of the cooling circuit subsystem in isolation from the other subsystems, only the water sources presently available to the subsystem were considered in the optimisation. Any water sources currently used by the other subsystems, but not used in the optimised scenarios were considered unavailable to the cooling circuit subsystem at this stage. The objective function for the optimisation of the cooling circuit subsystem may thus be stated as follows:

The system comprises process modules representing the four cooling towers located on the chlor-alkali complex and their associated cooling circuits. Given a single external source of water, the task is to identify an optimal network configuration which is able to supply sufficient water to each of the cooling towers, subject to the associated quality constraints, at minimum cost. This cost includes the costs associated with the purchase of the water and the disposal of the blowdown effluent produced by the subsystem. Thermal effects are not considered in the optimisation.

Table 6.7 presents the comparison between the results obtained from the optimisation problem and the current operating scenario while Figure 6.11 presents the proposed network configuration for the cooling circuit subsystem.

Table 6.7 : Comparison of the water requirement and effluent production associated with the existing network configuration and the optimal network configuration for the cooling circuit subsystem.

	Unit	Existing Configuration	Optimised Configuration
Umbogintwini River Water	[t/d]	846.62	828.16
Effluent	[t/d]	128.12	109.66

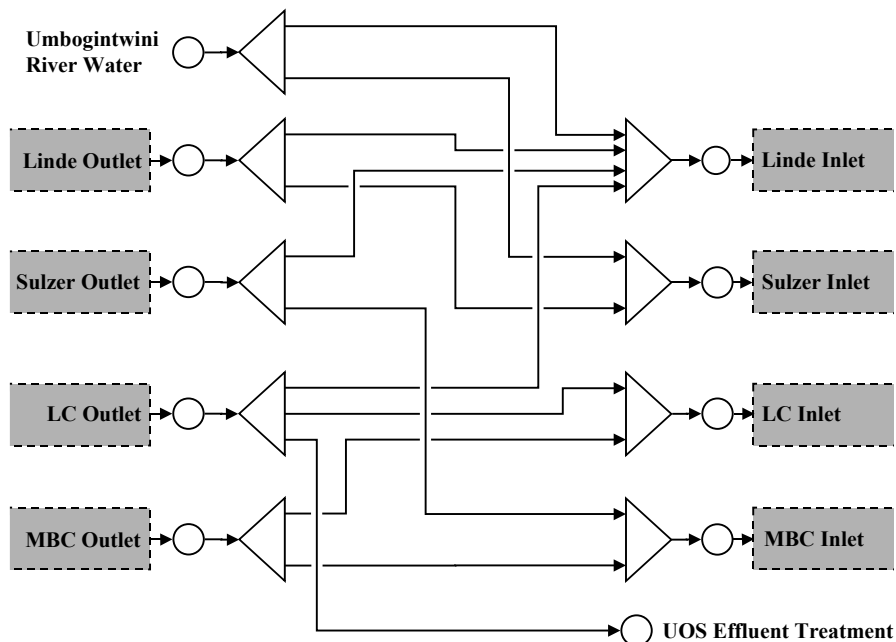


Figure 6.11 : The optimised network configuration for the cooling circuit subsystem.

6.2.7 Subsystem integration

Having considered the optimisation of the three individual subsystems in isolation from each other, attention now shifts to the integration of these subsystems. Before the strategy for integrating the subsystems is described, it is necessary to consider some of the effects arising from the optimisation of the individual subsystems.

The first of these effects relates to the decrease in demand for demineralised water by the chemical production subsystem, which means that the rate of production of demineralised water should decrease.

There were a number of good quality water sources present within the chemical production subsystem which might be more effectively used in the demineralisation plant subsystem. In the network configuration proposed by the optimisation of the chemical production subsystem in isolation from the other subsystems, these water sources were routed to the Hydecats destruction plant. It was however feasible to use Umbogintwini River water for this purpose instead, releasing the better quality water for the demineralisation plant.

The use of demineralised water in the cooling circuit subsystem has the effect of increasing the overall demand for demineralised water. This results in an increase in the regeneration frequency of the demineralisation plant. With this increase in regeneration frequency, the proportion of the total feed water to the demineralisation plant supplied by the chemical production subsystem decreases and the unit cost of the demineralised water increases once again. As such, the use of demineralised water is only economically feasible as long as the unit cost for demineralised water remains below R2.695 per ton. It is thus possible to use any additional demineralised water in the cooling circuit but only to the extent that the unit cost does not rise above the threshold value. This value is thus a significant point in the integration strategy since it marks the change in the pattern of use of the demineralised water.

One further effect of the changing regeneration frequency is that it changes the amount of caustic soda required for the regeneration of the demineralisation plant. This amount must be supplied from the chemical production subsystem. A decrease in the regeneration frequency results in a decrease in the demand for caustic soda by the demineralisation plant. This in turn results in an increased throughput of caustic soda to the caustic evaporators. More steam is required to effect the evaporation and more condensate is produced from the evaporation process. The increase in the amount of condensate in turn will affect the amount of good quality water available for export to the demineralisation plant and thus brings further change in the regeneration frequency of the demineralisation plant.

In light of these considerations, an iterative procedure is required for the integration of the subsystems. This strategy is outlined as follows:

- 1) Initially, the assumption is made that there is no export of water from the chemical production subsystem to the demineralisation plant subsystem. In addition, it is assumed that the caustic soda demand from the demineralisation plant is the same as that of the existing network configuration. The unit cost of demineralised water is similarly assumed to be the same as that associated with the existing network configuration.
- 2) From the optimisation of the demineralisation plant subsystem, the quantity of water available to the rest of the plant, the amount of caustic soda required for regeneration in producing this quantity of water and the unit cost of demineralised water are recorded.
- 3) From the optimisation of the chemical production subsystem, the daily quantity of water available for export from the chemical production subsystem and the demand for demineralised water by those elements of the subsystem included in the optimisation model are recorded. The total daily demand for demineralised water by the chemical

production subsystem is determined by incorporating the demand associated with those elements not included in the optimisation model.

- 4) Based on the chemical production subsystem's annual demand for demineralised water, the number of regeneration cycles per annum and the total cycle time for the demineralisation plant are calculated. The amount of water available for export to the demineralisation plant subsystem from the chemical production subsystem during this period is then determined.

The demineralisation plant subsystem model is updated to reflect this amount of water available from the chemical production subsystem and the model is optimised once more. As previously, the amount of caustic soda required for regeneration, the amount of demineralised water available to the rest of the plant and the unit cost of demineralised water are recorded.

- 5) Based on the results obtained from the optimisation of the demineralisation plant subsystem model, the daily demand for caustic soda is determined. The model for the chemical production subsystem is modified to reflect the updated unit cost of demineralised water and the updated caustic soda demand as derived from Step 4). From the optimisation of the chemical production subsystem, the daily quantity of water available for export and the daily demineralised water demand are recorded.
- 6) If the criteria for convergence is satisfied, the procedure stops at this point. If this criteria is not satisfied, Step 4 is repeated.

Table 6.8 presents a comparison between the annual material consumption and effluent production figures for various subsystems of the chlor-alkali complex in their existing configurations and those configurations proposed by the optimisation. These figures reflect the behaviour of the subsystems in combination with each other. The figures associated with the existing network configuration have been adjusted to reflect the performance of the various subsystems on an integrated basis. Table 6.9 combines the figures from Table 6.8 and presents a comparison between the two network configurations of the chlor-alkali complex in terms of the total consumption of materials and production of effluent.

The most notable features of these results are:

- The demineralisation plant shows a significant improvement in its performance with the decrease in the demand for demineralised water by the rest of the complex. Alongside this decrease, the frequency of regeneration decreases such that the normal cycle of operation is now 27.4 h instead of 16.6 h in the existing configuration. The unit cost associated with the demineralised water decreases from R 4.710 to R 3.193 per ton.
- A decrease in the amount of caustic soda required by the subsystem is observed compared to the demand associated with the subsystem when it is optimised in isolation from the other subsystems.
- In total, the potential economic savings associated with the proposed network configuration amount to R 945 727 per annum based on costs from the year 2000. This solution achieves a 14 % reduction in the amount of water used by the complex and a 42 % reduction in the amount of effluent generated.

Figure 6.12 presents a schematic diagram showing the interactions between the various subsystems as they exist in the proposed optimal configuration. The demineralisation plant subsystem now treats raw water and regenerates effluent from the chemical production subsystem.

Table 6.8 : Comparison of materials used and waste generated by the chlor-alkali complex in its existing network configuration and the optimal network configuration.

	Unit	Existing Configuration	Optimal Configuration	Improvement [%]
<i>Demineralisation Plant Subsystem</i>				
Umbogintwini River Water	[t/y]	55 582	58 967	-6
Umgeni Water	[t/y]	55 582	0	100
Total Water	[t/y]	111 164	58 967	47
Demineralised Water Produced	[t/y]	111 144	71 679	36
Caustic Soda (32% m/m NaOH)	[t/y]	170	94	44
Hydrochloric Acid (31% m/m HCl)	[t/y]	153	85	44
Effluent	[t/y]	9 779	3 361	66
NaCl Load in Effluent	[t/y]	85	47	45
NaOH Load in Effluent	[t/y]	0.96	0.49	49
Annual Saving* (AS1)	[R/y]	-	294 615	-
Unit Cost of Demineralised Water	[R/t]	4.710	3.193	32
Number of Regeneration Cycles	[/y]	436	282	35
Duration of Normal Operation	[h]	16.6	27.4	-
<i>Chemical Production Subsystem</i>				
Demineralised Water	[t/y]	104 308	68 507	34
Umbogintwini River Water	[t/y]	14 378	14 378	0
Total Water	[t/y]	118 686	82 885	30
Raw Salt	[t/y]	51 464	51 377	0.17
Sodium Carbonate	[t/y]	380.0	382.1	-0.54
Sodium Bisulphite	[t/y]	129.4	127.3	1.6
Caustic Soda (32% m/m NaOH)	[t/y]	24 196	23 881	1.3
Hydrochloric Acid (31% m/m HCl)	[t/y]	2 584	2 424	6.2
Chlorine	[t/y]	11 802	11 797	0.05
Hydrogen	[t/y]	260.4	260.4	0
Steam	[t/y]	25 487	25 828	-1.3
Flocculant	[kg/y]	2 797	2 890	-3.3
Alpha-Cellulose	[kg/y]	11 188	10 444	6.6
Effluent	[t/y]	86 655	39 287	55
NaCl Load in Effluent	[t/y]	5 047	4 945	2
NaOH Load in Effluent	[t/y]	14.36	30.22	-110
Solid Waste	[kg/y]	14 349	13 545	6
Annual Saving* (AS2)	[R/y]	-	584 844	-

Table 6.8 continued

	Unit	Existing Configuration	Optimal Configuration	Improvement [%]
<i>Cooling Circuit Subsystem</i>				
Umbogintwini River Water	[t/y]	304 782	298 136	2
Effluent	[t/y]	46 124	39 478	14
NaCl Load in Effluent	[t/y]	21.2	20.7	2
Annual Saving* (AS3)	[R/y]	-	66 268	-
Total Annual Saving (AS1 + AS2 + AS3)	[R/y]	-	945 727	-

This network configuration has the advantage that most of the retrofit work involves routing the effluent streams to the demineralisation plant. Once there, the piping is already in place to distribute the demineralised water to the appropriate demands.

Table 6.9 : Comparison between the total consumption of materials and waste generated across all subsystems of the chlor-alkali complex in its existing network configuration and the optimal network configuration.

	Unit	Existing Configuration	Optimal Configuration	Improvement [%]
Umbogintwini River Water	[t/y]	374 743	371 481	0.9
Umgeni Water	[t/y]	55 582	0	100
Total Water	[t/y]	430 325	371 481	14
Demineralised Water	[t/y]	104 308	68 507	34
Caustic Soda (32% m/m NaOH)	[t/y]	24 366	23 975	1.6
Hydrochloric Acid (31% m/m HCl)	[t/y]	2 737	2 509	8.3
Raw Salt	[t/y]	51 464	51 377	0.17
Sodium Carbonate	[t/y]	380.0	382.1	-0.53
Sodium Bisulphite	[t/y]	129.4	127.3	1.6
Chlorine	[t/y]	11 802	11 797	0.05
Hydrogen	[t/y]	260.4	260.4	0
Steam	[t/y]	25 487	25 828	-1.2
Flocculant	[kg/y]	2 797	2 890	-3.3
Alpha-Cellulose	[kg/y]	11 188	10 444	6.6
Effluent	[t/y]	142 557	82 126	42
NaCl Load in Effluent	[t/y]	5 153	5 013	2.7
NaOH Load in Effluent	[t/y]	15.3	30.7	-100
Solid Waste	[kg/y]	14 349	13 545	5.6
Annual Saving	[R/y]	-	945 727	-

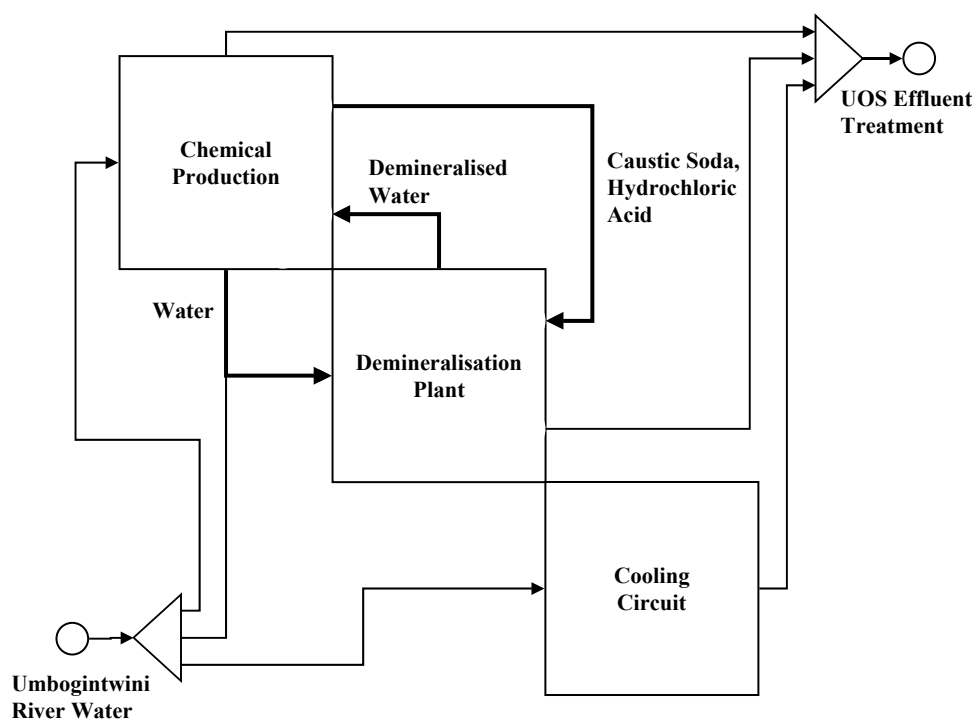


Figure 6.12 : Schematic diagram showing the distribution of water and collection of effluent from the subsystems of the chlor-alkali complex in its proposed optimal configuration.

6.3 Discussion and conclusions

This study represented the most comprehensive attempt to provide a thorough theoretical and practical treatment of the *process water pinch analysis* problem. The issue of utility water pinch analysis vs. process water pinch analysis was one which was encountered in some form in all the case studies undertaken during this project and WRC Project K5/851 that preceded it. It seems that, at least in the context of a water-poor country like South Africa, that the limitation to considering only utility water is a significant restriction. Clearly the extended theory is more complex and requires much more effort to apply. The individual process modules have to be individually crafted, and require much more insight and modelling skill than those which have been found adequate for utility water pinch analysis. The risks of making changes which will adversely affect the process involved are also greater.

Some perspective on these issues can be obtained from a utility water pinch analysis of the same chlor-alkali system carried out using the Linnhoff-March WaterPinch software, based on the same input data. A comparison between the results of the (utility) water pinch analysis results and the combined water and materials pinch analysis are shown in table 6.10.

The Water Pinch Analysis study was able to realise 57% of the total saving achieved by Combined Water and Materials Pinch Analysis. In terms of water abstraction and effluent generation, relatively small changes are observed between these two studies with the Combined Water and Materials Pinch Analysis achieving a further 3 % reduction in the total amount of water used and an additional 10 % reduction in terms of the amount of effluent generated. It is however in the area of chemical recovery and reuse where Combined Water and Materials Pinch Analysis outperforms Water Pinch Analysis and much of the additional cost saving is attributable to this.

Table 6.10 : *Comparison of potential savings achieved by Utility Water Pinch Analysis and Combined Water and Materials Pinch Analysis*

	Water Pinch Analysis [%]	Combined Water and Materials Pinch Analysis [%]
Umbogintwini River Water	7	0.9
Umgeni Water	42	100
Total Water	11	14
Demineralised Water	34	34
Caustic Soda (32% m/m NaOH)	0.2	1.6
Hydrochloric Acid (31% m/m HCl)	1.9	8.3
Raw Salt	0	0.17
Sodium Carbonate	0	-0.53
Sodium Bisulphite	0	1.6
Chlorine	0	0.05
Hydrogen	0	0
Steam	0	-1.2
Flocculant	0	-3.3
Alpha-Cellulose	0	6.6
Effluent	32	42
Solid Waste	0	5.6
Annual Saving [R/y]	542 881	945 727

7 TECHNOLOGY TRANSFER

The main thrusts of this project were technology evaluation and technology transfer. Water pinch analysis appeared in the literature as a technique that held much promise in the South African context, and the project sought to test it on South African processes, and promote its use by South African industries. Any theoretical aspects arose purely in response to problems encountered along the way. The chief *modus operandi* was to promote the water pinch concept to industries, and wherever possible to recruit engineering personnel from the companies involved to enrol for part-time MScEng degrees, undertaking water pinch analysis studies in their factories. Some more conventional academic projects involving full-time MScEng students and one PhD have served to generate theoretical support for situations where the current techniques were not completely adequate. In all cases the projects were centred on industrial case studies.

7.1 Industry based part time MScEng projects

The success of Thokozani Majozi's project at Sanachem, which was undertaken during the preceding water pinch project and presented in WRC report 851/01/03, prompted us to adopt the idea of enrolling process engineers who wanted to further their technical studies as part time postgraduate students on studies based at their own factories. The concept was that the project should be related to their normal work, and should be of interest to the company, to minimise conflicting priorities between work and study time. Four projects of this kind were started : Gladys Naylor (née Crampton) at Mondi Merebank, Maryna Mansfield at Sappi Tugela, Eric Slabbert at Sappi Ngodwana and Annelie Lourens at Sasol Secunda.

The concept appeared to work well at first, with good support from the companies involved. However, it seems that the 2 to 3 year time scale for a part time MScEng is significantly longer than the interest span of many companies. In most cases the priorities of the companies changed with time, and when the projects did not yield quick results, the students/engineers came under pressure to devote their attention to different areas which were considered to be more urgent or important than improving water efficiency. At the time of compiling this report, only Gladys Naylor had completed, and, as was noted in chapter 4, she did so in spite of the fact that company had by then completely lost interest in water efficiency, because of the way its supply contract with the Durban Water Recycling Scheme had been structured.

Clearly this is not a satisfactory state of affairs, and the concept needs to be rethought for the future. However it was successful in making the companies aware of water pinch analysis and exposing them to some of its practicalities. The work done by Maryna Mansfield at Sappi Tugela did lead to a paper presented at the WISA 2002 conference in Durban, and indeed all that remains to be done is the preparation of the thesis, which is progressing gradually. The work of Annelie Lourens at Natref also led to a paper at the same conference, however her emigration from South Africa probably ended any prospect of completing the project.

A significant later outcome was that, after completing his PhD, Paolo Gianadda was employed by Sappi in an R&D position dealing with optimisation of their operations, which includes the application of pinch analysis.

7.2 Workshops and courses

A pre-conference workshop for WISA delegates was also held at the University of Natal on the 19th of May, entitled *Water Pinch Analysis: A tool for the rational management of water and effluent in an industrial complex*. It was attended by 14 persons. A similar workshop was held at the University of Cape Town as part of WISA 2004. This was presented by Chris Brouckaert and Duncan Fraser, and attended by 10 persons.

At WISA 2002 there was a WRC sponsored workshop on *Tools for Cleaner Production*, in which a presentation was made on *Water Pinch Analysis as a Transparent Tool for the Co-regulation of Industrial Processes* (BROUCKAERT, C.J., SCHNEIDER, J., MANSFIELD, M. and BUCKLEY, C.A.). This forum gave the project and the technique very important exposure.

7.3 Conference presentations

The following paper was presented at *The International Water Association Conference on Water and Wastewater Management for Developing Countries*, Putra World Trade Centre, Kuala Lumpur, Malaysia, 29-31 October 2001, and subsequently accepted for publication in *Water Science and Technology*.

GIANADDA, P., BROUCKAERT, C.J., SAYER, R and BUCKLEY, C.A., The Application of Pinch Analysis to Water, Regent and Effluent Management in a Chlor-Alkali Facility

at the *Water Institute of Southern Africa Biennial WISA Conference and Exhibition*, Durban, 19-23 May 2002, the following posters and presentations were made:

LOURENS, A., The Application of Water Pinch at a Petrochemical Industry (Paper)

GIANADDA, P., BROUCKAERT, C.J., SAYER, R. and BUCKLEY, C.A., Process Water Pinch Analysis Guides Water, Reagent and Effluent Management in the Chlor-alkali Industry (Paper).

BROUCKAERT, C.J., SCHNEIDER, J., MANSFIELD, M. and BUCKLEY, C.A., Water Pinch Analysis as a Transparent Tool for the Co-regulation of Industrial Processes (Poster).

The last topic was also used as a presentation as part of a WRC sponsored workshop on Tools for Cleaner Production. This forum gave the project and the technique very important exposure.

At the *International Seminar on Advanced Achievements in Pinch Technology and Industrial Resource Management for Energy Savings, Pollution Reduction and Sustainable Development in Africa*, University of Durban-Westville, Durban, 18 - 20 November 2002 the following presentations were made:

BUCKLEY, C.A., BROUCKAERT, C.J., MANSFIELD, M. And GIANADDA, P. , Applying Water Pinch Analysis in the South African Context

GIANADDA, P., BROUCKAERT, C.J. And BUCKLEY, C.A., Conceptual Developments in the Field of Water Pinch Analysis - Selected Case Studies from the Chlor-Alkali

MANSFIELD, M., BROUCKAERT, C.J. And BUCKLEY, C.A., Water Pinch Analysis at the Sappi Tugela Paper Mill.

BROUCKAERT, C.J., BUCKLEY, C.A., HANEKOM, D.* and WOODHOUSE, C.*, Optimal Location of a Membrane Treatment Plant in a Power Station

At the *South African Chemical Engineering Congress, Chemical Engineers Competing in the Global Economy*, Sun City, South Africa, 3-5 September 2003

GIANADDA, P., BROUCKAERT, C.J. AND BUCKLEY, C.A., The Application of Combined Water and Materials Pinch Analysis to a Chlor-alkali Plant, (Paper)

GIANADDA, P., BROUCKAERT, C.J. And BUCKLEY, C.A., The Optimisation of an Ion-exchange Demineralisation Plant Using Combined Water and Materials and Pinch Analysis (Poster)

At the Waste Management Emissions & Recycling in the Metallurgical and Chemical Process Industries Conference, Mintek Conference Centre, Randburg, Gauteng, South Africa, 18-19 March 2004 :

BROUCKAERT, C.J., GIANADDA, P. and BUCKLEY, C.A., Process Integration for Water and Energy Management (Paper)

7.4 Publication

GIANADDA, P., BROUCKAERT, C.J., SAYER, R. and BUCKLEY, C.A., The Application of Pinch Analysis to Water, Regent and Effluent Management in a Chlor-Alkali Facility, *Water Science & Technology*, 46 (9), pp. 21-28, October 2002, ISBN 1843394286.

8 CONCLUSIONS AND RECOMMENDATIONS

In addition to the individual conclusions pertaining to each case study, which appear in the relevant chapters, the range and scope of the case studies undertaken during the project allows some broad conclusions to be drawn about water pinch analysis as a technique.

8.1 An assessment of the status of water pinch analysis theory and practice

Pinch analysis, whether applied to energy or water, is a special case of the more general technique of process optimisation. In most cases the problem of fully optimising all aspects of a process is so large that it is impractical to tackle as a whole. The strategy commonly adopted is to break up the full optimisation problem into a set of more manageable sub-problems which can be solved independently; pinch analysis seeks to address one of these sub-problems. It considers the optimisation of the utility systems in the process - either the thermal utility system or the water utility system.

As part of such a strategy, boundaries have to be set for each of the sub-problems. For instance, the usual assumption adopted in a pinch analysis is that, for the purpose of optimising the utility system, the process units are considered to be invariant. In terms of the overall optimisation problem, such boundary conditions are artificial, and involve approximations and assumptions concerning the behaviour of the parts of the system *outside the sub-problem boundary* which are excluded from the optimisation of the sub-problem (the division of the chlor-alkali complex into subsystem discussed in section 6.3.5 is also an example of this kind of strategy). The success of the strategy depends critically on how well these assumptions and approximations apply to the system under consideration.

The experience of the case studies undertaken in this project has been repeatedly that the standard assumptions of pinch analysis are somewhat restrictive. The continuous pressure to conserve water in South Africa means that many industries have already introduced measures to use water more efficiently, so the easy savings reported in the literature are often not available, and it becomes necessary to venture into more difficult areas to make further progress.

8.1.1 What pinch analysis promises

Pinch analysis was originally developed for the design of energy utility systems (Linnhoff and Hindmarsh, 1983). One of the more important features of pinch analysis is its ability to target minimum utility requirements for any process. Such *targets* may be set without the need for detailed design. (Hall and Linnhoff, 1994). The design of the utility can therefore be undertaken in two stages: determining the targets, for which only physical data are required, followed by detailed design, where all the other factors, such as economics, safety and operability must be taken into account.

Apart from its direct role in facilitating the optimal design of the utility system, this characteristic of pinch analysis provides a means for setting the boundary to separate the optimisation of the process units from the optimisation of the utility system. Since the utility target values are a function of the process units, and are easily and rapidly evaluated, they can be used to provide an approximate representation of the optimal utility design which is good enough to use in the comparative assessment of process design options.

So far the discussion has implicitly referred to the design of a new process. Pinch analysis methods have also been developed for redesigning a utility system to improve efficiency: the so-called *retrofit* situation. (Smith, 2000). Here the process design units are in place, and

would not be expected to change. What pinch analysis offers in this case are the targets which show how much improvement in efficiency can possibly be achieved by the redesign, and the design rules which allow one to pinpoint where structural inefficiencies exist in the current design, and so where to focus effort and investment to the best advantage.

8.1.2 Theoretical limitations encountered

The resounding success of numerous applications of energy pinch analysis suggests that its underlying assumptions work well in practice; the more limited success of water pinch analysis suggests that its assumptions are not as useful in many cases. Part of the reason for this is that water pinch analysis is based on an analogy between water and energy which is not exact. The behaviour of energy in a stream is represented in the analysis by two variables, the energy flow (kW) and the energy quality, that is its temperature. The boundaries to the optimisation problem are defined by the energy flows required by the process, together with the temperatures at which these flows are required; for the purpose of the energy utility subsystem optimisation, these requirements are considered to be fixed. For water pinch analysis, a similar structure is used to define the optimisation problem, with the key variables being contaminant loads (kg/s) in the water streams, and water quality represented by contaminant concentrations. The first problem with the analogy is that, while the quality of energy is uniquely represented by temperature, the quality of water is an altogether more complex and less well-defined concept. The second problem is that the boundary assumptions in terms of fixed contaminant loads and concentrations are less often appropriate in practice.

In energy pinch analysis, the formalism allows one to identify a *thermodynamic limit* (Smith, 2000) to energy recovery, which is independent of any economic considerations related to the energy utility system. Optimising the system can thus be handled in two steps: the first identifies the thermodynamic limit, and then the second examines how close one can get to this limit economically. It is this clear separation of the physical and economic effects that has contributed greatly to the conceptual appeal and practical acceptance of the technique.

When it comes to water pinch analysis, the lack of rigour in the thermodynamic analogy means that the equivalent of thermodynamic limit does not really exist independently of economic factors. The crucial issue is that of *quality regeneration*. In the case of energy, quality is regenerated by means of a heat pump, which is driven by an input of energy, and so can be analysed on the same thermodynamic basis as the rest of the system. In the case of water, quality is regenerated essentially by the input of energy (including chemical energy), which cannot be represented in terms of contaminant load and concentration. Reductions in the use of fresh water have to be balanced against the use of energy and/or chemicals in treating used water, and economic considerations are the usual means for determining the relative weighting of such disparate physical inputs. *Thus, the separation of physical and economic effects in the analysis is not possible, unless quality regeneration is excluded as a design option.*

This brings into question the nature of the “pinch” itself. In the energy pinch analysis the pinch is a limiting temperature, and in the simplest form of water pinch analysis it is a limiting concentration, but this depends on interpreting the limit in terms of the thermodynamic analogy. In response to the problem of water quality being a function of multiple contaminant concentrations rather than a single variable, the Linnhoff-March WaterPinch software, that features in chapters 2, 4 and 5 of this report, uses the sensitivities or *marginal costs* of the concentration limits to take the place of the pinch, however in chapter 5 it was demonstrated that these do not suffice, and that flow rate constraints also need to be considered. This leads to a concept of the pinch as *the set of all constraints which are active at the optimum*. (Active constraints are those for which the relevant variables are at

their limiting values). Unfortunately this does not have the elegance and intuitive appeal of the original pinch concept. Furthermore, the utility target values that it provides do not have the certainty associated with the original pinch concept, because they depend on what factors were included in the pinch analysis model.

When considering the question of the boundary assumptions for the subsystems to be analysed, the considerations are fundamentally similar for both energy and water pinch analysis. The *utility stream / process stream* distinction, as discussed in chapter 6, has an equally relevant counterpart in thermal pinch analysis. However, it does seem that in practice precluding process changes in the optimisation is more limiting in the case of water, perhaps because water is used for such diverse purposes.

The effect of these three issues (having to include economic effects early in the analysis; the consequent absence of a purely physical pinch limit; and the pressure to include process streams in the optimisation) is that water pinch analysis tends towards full process optimisation, which dilutes its status as a separate discipline. From a practical viewpoint, this means that the one cannot accept the general procedures and conclusions of the standard pinch analysis theory, and that each application needs to be evaluated on its particular merits.

It must be acknowledged that the above conclusions mostly reflect the experience of applying the analysis in the retrofit mode: i.e.. to improving water utilisation in existing, well established processes. In the case of a new design where process conditions have not yet been fixed, it may well be that the assumptions and approximations involved in the standard version of pinch analysis would be quite justified in view of the uncertainties about what the process conditions will be.

8.1.3 Practical strategies for applying water pinch analysis

How can water pinch analysis be applied so as to circumvent its theoretical limitations and realise its promise as far as possible? The case studies presented in this report suggest that there is no single answer to the question, and that an approach must be formulated according to the nature of the process involved.

The case study of **Ceres Fruit Juices** (chapter 3) demonstrated the most straightforward application of water pinch analysis, as the process conformed most closely to the classical assumptions of pinch analysis. The water involved is used for utility purposes of equipment washing and sterilisation and cooling (although some water is blended into the products, this could easily be excluded from the analysis). No wastewater treatment for quality regeneration was practised or contemplated. Total solids was considered as the single contaminant representing water quality.

From this example the first strategy for applying water pinch analysis can be formulated as:

- i) include only utility water streams in the analysis;
- ii) use a single, non-reactive contaminant to represent water quality.
- iii) exclude water treatment for the purpose of making it fit for reuse (treating the water to meet discharge standards may be considered);

This strategy avoids all the theoretical difficulties noted above, and allows one to use the classical pinch analysis methodology. This comes at the potential expense of the accuracy in locating the true optimum for the system design. Each option may be evaluated for its possible effect:

- i) Since this is a food process, risk factors would tend to preclude water reuse in any streams which come into direct contact with the product, so excluding process streams from the analysis is advisable in any case.

- ii) The use of a single contaminant could make the predicted water savings over optimistic, in that specific contaminants might prevent the reuse of water for specific purposes. This issue was noted in the case study, with the caution that the results should be seen as a first assessment, with such issues requiring further investigation. The justification for using a single contaminant is not really theoretical, as the methods for using multiple contaminants are readily available, it is more about the effort and expense of gathering the necessary data.

The case studies of the **AECI Bioproducts Lysine Plant** and the **Mondi Merebank Paper Mill** (chapters 4 and 5) illustrate a second possible strategy. These also considered only utility water, excluding process from the analysis, however they deviated from the simple strategy in several respects, thereby requiring the use of mathematical programming software. These deviations were:

- i) Excluding certain connections between specific sources and specific sinks. This is not the same as excluding a source or a sink: the source and sink involved remain in the analysis, and a constraint is added to the optimisation problem which is of a different kind to the concentration constraints in the standard pinch analysis.
- ii) The objective function was not simply the amount of fresh water supplied, but included costs of water supply and effluent discharge. Although neither of these case studies happened to involve regeneration for reuse, these factors had the same effect of moving away from considering the thermodynamic minimum for water use.
- iii) In the case of the lysine plant, multiple contaminants were considered.

These examples can be taken as representing the second strategy for approaching a water pinch analysis, in which mathematical programming is used to address all the restrictions except the exclusion of process streams and chemically reactive species. These exclusions allow the system to be modelled in terms of simple standardised elements, which makes it possible to use a generalised software package, such as WaterTarget used in these two studies.

The final case study of the **Sasol Polymers Chlor-alkali Plant** (chapter 6) accepted none of the restrictions noted above. While this resulted in the most rigorous approach to the problem, it was also the most complex and time consuming. In particular for process water containing reacting species, individual models of each process unit had to be developed which adequately represented process constraints and economics, which means that the development of a generalised software solution is much more difficult. It could be argued that this approach is no longer really pinch analysis, but borders on full process optimisation.

Although the three approaches were applied to different case studies in this project, the above argument suggests that they could be used sequentially as a progressive overall approach in a single project, in which one only moves to the next level of complexity if the results of the simpler analysis indicate that it is justified.

8.1.4 Other considerations

There are some observations concerning the application of water pinch analysis that are not related to its theoretical structure:

- 1) The direct economic drivers for water conservation are not as great as those for energy conservation, so industries are not as easily motivated to undertake water pinch analysis as energy pinch analysis.
- 2) In water-scarce situations, not uncommon in South Africa, there are indirect drivers related to the value chain of water, i.e.. the economic value derived from activities which could not take place without a sufficient supply of water of adequate quality.

- 3) In such situations regulators have the responsibility of balancing the water requirements of different users in an equitable way. The systematic and transparent methodology of water pinch analysis could be useful for establishing the water requirements of industrial systems for regulatory purposes. It must be emphasised that, in its present form, it is unlikely to be useful for non-industrial systems.

8.2 Recommendations

Recommendations that can be made fall into two categories: those that concern the application of water pinch analysis according to the current state of the art, and those that concern in what directions further development of water pinch is needed .

8.2.1 The application of water pinch analysis

- 1) A water pinch analysis of a system needs to be approached with a very clear understanding of the conceptual basis of the technique, its underlying assumptions, its range of applicability and its limitations.
- 2) Water pinch analysis is essential a *design tool*; it is useful for deciding how a water using system should be configured, or perhaps reconfigured. It does not have a useful role in managing the operation of a water using system.
- 3) As the case studies of this report demonstrate, pinch analysis encompasses a range of variants of the technique, each with a different set of modelling assumptions, and a different set of strengths and weaknesses. Care should be taken to select the most appropriate variant for a particular system, and a particular purpose. All the variants have been developed for application to industrial systems, and are intended to optimise the use of water in an industrial context. Any attempt to use it in a different context (for instance, in an environmental context) should be approached with great care to evaluate the appropriateness of its underlying assumptions.
- 4) A pinch analysis of a system is usually an iterative process with much uncertainty in the early iterations. It seems logical to start with the simplest form of the analysis, in spite of the sweeping assumptions involved; and bring in more sophisticated considerations as they are shown to be required.

8.2.2 The further development of water pinch analysis

- 1) Further efforts are required to encourage wider acceptance of water pinch analysis by South African industry. This should be undertaken in conjunction with industry on a case study basis.
- 2) Further work is needed to extend the water pinch analysis methodology to account for chemically reacting solutes and aqueous reagents.
- 3) Techniques for the early identification of the applicability of water pinch need to be further developed.
- 4) Techniques need to be developed to reduce the time and effort required to gather the data needed for a water pinch analysis.
- 5) The use of water pinch analysis as a tool for co-regulation should be explored. This will require studies in which regulatory authorities are involved as partners, and the development of a protocol for reporting the modelling assumptions and process limits used in an analysis in a transparent and auditable way, so that it can be used with confidence in negotiations between industrial and regulatory parties.
- 6) Local consultants should be encouraged to set up a water pinch analysis service to industry.

- 7) The energy efficiency of a process has a significant impact on its water use for cooling and the concomitant generation of saline effluents. The simultaneous optimisation of water and energy use is therefore an important direction for further investigation.

9 REFERENCES

- Allison, J.D., Brown, D.S. and Novo-Gradac, K.J. (1991) MINTEQA2/PRODEFA2, A geochemical assessment model for environmental systems: Version 3.0 User's Manual. (<http://www.epa.gov/ceampubl/mmedia/minteq/usermanu.pdf>.)
- Alva-Argaez, A., Kokossis, A. C., Smith, R. (1998) Process Integration for Wastewater Treatment Systems. *1998 AIChE Annual Meeting*. Miami Beach, Florida.
- Alva-Argaez, A., Kokossis, A. C., Smith, R.(1998b) Wastewater minimisation of industrial systems using an integrated approach. *Computers & Chemical Engineering* **22** Suppl. S741-S744.
- Alva-Argaez, A., (1999) Integrated Design of Water Systems, Thesis: Manchester Institute of Science and Technology: Manchester.
- Amidpour, M. and Polley, G.T. (1997) Application of problem decomposition in process integration. *Trans IChemE* **75** (A1) 53-63.
- Bagajewicz, M. and Savelski, M. (2001) On the use of linear models for the design of water utilization systems in process plants with a single contaminant. *Trans IChemE*, **79** Part A 600-610.
- Benkő N, Rev E and Fonyo Z (2000) The use of nonlinear programming to optimal water allocation. *Chem Engng Comm* **178** 67-101.
- Buehner, F. W., Rossiter A. P. (1996). Minimize waste by process design. *Chem. Tech*, (April): 64 - 72.
- Brooke. A., Kendrick D., Meeraus. A. and Raman R. (1998) GAMS A user's guide., GAMS Development Corporation, (<http://www.gams.com/docs/gams/GAMSUsersGuide.pdf>.)
- Brouckaert, C.J. And Buckley, C.A. (2003), The application of pinch analysis for the rational management of water and effluent in an industrial complex., *WRC Report No. 851/1/03*, Water Research Commission, Pretoria.
- Dericks, B.J., Savelski, M.J., Koppol, A.P.R. and Bagajewicz, M.J. (2001) Feasibility of zero-liquid discharge solutions in the process industry. *Proceedings of the 4th Conference on Process Integration, Modeling, and Optimisation for Energy Saving and Pollution Prevention* (PRES'01), Florence, Italy 7-12.
- Doyle, S.J. and Smith, R. (1997). Targeting Water Reuse with Multiple Contaminants. *Trans IChemE*, **75**, Part B, 181-189.
- El-Halwagi, M.M. (1995), Introduction to Numerical Optimization Approaches to Pollution Prevention, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor., McGraw-Hill: New York. 199-207.
- El-Halwagi, M. M. (1997). *Pollution Prevention through Process Integration. Systematic Design Tools*, Academic Press, San Diego.
- GAMS Development Corporation (2001) GAMS - The Solver Manuals. GAMS Development Corporation. (http://www.gams.com/docs/solver_man.pdf).
- Gardner, G.A., (2000) Liquid Waste Minimisation on a Chloro-alkali Complex, *MScEng Thesis*, University of Natal.

- Hall, S.G. and Linnhoff, B., (1994), Targeting for Furnace Systems Using Pinch Analysis, *Ind. Eng. Chem. Res.* **33** 3187-3195
- Hsiao, T. and Glatz, C.E., (1996) Water Reuse in the L-Lysine Fermentation Process. *Biotechnology and Bioengineering*, **49**(3) 341-347.
- Linnhoff, B., Hindmarsh, E. (1983). The pinch design method of heat exchanger networks. *Chem Eng Sci*, **38**(5) 745-763.
- Mann, J.G. and Liu, Y.A. (1999) Industrial water reuse and wastewater minimisation. McGraw Hill.
- Smith, R. (1995), Wastewater Minimisation, in *Waste Minimisation Through Process Design*, A.P. Rossiter, Editor. , McGraw-Hill: New York. 93-107.
- Smith, R. (2000), State of the art in process integration, *Applied Thermal Engineering* **20** 1337-1345
- Takama, N., Kuriyama, T., Shiroko, K., Umeda, T. (1980). Optimal water allocation in a petroleum refinery. *Comput. Chem. Eng.*, **4**: 251-258.
- Wang, Y. P., Smith, R., (1994). Wastewater Minimisation. *Chem Eng Sci.*, **49**(7): 981-1006.