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Innovative strategies to optimise water resources

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SUMMARY

1 Introduction

The focus on the rationalisation of the industrial consumption of energy and water has become central worldwide in the academic, governmental and industrial debate over the last 30 years.

Global population increase, development of emerging countries towards western standards and global warming due to climate change are challenges which force humanity to pursue and put in practice more sustainable production patterns consistent with the increasing demand of products without irreversibly damaging the environment.

According to the “World Water Development Report 2014” [1] (issued by the United Nations), freshwater withdrawals have tripled over the last 50 years.

Worldwide approximately 70% of freshwater is employed for cultivation, 20% for industry and 10% for domestic use. However, in industrialised nations, this balance is entirely different because manufacturing consumes more than 50% of available resources. For example, nowadays in Belgium, 80% of available freshwater is used for industrial purposes.

Demand for freshwater is globally growing by 64 billion cubic meters per year [2].

- Every year, the world’s population augment of roughly 80 million people [3].
- Mutations in lifestyles and consumption habits in recent years require more water consumption per capita.
- The sharp increase in biofuels production which occurred in recent years also had a significant impact on water demand. Among 1,000 to 4,000 litres of water are required to produce a single litre of biofuel [2].
- Energy (conventional and renewable) demand is accelerating with additional implications on water demand.

Water and energy are strictly interconnected and highly interdependent. Choices made and actions taken in one domain can significantly affect the other, positively or negatively.

Water is essential throughout the production, transportation and use of energy, which, in turn, affects the water cycle.

This concept which is known as “water-energy nexus” is nowadays the most shared approach applied to evaluate the general impact of improvement actions regarding energy and water management.

The same UN report [1] states that “*Global water demand (regarding water withdrawals) is projected to increase by some 55% by 2050, mainly because of growing demands from manufacturing (400%), thermal electricity generation (140%) and domestic use (130%)”.* Furthermore, *“Global Energy demand is expected to grow by more than one-third over the period to 2035, with China, India and the Middle Eastern countries accounting for about 60% of the increase. Electricity demand is expected to grow by approximately 70% by 2035. This growth will be almost entirely in non-Organisation for Economic Co-operation and Development countries, with India and China accounting for more than half that growth*”.

Water scarcity will become more and more critical worldwide, and the increasing energy demand involved by the industrialisation of developing countries will provide a substantial contribution to this phenomena.

Notwithstanding this, the industry does not make particular efforts to reduce the consumption of freshwater, mainly for the low profitability of water optimisation projects, but also for practical issues that industrial operators may face when pursuing the water optimisation goal in existing factories not originally designed with this target in mind.

However, this attitude might change in the short term either for economic or environmental issues: even in areas not yet characterised by water scarcity, new policies related to climate change and sustainability will probably drive the industrial operators to pay more attention to the management of freshwater resources and to start projects aimed to reduce its consumption.

This research aims to contribute to this framework highlighting the issues that might occur while applying the water consumption optimisation tools and techniques to actual industrial cases and suggesting practical strategies to overcome them.

In general, it is possible to pursue the goal of freshwater optimisation by applying various strategies and techniques, and the proper methodology depends on the nature of the industrial complex, on production targets and on the phase in which the study is carried out (new design or retrofit).

In principle, a water optimisation study should cover various aspects to reach its goals, whose relevance depends on the particular structure of the considered system.

- Identification and reconciliation of process data applying innovative algorithms, also able to manage heteroscedasticity and censored data (retrofit projects).
- Preliminary process stream configuration study (new design and retrofit) aimed to assess freshwater demand for different purity grades.
- Techno-economic evaluation – based on preliminary study results – aimed to deepen the alternative treatment strategies of the water streams undergoing regeneration (new design and retrofit).
- Sensitivity analysis aimed to highlight significant interventions with higher priority (retrofit projects).
- Rigorous mathematical modelling of the identified water and steam streams arrangement and the regeneration process units aimed to highlight the optimal treatment configuration (new design and retrofit).

1.1 State of the Art and Literature Review

The rationalisation of freshwater supply to industrial complexes involves the integration of different methodologies useful to:

- assess the actual flow rates of auxiliary and primary process streams,
- determine freshwater consumption target and saving potential,
- identify the optimal arrangement and plant topology in case of complex processing schemes,
- quantify the economic impact of the selected arrangement.

Various techniques and methodologies focused on these goals have been developed during the last decades of the previous century and are continuously improved.

The increasing computation capability and availability of plant data has driven the continuous evolution of these methodologies because these factors enabled their application to new problems of increasing complexity.

To contextualise the reader, the paragraphs of this section deepen the state of the art of the research areas which are meaningful for this study: Data validation and reconciliation, Pinch techniques and Optimisation Methods.

1.1.1 Data validation and reconciliation

The measurements of the process variables of chemical plants (flow rates, temperatures, pressures, levels, analytical tests and compositions) are subject to errors which can be either random or systematic: by consequence, the acquired plant dataset typically does not obey the laws of conservation of mass and energy.

Random errors are typically small and are due to the normal fluctuations of the process and instruments operation.

Systematic errors may be due to multiple reasons like departures from the steady-state operation, instrument failure, miscalibration, process leaks, poor sampling as well as clerical errors and may result in significant deviations from the actual value of the variable. Even though the last (also called gross errors) occur only occasionally and in small number compared to the number of instruments, they are the most dangerous ones because, if not correctly identified and handled, can bring to wrong conclusions concerning the actual behaviour of the monitored system.

The proper technical and economical monitoring of a plant, from effective control to business management, implies the knowledge of its actual state avoiding the distortions due to measurement errors.

Figure 1 lists the exercises requiring the application of plant information, the involved decisional processes and the time scale related to each activity level.

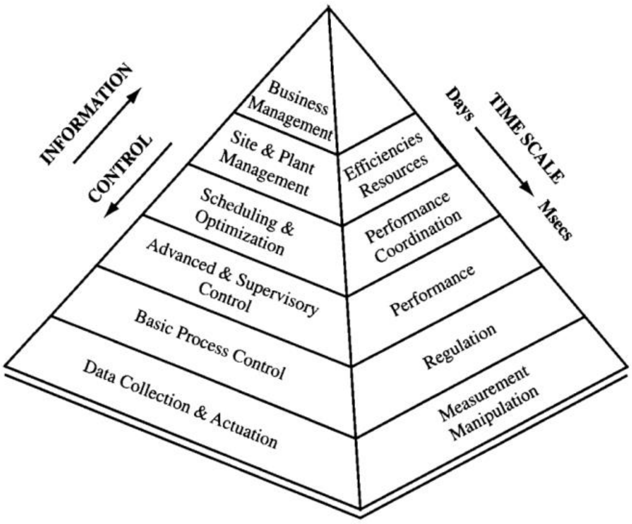


Figure 1 – Activity pyramid in a processing plant (from Busk, 1993) [12]

Modern plant data acquisition and management systems (DCS) permits the collection and storage of a considerable volume of data with sampling frequencies which can be extremely variable (from day to milliseconds).

Even though the implementation of these systems have dramatically increased the potential monitoring and control capabilities, the availability of this significant amount of data does not automatically mean knowledge, both because of the difficulty implied by monitoring thousands of variables at the same time and because of measurement errors which may lead to wrong conclusions.

It is fundamental to transform all this data into the information required to understand the actual state of the unit and to support the decisional processes involved with its management.

Data validation and reconciliation techniques (DVR) are aimed at highlighting gross errors and at adjusting the values of the relevant measurements to make them consistent with the conservation laws of mass and energy. Unfortunately, the presence of gross errors profoundly affects the results of this exercise. Thus gross errors must be identified and either corrected or discarded before running the data reconciliation process.

The aim of these techniques consists in elaborating the collected data to validate it and improve its accuracy.

References [11] and [12], list and describe the meaningful contributions to the development of these techniques starting from the sixties.

Data reconciliation is a constrained minimisation problem where the variables are the actual measurements the constraints are the balances related to the conservation laws of mass and energy (or other bounds required to handle the problem), and the Objective Function is a quadratic form of the adjustments to the measured values.

The constraints may be linear (in simple cases) but are generally non-linear; thus proper optimisation algorithms must be applied to identify the solution.

Various strategies have been proposed and used to treat the following circumstances:

- Gross errors identification with the support of statistical tests.

- Management of unmeasured flows distinguishing between those which can be infered with other measurements through the constraints (“observable” flows) and those which cannot (“unobservable” flows).
- Use of redundant data and the related statistical properties.
- Management of variations due to process variability (related to non-Steady State Conditions).

In this work, we started applying the methodology outlined by Crowe et al. [13] which foresees the direct elimination of unmeasured values in linear constraints before running the reconciliation process.

The method foresees:

- The preliminary identification and elimination of unmeasured variables from the reconciliation problem.
- The adjustment of the remaining flow rates by setting the mass conservation constraints and minimising the squared weighted of the corrections
- The estimation of the unmeasured flowrates through the application of the mass balance constraint around each node of the network.

The elimination of the unmeasured variables makes it possible to minimise the computational effort because it reduces the set of balance equations foreseen by the problem.

To reach this goal, Crowe proposed to build a Projection Matrix which is applied to blank out the unmeasured quantities automatically and produce a reduced set of balances.

The method foresees to include the statistical properties of the measured flow rates and concentrations (variance-covariance matrices) in the objective function of the minimisation algorithm so to put a higher penalty on deviations of variables that are measured more accurately.

The presence of gross errors affect the results of the method and should be previously identified and eliminated: it is possible to retrieve in literature various contributions proposing the application of some statistical tests to this purpose.

In principle, being random deviations, measurements should produce normally distributed residuals from the balances, but this does not always happen in case of gross errors which have the power of corrupting the results of the reconciliation process.

Almasy and Urhin analysed the “gross errors” concept and produced a list of the main deviation causes [14]:

- Malfunctioning instruments
- Measurement biases
- Model mismatches
- Process Leaks
- Departure from Steady State

Following their analysis, they concluded that gross errors are also random but on a different timescale. Various authors proposed the application of different tests like the Chi-square, Hotelling T^2 or Fisher F-test and also derived specific checks for this purpose like the Maximum Power (MP) and Generalized Likelihood Ratios (GLR) tests, while others introduced the concept of gross errors directly into the objective function. However, as in the case of data reconciliation, a fundamental prerequisite for the application of Gross Error Detection strategies is the availability of redundant measurements which increases the power of the statistical test.

1.1.2 Pinch Analysis

The academic world started to develop methods aimed at rationalising the use of energy during the late seventies, concurrently with the sudden increase in the price of fossil fuels. After the second world war, the western industry had been developed and rebuilt without caring much of the cost of energy which at that time was considerably lower than the price of equipment. The change of the relative value of energy and equipment (i.e. the increased the importance of OPEX against CAPEX) triggered the research for alternative design methods with a view to improving the energy efficiency of industrial facilities through the maximisation of the internal recovery of process heat.

One of the most practical tools that resulted in this field is the “Pinch Analysis”, which was initially developed to improve the efficient use of energy of industrial processes and whose concept was later on extended also to water (WPA), hydrogen (HPA) and more recently to carbon emissions (CEPA) [6] rationalisation.

Pinch analysis is nowadays a known and well-proven method in each of the following industry sectors:

- Oil refining
- Petrochemicals
- Chemicals
- Food & drink
- Pulp & paper
- Steel & metallurgy

This methodology analyses a commodity (typically energy, water or hydrogen), regarding quality (e.g. temperature level or purity) and quantity, assuming that the related cost will depend on both.

In general, a process consumes high-value utilities and rejects low-value utilities. Typically expensive fuels are burnt to provide the system with high-temperature heat while low-temperature heat is rejected through cooling equipment.

In the case of water, pure streams are fed to the process for various uses while contaminated effluents are treated to be compatible with environmental constraints.

Pinch analysis follows these sequential steps:

- Identification of process supplies and demands (sources and sinks) for the analysed commodity.
- Research on the optimal solution (minimising wastes) through the suitable matching of sources and sinks.
- Assessment of the matches suitability based on quality criteria (e.g. temperature or purity).
- Estimation of the investment cost associated with the optimal solution.

In general, the efficiency of a resource transfer depends intrinsically on the related entropy change: few heat transfers between sources and sinks with a high-temperature difference may reduce the overall heat recovery and are less efficient than more heat transfers with a low-temperature difference.

However, the optimal solution regarding transfer efficiency seldom involves the lowest investment cost: typically inefficient transfers require lower investments (e.g. heat transfer characterised by the high difference between hot and cold streams' temperatures requires less heat exchanging surface).

The first level of the analysis consists in the construction of the "composite curves" which are a graphical representation (quality vs quantity) of the cumulated contribution of all the supply and demand requirements of the analysed commodity.

In the case of energy, this representation graphs the temperature level of the hot and cold streams available for heat exchange (quality) versus the amount of exchanged heat.

Instead in the case of water, the composite curves graph the concentration of the meaningful contaminants (quality) versus the amount of water consumed by the process.

The cumulated curves are built summing the contributions of the various sources and sinks in the same quality range and are represented jointly in the same space (Figure 2). References [4], [5] detail the methodology applied to build these curves for the different types of application.

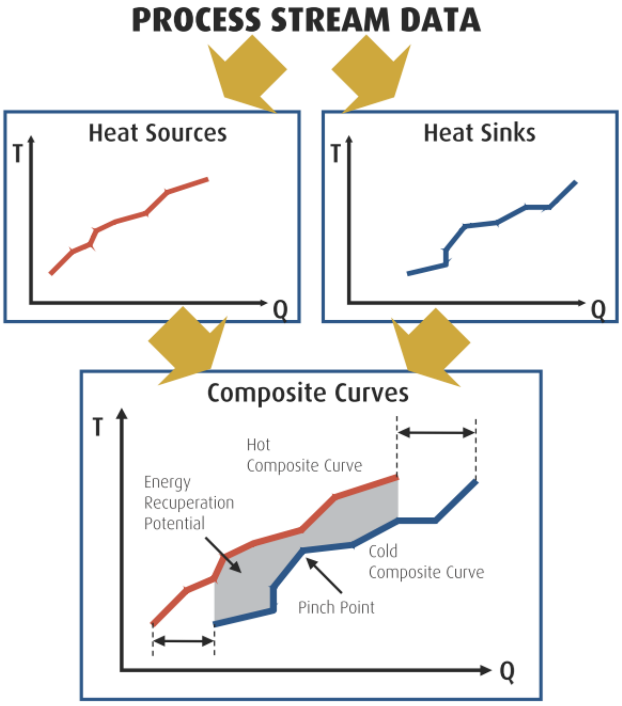


Figure 2 - Example of composite curves [4]

The overlap of the two curves quantifies the amount of commodity which can be recovered within the process while the non-overlapped zones quantify the external contributions needed (for example fuel for heaters or cooling). The goal is to identify a process configuration able to maximise the curve overlap considering at the same time the related equipment investment.

This kind of representation provide us with information about the process:

- The sink curve summarises the amount of utility required by the process at different quality levels (for example temperature, purity or concentration).
- The source curve summarises the amount of the same utility which is to be removed.
- The relative shift of the curves in the direction of the quantity axis results in the change of the extension of the overlapped zone and, consequently, in the variation of the amount of utility imported and disposed outside the process (Figure 3).
- The pinch point is the minimal quality difference between the two curves, and its level is a compromise (identified by the optimisation algorithm) between the utility recovery efficiency of the process and the relevant investment costs.
- The quality difference between source curve and sink curve at the pinch point is called, in the case of energy optimisation studies, approaching temperature

(ΔT_{min}) and its value (the lower, the better) provides an idea of the energetic efficiency of the process.

- The source curve must forcibly always be above the sink curve (because curves crossing would involve quality transfer with negative driving force). By consequence, the condition with pinch point equal to zero (with contact between the curves) permits to quantify the minimum theoretical amount of high-quality utility which the process requires as well as the minimum amount of low-quality utility to dispose of outside the process.

In practice, a heat transfer network characterised by pinch point with approaching temperature (ΔT_{min}) equal to zero is not possible, because it would require an infinite heat exchanging surface area, but it is possible to find standard data [7] based on experience detailing the typical ΔT_{min} values obtainable for various industries and processes.

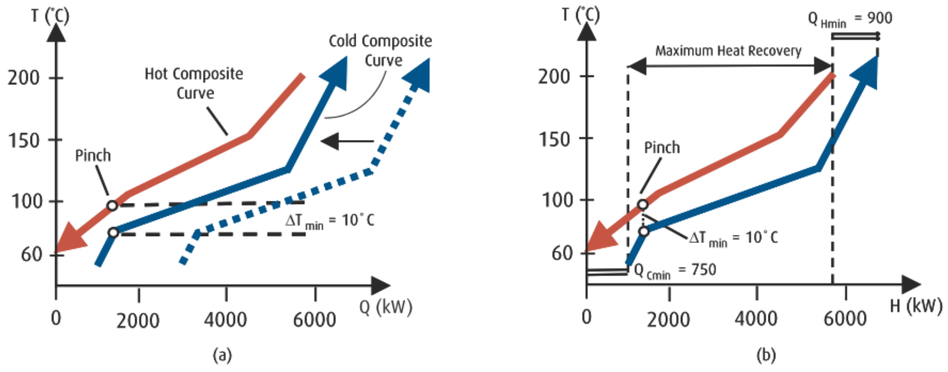


Figure 3 - Shifting curves to define the process energy target [4]

Since the initial applications of this concept in the early seventies, pinch analysis has developed, and its techniques improved. It provides tools enabling to investigate the energy streams within the process, and to highlight the most economical ways of maximising heat recovery and of reducing the external utility consumption (e.g., fuel, steam and cooling water). The methodology may be used to identify energy-saving projects within a process.

The ideal time to apply this technique is during the planning of process modifications that will require significant investments, and before the finalisation of process design. Indeed this technique enables to identify the most efficient equipment arrangement before running the rigorous thermodynamic calculations required by process design (for equipment sizing and heat and material balance definition).

In the case of new plant design, the application of this methodology produces the maximum improvements in efficiency, along with reduced expenditures since during this phase it is possible to evaluate many plant-layouts and overcome process constraints.

It is possible to apply also this concept in the case of a retrofit, but the existing equipment constrains the optimisation potential since in this case, it is necessary to find a trade-off between investments and utility saving.

These rationalisation concepts are nowadays mature, and engineering companies progressively integrate them into the standard practices applied to design new industrial complexes.

Many international Energy Agencies [4] strongly recommend these methodologies and more and more frequently list them among the mandatory requirements of process design tenders.

Compared to other innovations the technological transfer of these concepts to the industrial world was quite fast mainly because of the high economic returns involved.

The increased cost of energy resources as well as the concurrent availability of governmental incentives supporting the reduction of the environmental footprint of industrial processes characterised by high energy consumption resulted into minimal payback periods for many energy conservation projects and accelerated the integration of these technologies and concepts into Engineering companies’ best practices.

Furthermore, the increasing availability of process information (provided by modern data control systems) and of data elaboration techniques (simulation and reconciliation technologies) is another favourable environmental condition to the application of these technologies because of the enhanced the measurement capability as well as of the reliability of the calculations aimed to predict the actual utility savings.

Since its introduction Pinch Methodologies had an increasing number of applications in many different fields. Klemeš [8] published in 2018 an extensive review of the development of this methodology in various technological areas and industrial sectors; essential applications have been realised in the following areas:

- *Process Heat Integration*: optimisation of heat management within the same process unit
- *Total site Heat Integration*: optimisation of heat management between different process units of the same site
- *Heat Exchanger Network Retrofit*: improvement of the performance of an existing Heat Exchanger Network through the identification of the optimal arrangement.
- *Batch Transient and Semi-Continuous Integration*: application to batch and semi-continuous processes where the demand for heat supply and process flow depends on time.
- *Exergy Pinch*: synergic application of Pinch concept and Exergetic analysis.
- *Renewable Energy and Waste Heat Integration*: use of Pinch Methodology to study the optimal integration of renewable energy (e.g. Solar thermal, geothermal) in industry or to valorise waste heat.
- *Macro Energy Systems Planning*: application of Pinch Methodology for the Planning of macro-areas (like Regions or Countries) to fit the energy demand reducing at the same time Green House Gases Emissions.
- *Water Integration*: water demand minimisation, widely deepened in the next paragraph.
- *Production and Resource Planning*: application of the Pinch Principle to supply chains to optimise resource planning minimising inventory levels.

Emerging fields of application are:

- *Hydrogen Pinch*: use of Pinch Methodologies to optimise the Hydrogen Management inside industrial complexes. Even though Hydrogen Pinch Technology was introduced in 1999, these methodologies have not yet fully exploited notwithstanding the potential possibility to provide an overall overview of hydrogen reach streams flows and system limitations.
- *Power (Electricity) Integration*: extension of the Pinch Concept to power systems analysis, useful to determine the minimal requirement of power from external resources and the amount of storage required to manage with power production excess.

- *Water-Energy Integration*: Pinch Analysis applications aimed at considering in the same context both water consumption and heat integration, being these two aspects deeply interconnected.
- *Desalination*: application of Pinch Methodology to improve the design of Desalination Plants so to highlight solutions involving lower energy costs.
- *Emergy*: Pinch Analysis applications considering in the same context Energy recovery and environmental concerns. Emergy analysis applies PM to quantify on energy basis the value of ecosystems goods and services.
- *Financial Investment Planning*: the Pinch Principle is in this case applied to financial planning, comparing the cumulated Net Present Value versus cumulated investment.

1.1.3 Water pinch analysis

The pinch analysis method was first applied to address the problem of water management and rationalisation around mid-nineties by Wang and Smith [9]. Thus this application was conceived about 20 years later compared to the energy case.

Since the mid-eighties, there has been a change in attitudes toward the environmental impact of industrial operations: governments have introduced new legislation to improve the water footprint and established regulatory authorities with increased powers to enforce compliance.

Reducing waste has become one of the most significant challenges facing process industries, and since wastewater is one of the industry's major waste products, the ability to reclaim wastewater for reuse is an essential step toward overall waste reduction.

Water pinch is a systematic technique for analysing water networks and identifying projects to increase the efficient use of water in industrial processes.

Advanced applications make use of advanced software tools permitting to highlight and optimise the water network maximising water reuse, foreseeing partial regeneration (partial treatment of process water that allows its reuse), and effluent treatment opportunities.

Reference [5] (p.301) summarises the most relevant commercial tools available to date.

Since the seminal work of Wang and Smith [9], researchers developed various tools and methods allowing to examine the freshwater requirements of an industrial system and to quantify the Maximum Water Recovery (MWR) potential.

Researches developed mainly two approaches to state WPA problems: Fixed Load (mostly studied in the nineties) and Fixed Flow Rate (more recent applications) [19]:

- *Fixed Load problems*: water is primarily used as a mass separating agent to remove a specific impurity load from the rich stream. Typical examples are vessel cleaning, solvent extraction and gas absorption. The main concern is the impurity load removal from the rich stream, while water flow rate requirement of the process is a secondary concern and depends on contaminants removal goals. This approach best fits the cases where water loss and gain are negligible the inlet/outlet flow rates of the process are assumed to be uniform.

- *Fixed Flow Rate problems*: this approach addresses the question from the water sink and source perspective. Within the process, water consumption (Sinks) and production (Sources) points are classified and handled with various methods to minimise global consumption and waste discharge. Rather than focusing on impurity load removal, the flow rate is the primary constraint in the system. Inlet/outlet flow rates of the water-using processes may not be uniform, which is different from that of the fixed load problems.

Likewise the case of Energy Pinch, various tools have been proposed to define water recovery targets [5]:

- *Limiting Composite Curves*: [9] this tool foresees to represent process water requirements by plotting contaminant concentration vs removal load (Δm) diagram. Figure 4 shows an example. This graphical method permits to estimate MWR targets quickly and can be applied both for Fixed Load and or Fixed Flow Rate problems even though it requires some further elaboration to account for the Loss and Gains characteristic of the second ones.

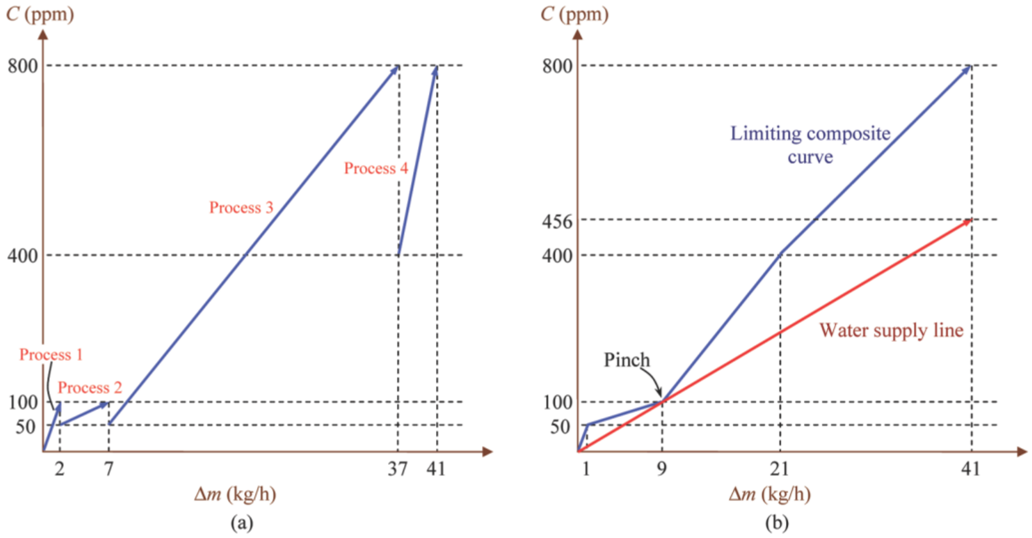
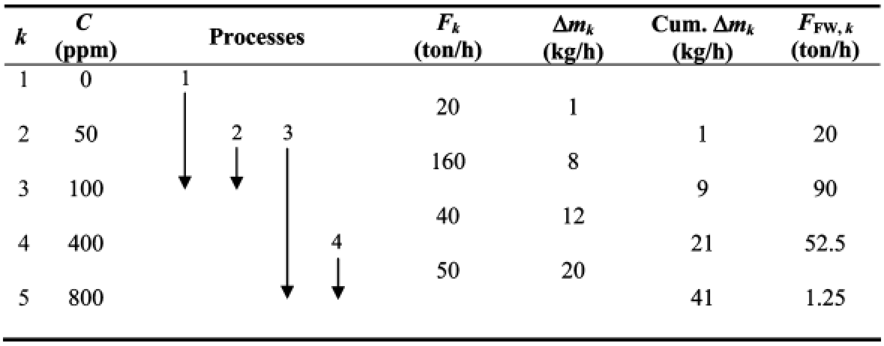


Figure 4 – Construction of Limiting Composite Curves [19]

- *Mass Problem Table*: [19] it is an algebraic targeting tool (introduced for Fixed Load Problems but adaptable also to Fixed Flow Rate Problems). It foresees the construction of a table (see Figure 5) reporting concentration levels in ascending order and the related demand (flow-rate) cumulated for the various processes in the following columns so to calculate the cumulative load (Cum.Δm_k) at each concentration level and finally the interval freshwater flow rate ($F_{FW,k}$).



k	C (ppm)	Processes	F_k (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)	$F_{FW,k}$ (ton/h)
1	0	1				
			20	1		
2	50	2 3			1	20
			160	8		
3	100				9	90
			40	12		
4	400	4			21	52.5
			50	20		
5	800				41	1.25

Figure 5 – Mass Problem Table Example [19]

- *Water-Source and Water-Sink Composite*: [19] this tool, developed for fixed Flow-Rate problems foresees to plot Sources and Sinks concentration levels (Y-axis) versus cumulative flowrate (X-axis) producing two step-curves. The Sink Composite (blue curve in Figure 6) is horizontally shifted to be entirely at the right side of the Source composite curve. This tool enables to identify the pinch (the contact point of the two curves) and to quantify the flow rate of freshwater (F_{FW}) and wastewater (F_{WW}), but these values are not absolute since this representation cannot highlight the potential flow rates reductions resulting from the mixing of the various sources. For example, Figure 6 (b) highlights the flow rates reductions obtainable through the mixing of SR2, SR3 and SR5.

SK$_j$				SR$_i$			
j	unit	F_j (ton/h)	C_j (ppm)	i	unit	F_i (ton/h)	C_i (ppm)
1	reactor	80	100	1	reactor	20	1000
2	cyclone	50	200	2	cyclone	50	700
3	filtration	10	0	3	filtration	40	100
4	steam system	10	0	4	steam system	10	10
5	cooling system	15	10	5	cooling system	5	100

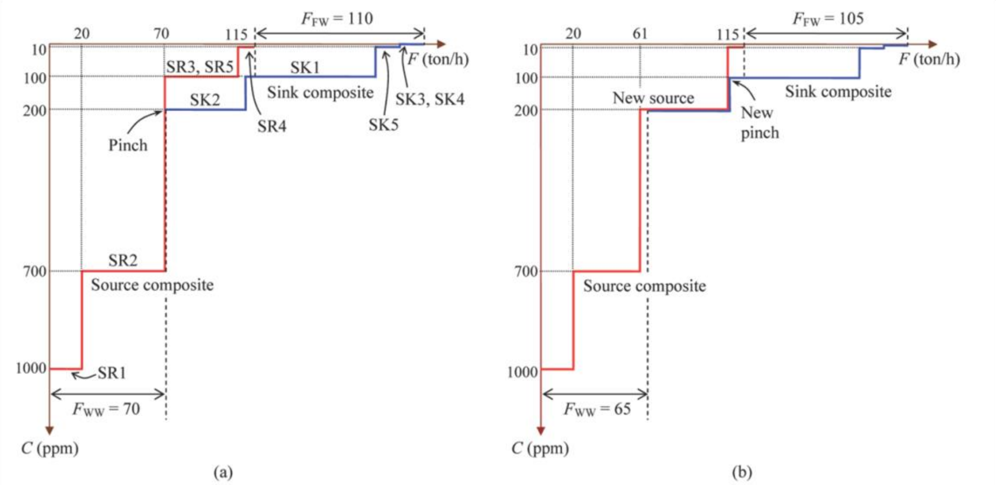


Figure 6 – Water-Source and Water-Sink Composite Diagram [19]

- *Water Surplus diagram*: [19] this tool, enables to identify the minimum water requirement but involves an iterative mechanism. The water surplus diagram reports the contaminant load excess available (Δm, X-Axis) in correspondence of different concentration levels (Y-Axis) (Figure 7 b). Reported Δm values depend on the surface difference between Source and Sink Composite Curves (Figure 7 a). Source Composite Curve is built assuming a given flow rate of freshwater F_{FW} which is iteratively adjusted to reach only positive values of Δm in the Water Surplus Diagram.

SK_j	F_j (ton/h)	C_j (ppm)	SR_i	F_i (ton/h)	C_i (ppm)
SK1	50	20	SR1	50	50
SK2	100	50	SR2	100	100
SK3	80	100	SR3	70	150
SK4	70	200	SR4	60	250

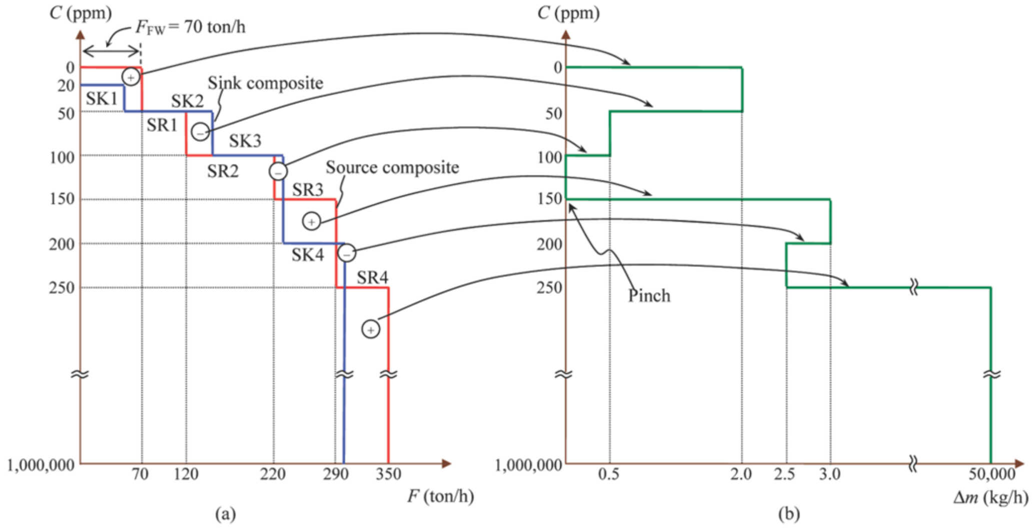


Figure 7 – Water-Surplus Diagram [19]

- *Material recovery Pinch diagram*: [19] this tool is not iterative and includes the simultaneous analysis of water flow rate and impurity load. This tool foresees plotting Sink and source composite curves on a cumulative impurity load (Δm) versus cumulative water flow rate diagram, arranging the slopes of the individual segments that correspond to the sink/source impurity concentrations in ascending order (Figure 8). The resulting Source composite curve is shifted in the X-Axis direction until it touches the sink composite curve (at the pinch point), with the source composite curve being below and to the right of the sink composite curve. This method allows targeting for single, multiple pure or impure fresh water feed: Figure 8b shows the impact of freshwater impurity

SK_j	F_j (ton/h)	C_j (ppm)	SR_i	F_i (ton/h)	C_i (ppm)
SK1	50	20	SR1	50	50
SK2	100	50	SR2	100	100
SK3	80	100	SR3	70	150
SK4	70	200	SR4	60	250

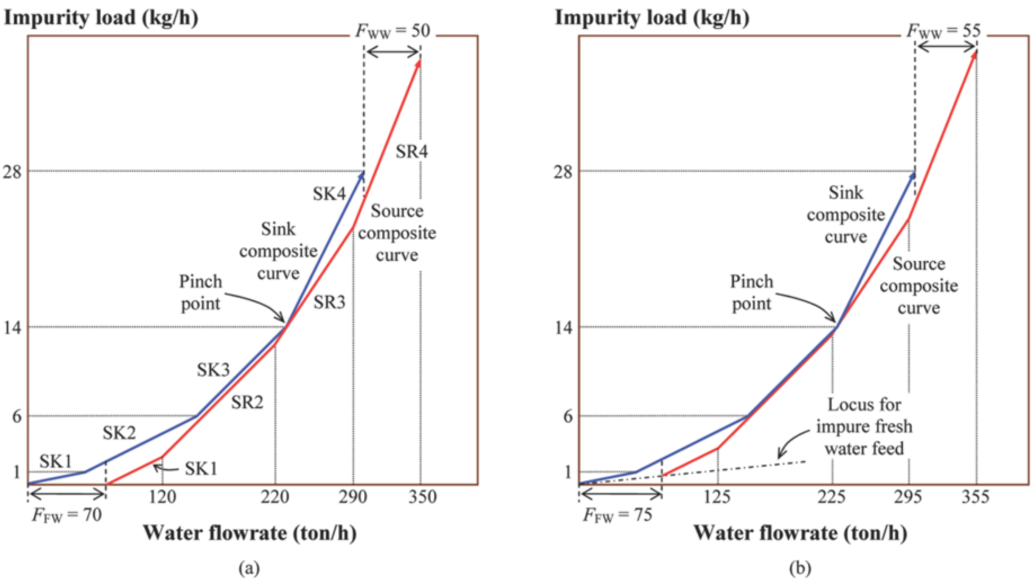


Figure 8 – Material recovery Pinch Diagram [19]

Water Cascade Analysis: [19] this technique was developed to overcome the iterative procedure in the water surplus diagram and is summarised by the table shown in Figure 9.

SK_j	F_j (ton/h)	C_j (ppm)	SR_i	F_i (ton/h)	C_i (ppm)
SK1	50	20	SR1	50	50
SK2	100	50	SR2	100	100
SK3	80	100	SR3	70	150
SK4	70	200	SR4	60	250

k	C_k (ppm)	$\Sigma_j F_j$ (ton/h)	$\Sigma_i F_i$ (ton/h)	$\Sigma_i F_i - \Sigma_j F_j$ (ton/h)	$F_{C,k}$ (ton/h)	Δm_k (kg/h)	cum Δm_k (kg/h)
					$\mathbf{F_{FW} = 70}$		
1	0						
					70	1.4	
2	20	50		−50			1.4
					20	0.6	
3	50	100	50	−50			2.0
					−30	−1.5	
4	100	80	100	20			0.5
					−10	−0.5	
5	150		70	70			**0.0** **(PINCH)**
					60	3.0	
6	200	70		−70			3.0
					−10	−0.5	
7	250		60	60			2.5
					$\mathbf{F_{WW} = 50}$	49987.5	
8	1000000						49990.0

Figure 9 – Water Cascade Table [19]

The most critical driver for performing a water pinch study is reducing flows to the wastewater treatment plant and avoiding capital expenditures in new plants.

During a water pinch study in an industrial facility, several types of water reuse solutions, with or without water treatment, are successively investigated:

- The initial step consists of the assessment of freshwater requirement under the assumption that the present contaminant inlet concentration of all site processes/equipment is the maximum acceptable (concentration of water sinks resulting from data extraction phase). This analysis indicates the minimum water usage under currently imposed constraints on inlet concentrations. This stage typically highlights low-cost opportunities involving only pipework modifications but generally results in a few water reuse opportunities.
- A further step foresees a sensitivity analysis aimed at highlighting more massive water savings by increasing the upper concentration limits to selected sinks. The challenge consists in identifying the maximum acceptable level of contamination for each unit operation. Discussions between plant operators and engineers are essential to evaluate the risk of quality or corrosion problems. Projects carried out to this stage permit to define the big part of water network modifications. These projects mainly involve simple piping modifications, but will generally lead to significant water savings.
- After evaluating reuse options, it is then possible to determine the potential offered by the many different combinations of regeneration and reuse projects. These projects consist of partially treating some process water streams before their reuse, and involve an analysis aimed at the identification of the critical streams for possible treatment in a regeneration process. The study can evaluate both existing and new water treatment units with the goal of reducing overall water consumption. Projects identified at this stage will involve capital expenditure for localised treatment steps.
- The final step consists in the evaluation of distributed effluent treatment options. Instead of mixing all waste streams and sending them to a single treatment unit, it might be more efficient to segregate streams in function of the contained contaminants and treat them appropriately before mixing with other streams. In this way, several small-scale treatment units will operate on undiluted effluent streams, rather than one single treatment unit operating on very dilute effluent, thus improving the overall efficiency.

Unlike the energy case savings in freshwater and wastewater are unlikely, on their own, to justify the cost of carrying out a detailed water pinch study and implementing the recommended projects, and this resulted in a slower integration of these concepts into the standard industrial design procedures, particularly in the case of retrofit projects focused on existing facilities.

Furthermore, the water networks slaved to existing and not recently built industrial complexes, typically dispose only of the minimal instrumentation required by the operation, and the measurements of most of the water streams flow are not available. This lack of information hampers the execution of retrofit projects starting from the data extraction phase [5] when it is fundamental to assess with good reliability the freshwater grades and flow rates supplied to process units and to treatment facilities in the actual state.

However, this tendency is not uniform for all cases: there are some industrial sectors (for example pulp and paper) involving relevant freshwater consumption and regional areas characterised by water scarcity (for example middle east) which have seen the flourishing of various project and applications aimed to the optimisation of this resource.

In the past, in most of the industrialised world, freshwater was assumed to be a limitless and low-cost commodity, and engineers have designed water systems on this assumption, with no particular attention to treatment efficiency and reuse or recycling options.

This attitude is now changing driven by the awareness that, because of climate change and the industrialisation of developing countries, water resource is not unlimited. There are countries in the world where water scarcity hampers the industrial development or where the actual cost of freshwater is, in absolute terms, higher or comparable to the cost of energy: in our perspective, the availability of practical methodologies permitting to optimise the management of water resource will become more and more critical in the next decades.

1.1.4 Optimisation methods

Water pinch methodologies are very powerful because, after extracting the required information, enable to dispose very quickly of a comprehensive insight of the water saving potential of a given system. The main drawback is that these methodologies work well with single contaminant problems but are difficultly applicable if the analysis is focused on multi contaminant systems.

As an alternative or as a complement to pinch analysis, mathematical programming methods, based on a water network superstructure including all feasible options, can be used: the first who introduced this approach was Takama in 1980 [16] who applied this methodology to identify the optimal water allocation of a Refinery. In this work, they developed an optimisation model including structural variables (indicating the effective use of water treatment options) and split ratios (if dividing in more than two streams), aimed at identifying the network configuration which, given refinery process conditions, minimises the total operative cost.

Various authors extended the use of these methods to different industrial cases including wastewater minimisation (Wang and Smith in 1994) [9], heat recovery optimisation (Varbanov et al. in 2004) [17] and total site analysis (Čuček et al. in 2014) [18].

Extensive reviews on the optimisation of water resources published between 2009 and 2012 are available and describe in detail the applications in this field. Foo (2009) reviewed the state-of-the-art of Pinch Analysis techniques for water network synthesis [19], Jeżowski (2010) produced a review of water network design methods [21], Klemeš (2012) summarised the current opinion in chemical engineering concerning the recycle/reuse of industrial water.

In the section describing the Optimisation-based methods, Jeżowski [21] lists the difficulties associated with the general solution of this problem and suggests various strategies to address them.

As discussed by Biegler, Grossmann, and Westerberg (1997), the optimum design can be identified using an optimisation algorithm capable of dealing with suitable nonlinear, generally nonconvex objective functions and constraints including both continuous and discrete variables. The latter corresponds to binary variables which specify the presence/absence of the option associated with the variable in the superstructure, as well as variables that are intrinsically integer, such as the number of units of a particular operation.

The resulting model is a MINLP optimisation problem, for whose solution the most frequently used algorithm is BARON, proposed in 2005 by Tawarmalani and Sahinidis [35] and available in GAMS environment [36], which can provide the global optimum solution of the network.

In the food industry, there is generally a double use of water. Water streams can be (and typically are) part of the usual utility system but are frequently also incorporated in the products. Thus, in this specific case there arise additional difficulties compared to the case in which water is only a system utility because the amount of contaminants transferred from process streams to the water streams is subject to a double constraint: the quality of products and wastewater concentration which may need regenerating before being discharged.

A typical application which is addressed with mathematical programming is the identification of the optimal arrangement of Reverse Osmosis Networks, which is an example of Process Synthesis.

Given the quality of the feed, treatment goals, type of membrane modules and operative constraints it is possible to identify alternative arrangements (with different number of permeate treatment steps, retentate treatment stages, recycles and mixes) with different investment and operating costs and, due to characteristics of the problem, it is not straightforward to identify the optimal solution.

Although various works aimed at addressing this problem through mathematical programming techniques are available in the literature, a universally recognised approach is not yet available to generalise RON process synthesis problems.

Evangelista [37], proposed a short-cut method for the design of Reverse Osmosis Desalination Plants. This method provides straightforward formulas for the mathematical model useful for the direct estimation of permeate yield and quality depending on pressure drop across the module, osmotic pressure and feed flow rate.

The RON optimisation problem is usually formalised through "superstructures" inclusive of all the different alternative combinations (see example in figure [39]); within the mathematical model, with binary or integer variables representing the possible alternative configurations.

The result is a mixed integer, non-linear (MINLP) problem which typically is not convex.

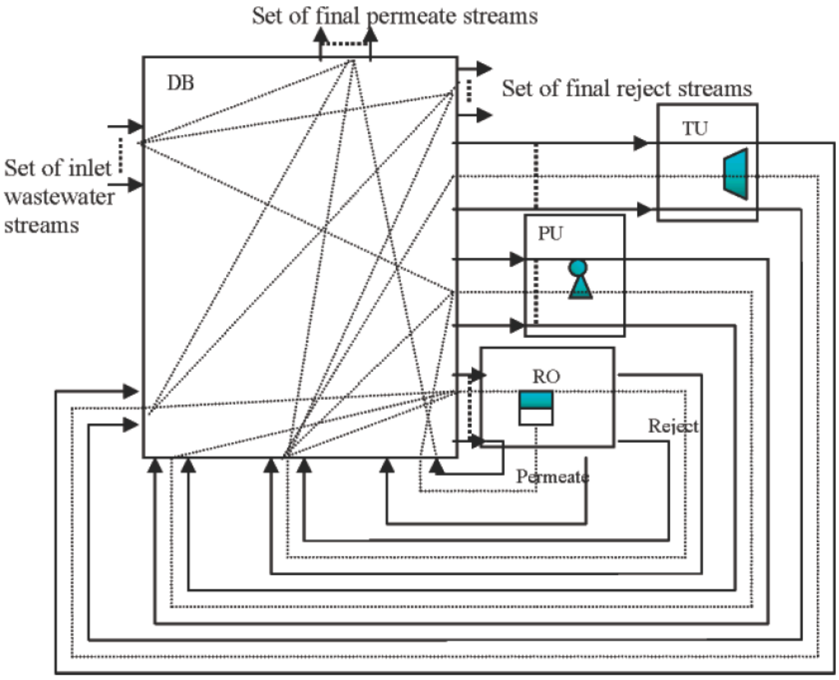


Figure 10 – Superstructure representation of a RON layout [39].

This approach was firstly introduced in this field by El Halwagi [38] who proposed an adequate superstructure for the RON problem. This idea was then further deepened and extended in subsequent works.

More recently Saif [39] describes the methodology applied to formalise the RON problem for a desalination unit through a superstructure and indicates the strategies put in practice to find the optimal solution (convex relaxation, and tightening of various constraints) and the optimisation algorithm applied for its resolution (spatial branch and bound).

A similar approach is also presented by Kohr [40] who presented the application of a superstructure model aimed to represent the reverse osmosis network (RON) for water regeneration for an operating oil refinery in Malaysia.

However, most of the numerical examples reported in these works refer to quite simple configurations whose representation requires a limited number of variables, while industrial practice often needs to confront and manage more complex problems.

The identification of the optimal RON arrangement through a superstructure requires the concurrent management of:

- integer variables (representing the number of modules contained in each stage),
- binary/combinatory variables (modelling weather some treatment sections are considered or not),
- continue variables (modelling streams flow rates, concentrations and operative conditions),
- operative goals and constraints (which during the optimisation run can be fixed or variable depending on the related configuration),
- the objective function (usually economic representing the investment and operation cost associated with each configuration).

The objective function has a discrete and multimodal trend (due to the concurrent existence of combinatorial and integer variables and of non-linear constraints) and the problem is “non-convex”.

Therefore, it is necessary to use algorithms able to manage this type of problems and to identify feasible solutions (able to satisfy all the constraints) and possibly to avoid to incur in sub-optimal results.

1.2 Project focus and Case Studies

The context of this study is the area on the rationalisation of industrial water consumption, with a specific focus on the food industry which has interesting peculiarities concerning to water quality requirements and mass balance assessment.

During the execution of this PhD research project, two practical examples have been studied, one concerning a retrofit case and one focused on a new design case:

- The first example covers an existing industrial complex in the food industry (maize milling factory producing starch, sugars and co-products), where the problem of flowrates data reconciliation have been deepened. In this context, the issues related to the lack of measurements and fluctuating water (unavailability of direct analysis of water content in feedstock and product streams) have been addressed. A suitably modified data reconciliation approach, able to fit these specific requirements have been developed.
- The second example covers the new design of a Reverse Osmosis Network (RON), where the problem related to the identification of the optimal arrangements of RO modules considering the goals of the treatment, the economics and the specific technical constraints of the system and RO modules have been studied. In this context, a numerical modelling algorithm suitably modified to reach robust and reliable solutions have been developed.

The project focused on the first example also foresees a future phase aimed at reducing the freshwater consumption by maximising internal recycling between process phases with the support of water pinch analysis.

1.3 Thesis structure

The next sections of the thesis describe the application of these rationalisation techniques to the actual industrial examples introduced in the previous paragraph.

This research aims to test the effectiveness of State of the Art methodologies in the case of actual industrial problems to propose solutions to the technological gaps and limitations which might hinder their application.

Chapter 2 describes the application of Data Reconciliation and Validation techniques to the case of a Corn Refinery producing starches, starch derivates, sugars and fermentation products marketed in various sectors like human and animal food, chemical and pharmaceutical industry.

This example is particular for the dual role played by freshwater which can be at the same time a reactant and a utility (acting as mass or heat transfer vector) and for the need to manage different freshwater purity grades to fit production requirements.

Concurrent lack of measurement of freshwater streams, processing scheme complexity and occasional analysis of water content in finished and unfinished products makes the data reconciliation activity particularly challenging.

A relevant result of this research is the improvement of the DVR methodology through an innovative approach which considers the statistical variability of intermediate and finished products water content (resulting from the a-posteriori elaboration of the standard quality control tests) within the reconciliation algorithm.

Chapter 3 describes a Water Pinch application focused on the milling phases of the Corn Refinery described in Chapter 2.

This study aims to quantify the freshwater saving potential in the current case (base case) and assuming to treat some wastewater streams and to recycle the purified part to the main process phases (retrofit case).

The contaminant considered in this context is the COD, and the retrofit case highlighted a potential saving of 8.5 % of freshwater demand.

Chapter 4 describes a process synthesis application useful in the case of the design of new water treatment units.

An Optimisation model has been developed to identify the arrangement of a Reverse Osmosis Network (RON) so to minimise the investment and operative costs given the quality of the feed, the characteristics of membrane modules, the operative constraints and the treatment goals.

This type of problem is particularly challenging to solve because it is a mixed integer, non-linear (MINLP) and not convex.

At an initial stage, the problem has been formalised through a “Super Structure” representative of all possible alternative configurations, but it was not possible to reach a robust and stable solution applying the BARON algorithm which is purposely devoted to managing this type of problems.

It was, therefore, necessary to set-up a combined strategy concurrently simplifying the problem (splitting it into subproblems to be solved in parallel) and identifying an alternative optimisation algorithm (modified Simulated Annealing) which was adequately adjusted to handle the type of variables required by this specific problem.

Chapter 5 summarises the most significant results of this research work.

2 Integrated Data Reconciliation of Water Flows

The first example studied during the PhD work deals with the food industry; this industry is characterised by relevant freshwater consumption, high purity requirements and by the need to manage in the same context different grades of freshwater.

Furthermore, in most food industrial complexes, water is both a utility and a reactant and can flow out the process in the form of product, waste or evaporation loss.

This behaviour poses particular issues when trying to establish the material balance of the complex, both for what concerns the identification and management of the measurements and regarding the assumptions required to handle the parameters which can not be measured directly.

A food industry company expressed its interest in a holistic study aimed at rationalising the use of freshwater resources so to minimise the global demand and provided the necessary data.

The identified industrial complex is part of a multinational company operating in the biorefinery sector, transforming renewable raw materials from agricultural activities (cereals, tubers, vegetables) into products for the pharmaceutical, cosmetics, food industries and generating biogas.

Internationally the group is among the major producers of starches, glucose, dextrose and maltodextrins syrups, and is a leader in the production of polyols (e.g. Sorbitol, Mannitol, Xylitol, Maltitol).

The specific activity carried out by the studied industrial complex is Corn Refining producing starches, starch derivates, sugars and fermentation products marketed in various sectors like human and animal food, chemical and pharmaceutical industry.

Notwithstanding the high level of attention dedicated by the Corporate to the environmental impact of the industrial activity, nobody had ever carried out a comprehensive study on the use of water resources.

The industrial complex started its operation more than sixty years ago, and since the original establishment the farm has grown up both regarding capacity and complexity, and freshwater consumption naturally followed this trend.

Due to the limited cost of this utility, during the evolution of the industrial complex freshwater supply and treatment facilities have been adjusted to the primary processes requirements, but mostly through action aimed to the increase of the supply (number of aquifer wells or river in-take points).

Due to the continuous research of more sustainable patterns, recently the Company put a greater emphasis on the achievement of efficient water systems throughout its organisation, aiming to increase the efficiency in water reuse and recycling.

Therefore recently the Company launched various projects aimed at maximising internal water recyclings so to reduce the global water footprint, and the first step to proceed in this direction requires to dispose of an overall, and trustable material balance of water uses within the complex, covering both auxiliary and production processes.

The reconciliation of water streams uses carried out during this research project is part of this general strategy.

From the research perspective, the case is stimulating because it requires facing the various issues sometimes not considered from a theoretical perspective but occurring in reality.

These issues, typically occurring because the original complex designer did not foresee for the auxiliary systems the required monitoring instrumentation, risk jeopardising the successful result of the optimisation project.

Details of the industrial process are not mentioned in this context due to the confidential agreements put in place at the beginning of this work.

2.1 Food industry and fluctuating water

The food industry is “water-intensive” because it requires a significant and continuous supply of energy and of freshwater which is needed:

- as a raw material to be integrated into the finished products (fluctuating water),
- as a separating agent (e.g. extraction, absorption, scrubbing and stripping operations),
- as a washing medium for contaminant removal and other,
- for auxiliary scopes (steam heating, water cooling, power generation).

The concurrence of many of these operations within the same Complex involves the management of separate networks with different grades of water as well as the availability of supply water treatment processes enabling the production of the suitable amounts of water streams with the demanded purity levels.

The global water material balance of a system must account for both “pure” water streams (which can be of different types and handled through separated networks because of different Contaminants levels) and for “mixed” streams which can be raw materials or products containing water.

The content of water in mixed streams typically is not measured concurrently with the other data used to carry out the reconciliation process, is not constant and is subjected to variations related to the process operative conditions and the quality of the feedstock.

Consequently, the usual techniques for data reconciliation and for minimising the overall water consumption are to be modified to account for these fluctuations.

Furthermore, the presence of chemical reactions in the balance equations can give rise to severe nonlinearities which are to be accounted both in the preliminary reconciliation of the process measurements, as well as in the following optimisation studies.

2.2 Industrial complex description

The case study considered represents a large-scale plant involving eleven water using units (corresponding to six processing phases), seven treatment units (four for incoming water preparation and three for wastewater treatment) and one main contaminant.

The plant is a biorefinery which transforms raw corn into starches, starch products, sugars and fermentation products marketed in several sectors like food, animal nutrition, chemical and pharmaceutical industry.

The initial transformation phases are the physical separation processes (wet milling for corn steeping and by-products separation, and dry milling for final starch products) while the following steps are physical-chemical, chemical or biochemical processes (acid and enzymatic starch liquefaction, hydrolysis and fermentation).

The Complex disposes of a corn wet milling process separating the raw material into its constituent components: starch (~70%), germ (~4%), fibre (~2%), and protein (mainly gluten ~10%) [23]. The remaining part (~14%) is water.

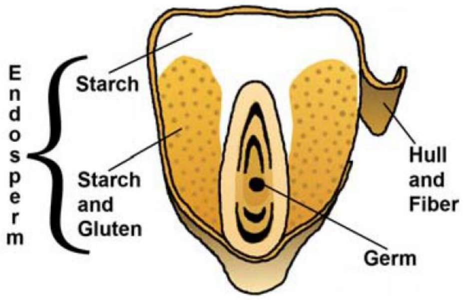


Figure 11 – Corn components [23]

Figure 12 summarises the main corn refining processing steps: wet milling, co-products separation and dry milling (starch purification and drying) are the highest water and energy-intensive processes.

These three phases absorb 57% of freshwater demand and 57% of energy demand (heat and power), generate 48% of wastewater and 37% of water evaporation loss.

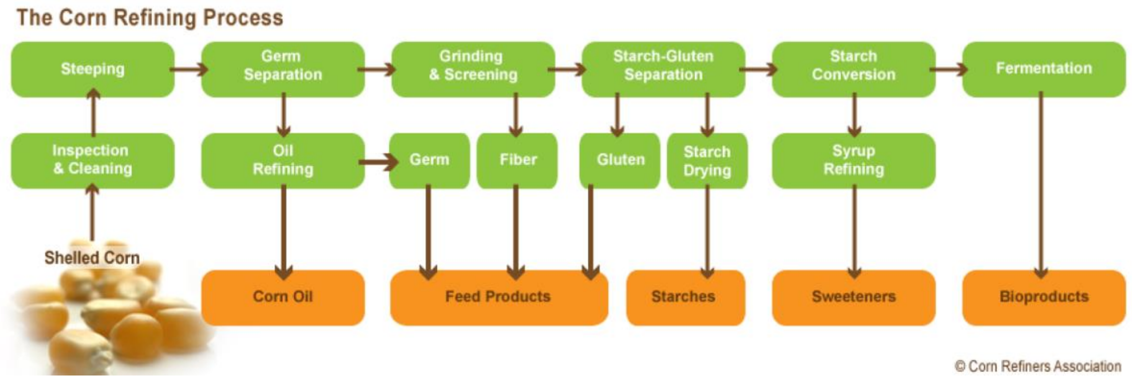


Figure 12 – Corn refining steps [23]

The bio-refinery also disposes of further treatment facilities for Starch conversion through enzymatic and acid liquefaction and downstream refining treatments to produce various sugars and syrups which are either marketed as finished products or fed to downstream fermentation units to generate added value products like Sodium Gluconate, Gluconic Acid and Glucono Delta Lactone (solid and liquid).

Liquefaction and sugar refining treatments absorb 25% of freshwater demand and 28% of energy demand (heat and power), generate 28% of wastewater and 50% of water evaporation loss.

Final fermentation treatments absorb 18% of freshwater demand and 15% of energy demand (heat and power), generate 24% of wastewater and 13% of water evaporation loss.

Overall, the processing of one ton of raw corn involves the consumption of 4.2 ton of freshwater and 1.3 MWh of energy (cumulated heat and power), the generation of 2.8 ton of wastewater and the evaporation of 1.5 ton.

Beyond the above-described activity (which is the main one) the industrial complex also disposes of:

- Auxiliary units for captive power and steam generation (two cogeneration units a standard boiler fed with natural gas and a cogeneration unit supplied with the biogas produced by the anaerobic treatment of a part of the wastewater).
- Production of organic products (e.g. succinic acid) from biological sources through intermediate sugars fermentation.

Water is supplied to the plant from superficial and deep aquifers, from a nearby stream and to a lesser extent from the public water supply.

The incoming freshwater treated differently depending on its origin and its use. In particular:

- Deep aquifer water goes directly to the raw water (R) circuit for the production process.
- Superficial aquifer water gets purified through filtration and then goes to the raw water circuit for the production process.
- Nearby stream water goes to the internal cooling circuit and then returns to the river: the water consumptions mentioned previously do not include this flow rate.
- Raw water is fed to reverse osmosis, softening units, and demineralisation columns (anionic, cationic, decarbonisation) to produce demineralised (D) and soft (S) water.
- Demineralised water is used to produce process steam (P).

Figure 13 reports a simplified Block Flow Diagram representing the production facilities covered by the study: the scheme details the grade of water consumed by each unit (as per legend).

Beyond the grades mentioned above the scheme highlights the production/consumption of recycled water streams (Y) as well as evaporation losses (L) and wastewaters (W) generated by product washing treatments.

To simplify the representation, only one recycled water (Y) entering or exiting the various blocks has been reported, but in practice, it represents multiple flows with different origins and purity levels: typical examples are washing and purification water or exhaust steam. Therefore the specific contaminant level of each water stream exiting a process must be carefully considered in the framework of the water optimisation study.

Wastewaters undergo anaerobic and aerobic treatments to reduce the contaminant content up to permitted concentration before being discharged.

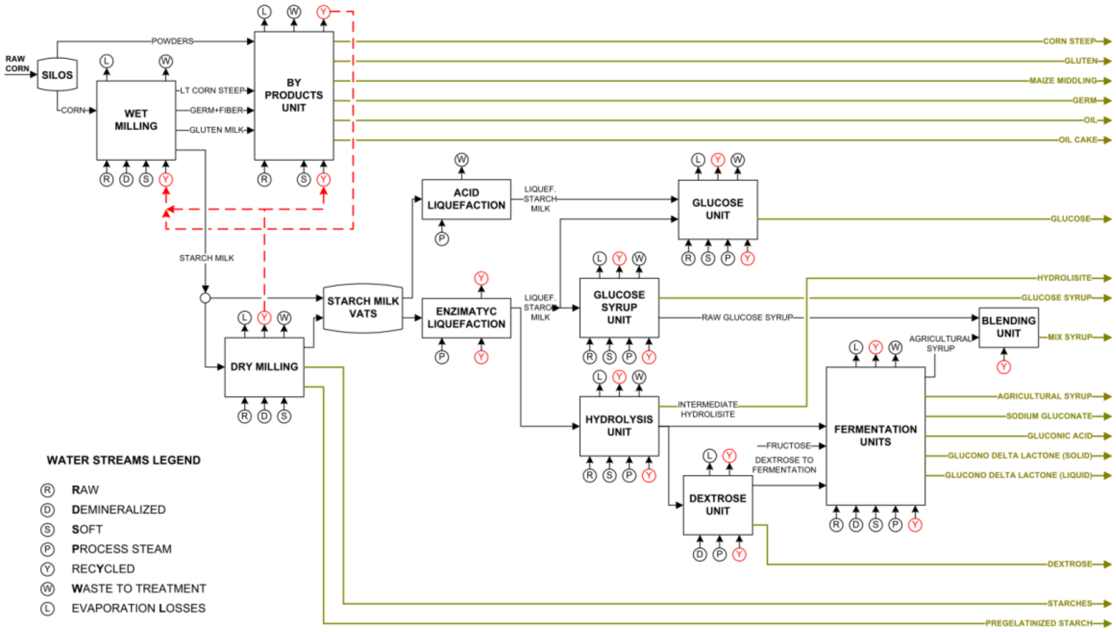


Figure 13 – Simplified Block Flow Diagram

Figure 14 summarises the processes available to treat the fresh water supplied to the complex and to purify the wastewater before discharge.

Both process phases and freshwater treatments generate wastewater: the amount produced to condition the incoming freshwater is about 20% of the overall wastewater production.

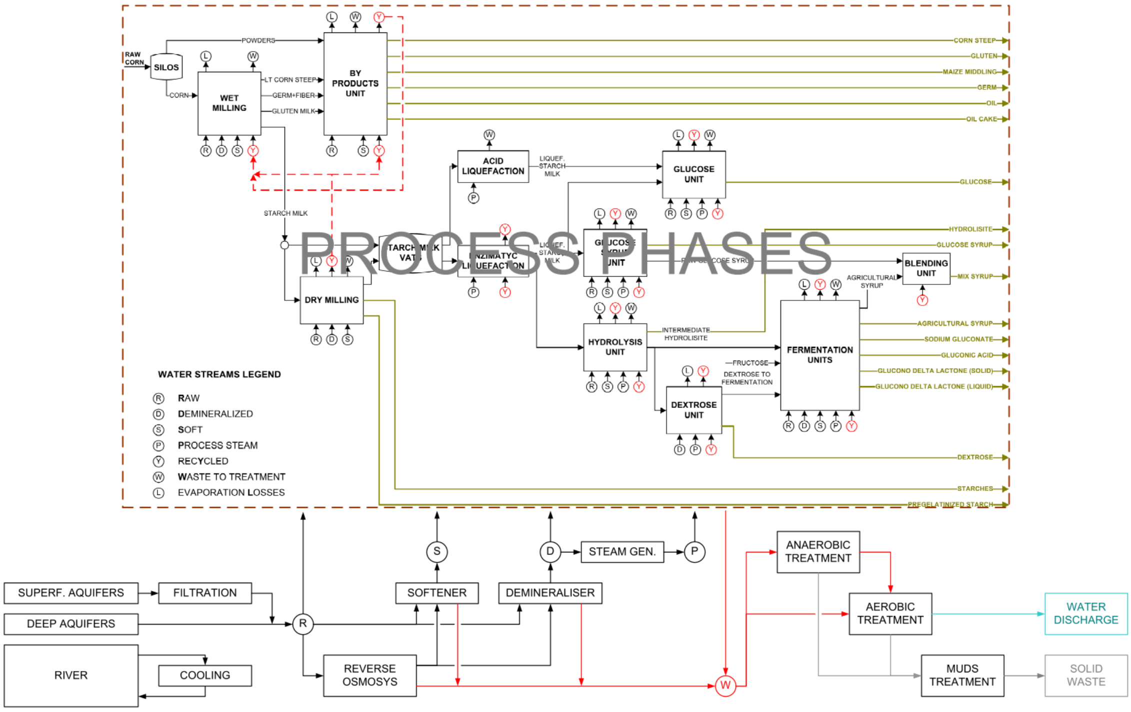


Figure 14 – Auxiliary freshwater and wastewater treatments

2.3 Integrated water material balance definition

During the initial phase of the project, the company agreed to disclose the information required to carry out the study, but neither simplified process flow diagrams (detailing the arrangement of process equipment inside each process phase) nor an overall material balance inclusive of freshwater supply and treating facilities were available.

Therefore, during the first step of the study, the available data sources have been assembled to build a complete material balance.

The information protection policies in place within the organisation, despite the secrecy agreements put in place, did not allow the disclosure of the detailed P&ID schemes which are usually considered by the internal technical staff confidential policies. Consequently, in the framework of the study, each process phase has been forcibly considered as a black box transforming incoming feedstock into outcoming streams without getting into the details of the detailed operations occurring inside each process phase.

The information useful for the definition of the overall material balance was available in multiple reports generated by different production services (operation, technological, environmental protection) for different purposes (production monitoring, achievement of environmental permits or other).

The following information has been used to execute this activity (not annexed to this dissertation for confidentiality agreements):

- Heat and material balances for each processing phase related to the production activities carried out in the year 2015 (for the main production activity which is corn milling and downstream treatments).
- Block Flow Diagram and standard water balance of the industrial plant detailing supply sources (deep and superficial aquifer wells and river), freshwater and wastewater treatment units, production of water grades, supply to processing phases, wastewater treatment and discharge.
- Monthly detail of water streams measurements for the year 2015

The analysis and deepening of this information took a long time: throughout different documents, the data was structured and grouped with different criteria and result in some instances inconsistent.

Due to the lack of reference process schemes of the various phases, it has been particularly complex to identify precisely the water or process streams corresponding to reported data in the different sources.

This kind of issues can constitute significant impediments to the successful execution of water rationalisation in case of retrofit projects.

The required information is frequently not available or duly structured.

To execute in the following stage a more in-depth process analysis highlighting potential optimisation areas, we decided to proceed with a data reconciliation activity inclusive in the same environment both freshwater treatments and primary process streams.

The two systems are complex and intimately integrated, and it is not advisable to model them separately because of the concurrent existence of material transfers from the water network to products and of significant evaporation losses.

This analysis led to the definition of an incidence matrix constituted by **20 nodes** and **108 streams** representing the overall water material balance from aquifers to wastewater treatment including the process phases: to quantify the contribution of mixed streams (like corn, products or chemicals) it has been necessary to make assumptions about the water content of each of them.

The water content of mixed streams is not constant and is subject to fluctuations which can be related to various factors linked to variations in feedstock quality, environmental and plant operating conditions.

The incidence of these fluctuations in the overall data reconciliation process can be even higher than that of measurement errors and must be correctly addressed, also because of the presence of evaporation losses (which cannot be measured) involves a compensation effect which might hide the unbalances due to water content oscillations.

2.4 Basic reconciliation software

The methodology outlined by Crowe et al. [13] already described at the Data Validation and Reconciliation paragraphs have been coded to handle the data reconciliation problem.

This method applies Linear Algebra Techniques to execute mathematical operations over the data matrices characteristic of the reconciliation model: details on Linear Algebra Methodologies are available at [24], the textbook which has been used to refresh these mathematic techniques.

The programming language applied to code Crowe's method is Fortran G95, primarily because of the availability on the internet free routines performing very fast the basic Linear Algebra operations. In particular, the material made available by the LAPACK library has been used [29].

The developed code is available in Appendix 8.1, while the detail of the type and source of the external routines included in the software is in Table 1.

ROUTINE	DESCRIPTION	SOURCE
MMUL	This subroutine computes the matrix product A*B and stores the result in the array C.	[25]
SVDRS	This subroutine computes the singular value decomposition of the given M1 x N1 matrix, A, and optionally applies the transformations from the left to the NB column vectors of the M1 x NB matrix B.	[26]
DGEQP3	DGEQP3 computes a QR factorisation with column pivoting of a matrix A: A*P = Q*R using Level 3 BLAS.	[27]
MATINV	Computing the inverse of a general n by n matrix in place, i.e., the inverse overwrites the original matrix.	[28]

Table 1 - Routines from external libraries

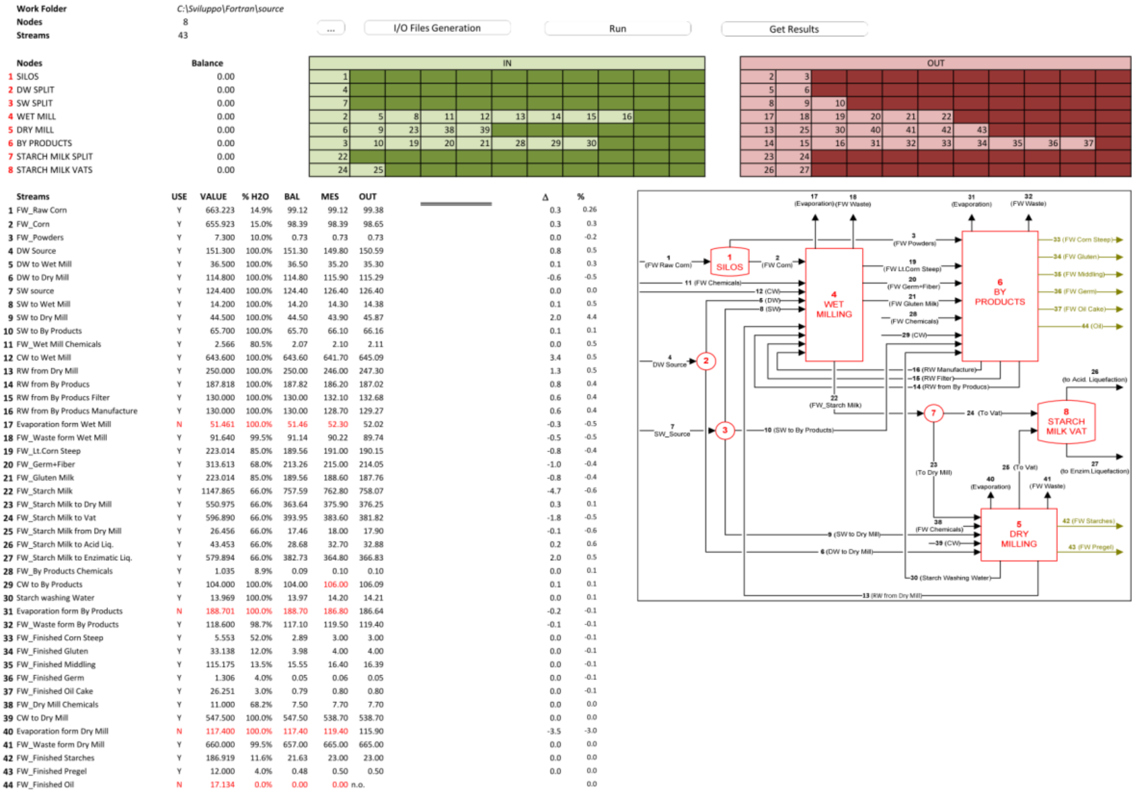
The software acquires input data, runs the reconciliation process and produces a report with the results.

The input text files are structured as follows:

- mat_hss_t.txt: containing a matrix detailing the structure of the network (nodes x streams with -1 for streams entering into a node, 1 for streams exiting from a node, 0 for the other cases),
- hss_t.txt: containing the list of measured flow rates (Stream identifier, value).

To simplify the use of this tool for the Company technical staff an interface, enabling the input setting and result reading from MS Excel environment have also been developed.

A prototype of this software focused on the initial Phases involving physical separation of corn components (wet milling, co-products separation and dry milling which overall constitute the 57% of total freshwater demand) has been submitted to the Company for their technical evaluation and approval. Figure 15 shows the graphical user interface developed for this reconciliation problem which consists of 8 nodes and 43 freshwater streams.



Work Folder *C:\Sviluppo\Fortran\source*
Nodes 8
Streams 43

	Nodes	Balance
1	SILOS	0.00
2	DW SPLIT	0.00
3	SW SPLIT	0.00
4	WET MILL	0.00
5	DRY MILL	0.00
6	BY PRODUCTS	0.00
7	STARCH MILK SPLIT	0.00
8	STARCH MILK VATS	0.00

IN										
1										
4										
7										
2	5	8	11	12	13	14	15	16		
6	9	23	38	39						
3	10	19	20	21	28	29	30			
22										
24	25									

OUT										
2	3									
5	6									
8	9	10								
17	18	19	20	21	22					
13	25	30	40	41	42	43				
14	15	16	31	32	33	34	35	36	37	
23	24									
26	27									

	Streams	USE	VALUE	% H2O	BAL	MES	OUT	Δ	%
1	FW_Raw Corn	Y	663.223	14.9%	99.12	99.12	99.38	0.3	0.26
2	FW_Corn	Y	655.923	15.0%	98.39	98.39	98.65	0.3	0.3
3	FW_Powders	Y	7.300	10.0%	0.73	0.73	0.73	0.0	-0.2
4	DW Source	Y	151.300	100.0%	151.30	149.80	150.59	0.8	0.5
5	DW to Wet Mill	Y	36.500	100.0%	36.50	35.20	35.30	0.1	0.3
6	DW to Dry Mill	Y	114.800	100.0%	114.80	115.90	115.29	-0.6	-0.5
7	SW source	Y	124.400	100.0%	124.40	126.40	126.40	0.0	0.0
8	SW to Wet Mill	Y	14.200	100.0%	14.20	14.30	14.38	0.1	0.5
9	SW to Dry Mill	Y	44.500	100.0%	44.50	43.90	45.87	2.0	4.4
10	SW to By Products	Y	65.700	100.0%	65.70	66.10	66.16	0.1	0.1
11	FW_Wet Mill Chemicals	Y	2.566	80.5%	2.07	2.10	2.11	0.0	0.5
12	CW to Wet Mill	Y	643.600	100.0%	643.60	641.70	645.09	3.4	0.5
13	RW from Dry Mill	Y	250.000	100.0%	250.00	246.00	247.30	1.3	0.5
14	RW from By Producs	Y	187.818	100.0%	187.82	186.20	187.02	0.8	0.4
15	RW from By Producs Filter	Y	130.000	100.0%	130.00	132.10	132.68	0.6	0.4
16	RW from By Producs Manufacture	Y	130.000	100.0%	130.00	128.70	129.27	0.6	0.4
17	Evaporation form Wet Mill	N	51.461	100.0%	51.46	52.30	52.02	-0.3	-0.5
18	FW_Waste form Wet Mill	Y	91.640	99.5%	91.14	90.22	89.74	-0.5	-0.5
19	FW_Lt.Corn Steep	Y	223.014	85.0%	189.56	191.00	190.15	-0.8	-0.4
20	FW_Germ+Fiber	Y	313.613	68.0%	213.26	215.00	214.05	-1.0	-0.4
21	FW_Gluten Milk	Y	223.014	85.0%	189.56	188.60	187.76	-0.8	-0.4
22	FW_Starch Milk	Y	1147.865	66.0%	757.59	762.80	758.07	-4.7	-0.6
23	FW_Starch Milk to Dry Mill	Y	550.975	66.0%	363.64	375.90	376.25	0.3	0.1
24	FW_Starch Milk to Vat	Y	596.890	66.0%	393.95	383.60	381.82	-1.8	-0.5
25	FW_Starch Milk from Dry Mill	Y	26.456	66.0%	17.46	18.00	17.90	-0.1	-0.6
26	FW_Starch Milk to Acid Liq.	Y	43.453	66.0%	28.68	32.70	32.88	0.2	0.6
27	FW_Starch Milk to Enzimatic Liq.	Y	579.894	66.0%	382.73	364.80	366.83	2.0	0.5
28	FW_By Products Chemicals	Y	1.035	8.9%	0.09	0.10	0.10	0.0	0.1
29	CW to By Products	Y	104.000	100.0%	104.00	106.00	106.09	0.1	0.1
30	Starch washing Water	Y	13.969	100.0%	13.97	14.20	14.21	0.0	0.1
31	Evaporation form By Products	N	188.701	100.0%	188.70	186.80	186.64	-0.2	-0.1
32	FW_Waste form By Products	Y	118.600	98.7%	117.10	119.50	119.40	-0.1	-0.1
33	FW_Finished Corn Steep	Y	5.553	52.0%	2.89	3.00	3.00	0.0	-0.1
34	FW_Finished Gluten	Y	33.138	12.0%	3.98	4.00	4.00	0.0	-0.1
35	FW_Finished Middling	Y	115.175	13.5%	15.55	16.40	16.39	0.0	-0.1
36	FW_Finished Germ	Y	1.306	4.0%	0.05	0.06	0.05	0.0	-0.1
37	FW_Finished Oil Cake	Y	26.251	3.0%	0.79	0.80	0.80	0.0	-0.1
38	FW_Dry Mill Chemicals	Y	11.000	68.2%	7.50	7.70	7.70	0.0	0.0
39	CW to Dry Mill	Y	547.500	100.0%	547.50	538.70	538.70	0.0	0.0
40	Evaporation form Dry Mill	N	117.400	100.0%	117.40	119.40	115.90	-3.5	-3.0
41	FW_Waste form Dry Mill	Y	660.000	99.5%	657.00	665.00	665.00	0.0	0.0
42	FW_Finished Starches	Y	186.919	11.6%	21.63	23.00	23.00	0.0	0.0
43	FW_Finished Pregel	Y	12.000	4.0%	0.48	0.50	0.50	0.0	0.0
44	FW_Finished Oil	N	17.134	0.0%	0.00	0.00	n.o.		0.0

Figure 15 – Reconciliation Software prototype – MS Excel GUI

2.5 Management of water content fluctuations

As described in the previous paragraph, this reconciliation exercise if focused on the overall freshwater balance, inclusive of the amount of water contained in process streams: therefore, for this purpose, it is necessary to consider in the same context both freshwater and mixed streams.

The peculiarity of this reconciliation problem is due to the impossibility to directly measure the water content of process streams (raw materials, intermediate and finished products) which must be considered jointly to the flow rate of the process stream to estimate the actual water flow in input to the reconciliation process.

Freshwater streams can be of different types and grades (e.g. raw water, sweet water, demineralised water, recycled water, exhaust steam) but have a water content greater than 99.9% anyhow.

Mixed streams are:

- Feedstock (raw corn average water content ranges between 13 to 15% depending on the origin and storage conditions [30]),
- Intermediate products (in our case with water content ranging between 10% to 85% depending on the product and operative conditions),
- Finished products (in our case water content ranging between 0% to 54% depending on the product and operative conditions),
- Chemicals (in our case water content ranging between 0% to 81%).

Furthermore, in the case of finished products, it is also necessary to take into account the commercial specifications which are binding the maximum water content of the various products.

Therefore, most of the water content laboratory tests are carried out on finished products while less information is typically available to determine the water content of intermediate products.

The existence of commercial specifications binding the maximum water content of the finished products does not mean that this amount can be considered fixed, but only that there is a higher level of attention from the production side to avoid “out of spec production”.

Notwithstanding the availability of characterisation data for the finished products, this information is considered “sensitive” for the related commercial implications, and the Company decided not to disclose it in the framework of this study.

However, water content data, even if with variable sampling frequency for the different streams, should be made available by ordinary quality control activities. The resulting statistical information can be applied to improve the efficiency of the reconciliation process.

The Data Reconciliation of steady-state processes is frequently carried out using adequate statistical objective functions (typically a likelihood function) which are optimised subject to constraints due to steady-state equations provided by material balances.

If additionally, only one component is considered (which is precisely the case of the water resources which we examined in our case), the mass balances provide a set of linear equations, and the maximisation can be carried out analytically, which makes it possible to detect and remove gross errors.

Suppose x' are measurements of process water flow-rates and $\hat{x}$ are the corresponding rectified values. They satisfy the set of steady-state material balances

$$A\,\hat{x} = 0 \tag{1}$$

Where A is the incidence matrix and $\hat{x}$ the flow rates of all the water streams of the process. The number of rows of A, m, is equal to the number of units for which a material balance is considered, whereas the number of its columns, n, is given by the total number of streams present in the process.

The element a_{ij} is given by:

$$a_{ij} = \begin{cases} 1\ if\ the\ stream\ j\ enters\ the\ unit\ i \\ -1\ if\ the\ stream\ j\ leaves\ the\ unit\ i \\ 0\ otherwise \end{cases}$$

However, the fluctuating content of water in the products – which affects the value of some of the $\hat{x}$ in equation (1) – is not measured concurrently to the other flow rates measures which are considered to determine the net input value x'; rather, samples are periodically collected and subjected to a quality control procedure that determines the water content.

Thus, their average statistical properties (including the components of their variance-covariance) over the interval of time corresponding to the sampling frequency are available, the relevant information cannot be used directly but has to be adequately adjusted.

The water content fluctuations detected in the quality control procedure can be elaborated to determine the relevant statistical information which in turn can be employed to construct an a priori likelihood function $P_0(\hat{x}_P) = P_0(y)$ which is supposed to be:

$$P_0(y) \propto e^{-y^T V_P^{-1} y} \tag{2}$$

where the subscript P is the index for the product flow rate vectors.

The a priori likelihood function is combined with the distribution resulting from dynamic fluctuations (as proposed by Sisi Guo et al. [32]) using Bayes' theorem, with the information provided by the measurements.

In this context, it has also been assumed that the experimental errors of the water content measures are also normally distributed. Basing on this assumption is possible to define the a posteriori likelihood function as follows:

$$e^{-(\hat{x}-x')^T V^{-1}(\hat{x}-x')} \cdot e^{-y^T V_P^{-1} y} \tag{3}$$

Where V is the variance-covariance matrix of the process subject to $A\hat{x} = y$.

Equivalently, it is possible to find the solution minimising:

$$(\hat{x} - x')^T \, V^{-1}(\hat{x} - x') + y^T V_P^{-1} y \tag{4}$$

subject to

$$A\hat{x} = y \tag{5}$$

It is possible to solve this problem in closed form for $\hat{x}$

$$\hat{x} = [A^T V_P^{-1} A + V^{-1}]^{-1} \cdot V^{-1} x' \qquad (6)$$

If some measurements are missing, the Matrix Projection approach described by Crowe, Garcia Campos, and Hrymak [13], which has been summarised in the previous paragraphs, can be used to reconcile the values that are identifiable.

While the matrix V_P is evaluated directly from the ordinary test executed by the quality control service, a tuning procedure for the determination of the incidence matrix V can be established following the strategy proposed by Dovì and Del Borghi [33].

In this work, which is aimed at accounting for the departure from steady state condition due to the variation of hold-ups, fluctuations are taken account of directly in the reconciliation procedure, whereas their statistical properties are determined using a tuning method that makes use of the usual chi-tests.

Constraining the sum of squared deviations of a train of measurements (including q data sets) to satisfy the chi-square distribution provides the optimisation criterion:

$$\Phi = \sum_q \varphi_q^2 = min \qquad (7)$$

Therefore:

$$\sum_q \left\{ x_q^T \left[\left(A^T V_p^{-1} A + V^{-1}\right)^{-1} V^{-1} - I \right]^T V^{-1} \left[\left(A^T V_p^{-1} A + V^{-1}\right)^{-1} - I \right] x_q - v \right\}^2$$

$$= min \qquad (8)$$

Where:

q is the number of considered experimental samples

v is the dimension of x

I is the identity matrix

The minimisation concerning the elements of V can be efficiently carried out using a Gauss-Newton algorithm.

However, minimising Φ does not necessarily satisfy the chi-test (although the resulting distribution is as close as possible to the χ^2 distribution, it might be not close enough).

To this purpose, the Kolmogorov-Smirnov test [34] can be used (Dovì and Del Borghi, 2001 [33]) to verify whether there is enough experimental evidence or the number of the data sets in the training period is to be increased.

3 WCA study for potential savings targeting

Aiming to quantify the maximum water recovery target obtainable in the case considered, a Water Cascade Analysis focused on the corn refinery previously described has been carried out.

In particular, the Water Cascade Analysis deepens the case of the initial transformation phases (wet milling for corn steeping and by-products separation, and dry milling for final starch products) which overall absorb 57% of freshwater demand.

Manan et al. initially proposed the WCA methodology applied in this context in 2004 [20].

Reference [5] describes in detail the WCA methodology which foresees to rank the cumulated flow rates of water consumption (sinks) and production (sources) streams for increasing contaminant levels.

This particular data arrangement and elaboration makes it possible to calculate the make-up assuring the required supply of freshwater for each contaminant level considered within the analysis.

The contaminant considered is COD (Chemical Oxygen demand) which is the amount of oxygen required for the total chemical oxidation of compounds contained in the water sample. Even if not the sole one, the COD is one of the most significative contaminants considered within the industrial complex and, for a preliminary analysis is the one which best fits the purpose of this study.

Unlike the reconciliation exercise previously described, which involved the concurrent evaluation of water and mixed streams (raw materials or products containing water), this analysis is carried out only on water streams.

As described in the previous sections, the corn refining process requires three different types of water: raw, sweet and demineralised but, in practice, the only grade of water supplied to the industrial complex is raw water which is fed both to process and purification units.

It is, therefore, reasonable to simplify the analysis by relating directly to raw water the consumption of other water purified water streams (sweet and demineralised water).

The following criteria, deduced from the results of the reconciliation step, have been applied to relate sweet and demineralised water to raw water:

- The production of 1 ton of Sweet Water involves the consumption of 1.176 ton of Raw Water and the generation of 0.176 ton of wastewater.
- The production of 1 ton of Reverse Osmosis Permeate involves the consumption of 1.461 ton of Raw Water and the generation of 0.461 ton of wastewater.
- The production of 1 ton of Demineralised Water involves the consumption of 0.902 ton of Reverse Osmosis Permeate and 0.488 ton of Raw Water and the generation of 0.350 ton of wastewater, thus (considering the previous parameters) overall the consumption of 1.350 ton of Raw Water.

Table 2 reports the COD levels considered for this analysis: since not all values have been made available, it has been necessary to estimate the COD of some streams; additionally, some reasonable roundings and approximations have been made to contain the number of levels, as explained below.

COD Levels for Water Streams	
Raw Water	20
Currently recycled water	80
Reverse Osmosis, Demineralisers wastewater	60
Sweeteners wastewater	100
Starch washing water	100
Treatable Wastewater	300
Wastewater treatment RO permeate	20
Wastewater treatment RO retentate	650
Total wastewater	1000
Non treatable Wastewater	1120

Table 2 - COD of water streams

After this preliminary elaboration, the flow rates of the water liquid streams resulting from the reconciliation exercise have been grouped for different levels of COD and cumulated so to determine the total water consumption and production in correspondence of each level.

The WCA has been executed for two cases; base and retrofit:

- The base case assumes that it is not possible to increase the contaminant level of the water streams fed to the process beyond the current levels and does not foresee treatments reducing the COD to a level acceptable by process units.
- The retrofit case studies the impact of the addition of treatment units (typically Reverse Osmosis) reducing the contaminant content of some “treatable” waste streams.

3.1 Base Case

Table 3 lists the Sinks and resulting from the reconciled material balance of Wet Milling, Dry Milling and By Product Phases. Flow rate (F_j and F_i) values are in ton/h, COD values in mgO_2/litre.

This case considers five contaminants levels. All wastewater streams from process units are in correspondence of the higher level (COD = 1000) because of the absence of sinks for COD > 100.

The big part of the demand is at Raw Water purity level, and the sinks at mid purity levels are saturated.

Water Sinks and Sources					
Sinks			**Sources**		
	F_j	C_j		F_i	C_i
SK_1	187.4	20	SR_2	6.0	60
SK_3	79.5	80	SR_3	79.5	80
SK_4	1.6	100	SR_4	4.2	100
			SR_5	99.8	1000

Table 3 - Sinks & Sources Base Case

Table 4 shows the results of the WCA which confirms that in the base case it is not possible to achieve water savings keeping the current COD constraints for the water streams entering the process.

The pinch point (highlighting the maximum COD concentration which can be absorbed by the system) occurs in correspondence of COD = 100; thus the only way to save water is to treat wastewater streams to generate streams with low COD values.

The resulting freshwater demand is equal to 187.4 ton/h while the wastewater flow rate is 105.8 ton/h, corresponding to 56.4% of the supply.

Water Cascade Analysis - Base Case

K	C_K [ppm]	ΔC_K	ΣF_{sink} [ton/h]	ΣF_{source} [ton/h]	ΣF_{source}+ ΣF_{sink} [ton/h]	$F_{C,k}$ [ton/h]	Δm [kg/h]	Cum Δm [kg/h]	$F_{FW,cum}$ [ton/h]	$F_{C,k}$ [ton/h]	
						0.0			F_{FW} =	**187.4**	
1	20		-187.4		-187.4			0.0			
		40				-187.4	-7.5			0.0	
2	60			6.0	6.0			-7.5	-187.4		
		20				-181.4	-3.6			6.0	
3	80		-79.5	79.5	0.0			-11.1	-556.3		
		20				-181.4	-3.6			6.0	
4	100		-1.6	4.2	2.5			-14.8	-737.7		**<< PINCH**
		900				-178.9	-161.0			8.6	
5	1000			99.8	99.8			-175.7	-195.3		
									F_{WW} =	**105.8**	
								-175.7			

Table 4 - WCA Analysis Base Case

3.2 Retrofit Case

The retrofit case assumes the insertion of proper treatment units aimed at producing low COD streams from “treatable” wastewater streams.

The analysis of the COD level of the various wastewater streams produced by the process units highlighted that about 10 % of the total wastewater exiting the initial transformation phases has a mid-low COD (about 300) and, if adequately segregated from the other wastewater streams can be purified to reach a COD comparable to that of Raw Water.

Similarly, it is possible to treat the wastewater streams produced by the generation of Sweet and Demineralised water.

The retrofit case assumes to segregate the wastewater streams characterised by a low COD level and to send them to dedicated new purification units (for example Reverse Osmosis) to concentrate the contaminants in the retentate and recycle the permeate upstream to processing phases.

Therefore, the new analysis foresees additional Sinks and Sources: previous wastewater source (99.8 Ton/h, COD = 1000) is split into two sources: treatable wastewater (14.7 Ton/h, COD = 300) and non-treatable wastewater (14.7 Ton/h, COD = 1120).

The additional purification treatment involves a new sink absorbing water with COD equal to 300 (SK_6), and two new sources at COD 20 (SR_1) and 650 (SR_7) respectively representing the water streams exiting the purification stage.

Table 5 shows the updated list of sinks and sources for the retrofit case; the elements modified from the base case are highlighted in red.

Water Sinks and Sources					
Sinks			Sources		
	F_j	C_j		F_i	C_i
SK_1	187.4	20	SR_1	15.9	20
SK_3	79.5	80	SR_2	6.0	60
SK_4	1.6	100	SR_3	79.5	80
SK_6	23.3	300	SR_4	4.2	100
			SR_6	14.7	300
			SR_7	7.3	650
			SR_8	85.1	1120

Table 5 - Sinks & Sources Retrofit Case

Table 6 shows the WCA table adjusted for the retrofit case. The figures written in red are the ones changed (or added) compared to the base case.

The insertion of the purification facility involves:

- the freshwater supply reduction of about 8.5% corresponding to 15.9 ton/h.
- the wastewater production reduction of 12.7% corresponding to 13.4 ton/h.

The pinch point still occurs in correspondence of COD = 100

Water Cascade Analysis - Retrofit Case											
K	C_K [ppm]	ΔC_K	ΣF_{sink} [ton/h]	ΣF_{source} [ton/h]	$\Sigma F_{source}+ \Sigma F_{sink}$ [ton/h]	$F_{C,k}$ [ton/h]	Δm [kg/h]	Cum Δm [kg/h]	$F_{FW,cum}$ [ton/h]	$F_{C,k}$ [ton/h]	
						0.0			F_{FW} =	**171.5**	
1	20		-187.4	15.9	-171.5			0.0			
		40				-171.5	-6.9			0.0	
2	60			6.0	6.0			-6.9	-171.5		
		20				-165.5	-3.3			6.0	
3	80		-79.5	79.5	0.0			-10.2	-508.4		
		20				-165.5	-3.3			6.0	
4	100		-1.6	4.2	2.5			-13.5	-673.9		**<< PINCH**
		200				-162.9	-32.6			8.6	
5	300		-23.3	14.7	-8.6			-46.1	-230.3		
		350				-171.5	-60.0			0.0	
7	650			7.3	7.3			-106.1	-303.1		
		470				-164.1	-77.1			7.4	
8	1120			85.1	85.1			-183.2	-389.9		
									F_{WW} =	**92.4**	

Table 6 - WCA Analysis Retrofit Case

Recently the Company is experiencing in some seasons water scarcity problems and has foreseen to build additional water wells to overcome this limitation.

In this context, it might be convenient to consider whether the segregation of “treatable” wastewater streams and the insertion of dedicated purification facilities provides a valid and economical alternative to the increase of water supply capacity

To deepen the potential existence of a seasonality effect on freshwater demand (the reconciled information is determined on yearly base), a preliminary Principal Components Analysis (PCA) study on the water streams monthly flowrates have also been carried out.

Appendix 8.2 reports a brief discussion of the results of the PCA analysis.

This study highlights a potential seasonality trend, but to understand the causes of this behaviour, it would be necessary to plan further analysis also covering the monthly balances of the primary process streams.

This analysis will enable to understand if the observed trend is related to production causes (different production asset due to raw material quality of products demand) or the global environmental conditions (temperature or humidity).

Unfortunately, the Company did not disclose the information required to explore further this subject.

4 Optimisation of Reverse Osmosis Network

During the second part of the research project, the problem of optimising the configuration of Reverse Osmosis Networks (RON) for water treatment plants has been addressed, which is a useful application in the field of new treatment units design.

The RON configuration problem is general, and in principle, a well-performing algorithm would apply to different water treatment areas (desalination, purification or wastewater treatment).

The water scarcity issue of the corn refining complex previously described, can be addressed through dedicated RON properly configured to assure the simultaneous removal of more contaminants.

Therefore, the opportunity to study this application starting from the available technical and economic information to define the boundaries and requirements of the actual industrial problem has been seized.

The goal of the research is to develop a “working” algorithm able to identify, by technical and economic parameters, the optimal arrangement of the modules of a Reverse Osmosis Network for the treatment of the various grades of wastewater (with variable and multiple contaminants content).

The confidentiality agreements in place do not permit to publish a case study based on the data of this industrial complex, therefore, in this context, the results of the application obtained for another industrial case have been presented: the treatment of production wastewater (generated within an on-shore oil extraction field).

Even though the contaminants type and concentration are different, this case is quite similar to the previous one. Some reference information detailing the quality of this wastewater is readily retrievable in published sources.

RON optimisation is a particular example of process synthesis that does not foresee the management of chemical reactions but just the separation of contaminants: while some procedures have been proposed in the literature, there is not yet an off-the-shelf software capable of directly solving this problem.

It is possible to address this problem with the support of mathematical programming techniques able to simultaneously consider the following types of variables:

- Integer and binary: to describe the structural and operational alternatives of the process.
- Real: to describe the other continuous parameters of the process.

Generally, these are Mixed Integer, non-linear and non-convex problems which are difficult to solve with standard optimisation algorithms which risk identifying sub-optimal results (the existence of multiple minima characterises the objective function in correspondence of different regions of the solutions domain).

The objective function (to be minimised) is economical and accounts for the following cost elements:

- water supply
- water treatment operation (chemicals and energy)
- water treatment facilities investment (both for the water incoming and exiting the industrial complex).

As a first step, the problem has been formalised. The Branch-And-Reduce Optimization Navigator (BARON) solver [35] (available in the commercial software environment GAMS [36]) was first used for the identification of the optimal configuration.

This algorithm, developed for the resolution of non-linear (NLP), Mixed Integer (MIP) and non-convex problems in acceptable computing time, applies methodologies aimed at quickly and exhaustively exploring the solution domain to identify the "global" optimal solution, and is considered one of the most effective algorithms.

Concerning this solver, GAMS website states: that "*While traditional NLP and MINLP algorithms are guaranteed to converge only under certain convexity assumptions, BARON implements deterministic global optimisation algorithms of the branch-and-bound type that are guaranteed to provide global optima under fairly general assumptions. These include the existence of finite lower and upper bounds on nonlinear expressions in the NLP or MINLP to be solved.*"

While BARON is expected to attain convergence in a wide range of cases, it failed to find the optimal solution in a reasonable amount of time, unless the initial value was very close to the actual optimum (identified as described below).

Due to this unforeseen obstacle, it has been necessary to put in place strategies to work around this constraint and reduce the computation time:

- reducing problem complexity
- finding an alternative solver better fitting this specific problem.

In principle, the global target of the optimisation problem turned from "identifying the absolute global optima" into "identifying good enough solutions", which is more acceptable also from an industrial perspective.

The applied general strategy to reach this goal consisted in:

- Transforming integer variables into "constrained" real variables (which helps to improve the performance of the solver).
- Reduction of the solution domain by dividing the problem into more simple sub-problems to be optimised in parallel.
- Identify an alternative algorithm to solve the problem adapting it to its specific requirements.
- Resolution of the problem in successive steps so to introduce part of the constraints in a second phase step after identifying the feasible solutions domain.

4.1 The process synthesis problem

The academic community started discussing the use of mathematical programming to solve process synthesis problems in the sixties. Since the preliminary works, many applications and progress have been achieved, also thanks to the fast development of computer calculation capabilities which enabled to increase the complexity of the investigated problems [42].

For a given chemical process with defined goals (regarding products yield and quality), process synthesis aims to determine the assembly and interconnection of the components (heat transfer, mass transfer, separation, reaction) into a network to produce the desired outputs with the goal of optimising either economic or environmental impact.

The typical approach foresees the formalisation of an optimisation model representing a “superstructure” able to express all the possible alternative configurations and enabling the calculation of the process results associated with each solution.

The main issues that the researchers have tried to address in this domain are:

- Coverage of solution domain: depending on the application and considering the high number of interconnection possibilities and alternative processing strategies, the superstructure must be conceived to cover all the meaningful solutions and to avoid the meaningless ones (which have the effect of increasing the computational burden).
- Nature of the related optimisation problem: typically the problem resulting from the superstructure requires integer variables and non-linear constraints (MINLP problems). These problems can arise very difficult to solve, mainly when the objective function (which generally accounts for process economics) is “non-convex” (where the existence of multiple local optima complicates the global optima identification).

When the problem is “non-convex” and it is not possible to solve it within a reasonable time-frame, it possible to speed-up its solution, acting both on its structure (reducing the number of integer variables or linearising non-linear constraints) and on the solving strategy (splitting the resolution process in more steps so to reduce progressively the solutions domain).

Based on a recent review on Process Synthesis publications [43], main developments occurred in the field of Heat Exchanger Networks (HENS), Mass Exchange Networks (MEN) and Distillation Sequences (DS) but not many prominent papers appeared in the last decade.

Among newer contributions, there has been a particular success in the areas of dividing wall columns, reactive distillation, and water network synthesis.

Despite the progress achieved in various areas, there are still many open challenges and, a universally established approach does not exist.

The capability to robustly solve massive, industrially-relevant problems remains limited, and it is necessary to fine-tune each application to the particular problem requirements.

4.2 Reverse Osmosis Network Configuration

Reverse Osmosis is a process in which the solvent is forced to pass from a more concentrated solution to a less concentrated one through a special membrane capable of containing contaminants. The material transfer takes place by applying pressure able to overcome the resistance due to osmotic pressure.

The reverse osmosis module feedstock is separated into two streams, one with a higher concentration of solutes and high pressure called "retentate" and one with a lower concentration of solutes and pressure of the "permeate".

During the last decades this process established itself at industrial level for various applications (sea and brackish water desalination, wastewater treatment, industrial streams concentration), thanks to the high flexibility, scalability and reduced energy consumption compared to other separation processes.

It is possible to connect Reverse Osmosis modules in networks where the permeate and the retentate streams exiting from one module go to others. It is possible to set-up a Reverse Osmosis Network (RON) arranging modules both in series and in parallel.

Within the same RON, treated streams go in parallel to more modules; it is possible to foresee more treatment levels in series as well as recycling the retentate and permeate streams back to the previous treatment levels.

The RON is a system characterised by multiple pressure levels with pumps providing energy to the treated streams, turbines (or pressure exchangers) recovering energy from concentrated streams and Reverse Osmosis Membrane Modules separating the incoming streams.

The optimal RON arrangement depends on:

- the specific treatment’s goals,
- solutes concentration in the feed stream,
- general operative constraints (e.g. maximum inlet pressure or minimum inlet flow rate per module)
- overall treatment energy consumption,

- associated investment cost (number of RO modules required for a given arrangement).

4.3 Problem description

During this research, there has been the opportunity to carry out a case study focused on a real industrial RON optimisation problem: definition of the optimal RON configuration for treating the wastewater generated within an on-shore oil production field.

A maximum limit of dischargeable wastewater constrains the oil production facility thus the goal of the treatment is to minimise the final volume of wastewater by producing a right amount of pure water which is then recycled for other industrial uses.

Downstream the preliminary treatments (chemical, physical and biological) aimed at removing hydrocarbons and other undesirable contaminants; wastewater is fed to a Reverse Osmosis Unit so to produce demineralised water which is recycled back to the production cycle and minimise the volume of residual water sent to the final treatment before discharge.

In this framework, the goal of the study was to put in place a model able to identify the most appropriate RON arrangement given:

- Feed quality and operative conditions (flow rate, pressure and concentration of various contaminants),
- Technical parameters characterising the membrane modules,
- Operative constraints (global and of single modules),
- Treatment goals (permeate purity and retentate maximum flow rate),
- Operative costs,
- Investment costs.

Table 7 lists the information considered by the optimisation model; input data are grouped in the following families: economic, feed, bounds, permeate and membrane.

Type	Description	Unit
Economic	Specific yearly membrane cost	$\$/(m^2 \bullet year^{)}$
Economic	Purified water sale price	$\$/m^3$
Economic	Pumps and turbines investment cost calculation coefficients	$\$$
Economic	Pumps and Turbines efficiency	adimensional
Economic	Specific yearly membrane maintenance cost	$\$/(m^2 \bullet year^{)}$
Economic	Power cost	¢/kWh
Economic	Usage rate	days/year
Feed	Flow Rate	l/s
Feed	Ions concentration $(Na^+; K^+;Mg^{2+};Ca^{2+};Cl^-;Br^-;I^-;SO_4^{2-})$	g/l
Bounds	Flow Rate (min/max) for each RO module	l/s
Bounds	Maximal inlet pressure	Bar
Permeate	Minimum produced flowrate	l/s
Permeate	Ions concentration $(Na^+; K^+;Mg^{2+};Ca^{2+};Cl^-;Br^-;I^-;SO_4^{2-})$	g/l
Membrane	Single Module Surface	m^2
Membrane	Water permeability through the membrane (coefficient A)	$10^{-13} \bullet ms^{-1}Pa^{-1}$
Membrane	Solute permeability through the membrane (coefficient k)	$10^{-8} \bullet ms^{-1}$
Membrane	Coefficient γ	adimensional
Membrane	Stage head loss	Bar

Table 7 - RON Optimisation Model Input

Permeate, and retentate streams flow rates and concentration are calculated within the model applying Evangelista’s shortcut method [37].

The developed model enables to highlight the optimal arrangement of membrane modules specifying:

- the number of retentate treatment serial stages,
- the number of parallel membrane modules for each stage,
- the possible need for more permeate treatment steps,
- the possible need for upstream retentate recycling

Figure 16 shows an arrangement example: in the specific case, the arrangement foresees a first treatment step (with three retentate treatment stages) and by a second permeate treatment step (with two retentate treatment stages). Furthermore, part of the permeate can by-pass the following stages, and part of the retentate can be recycled upstream.

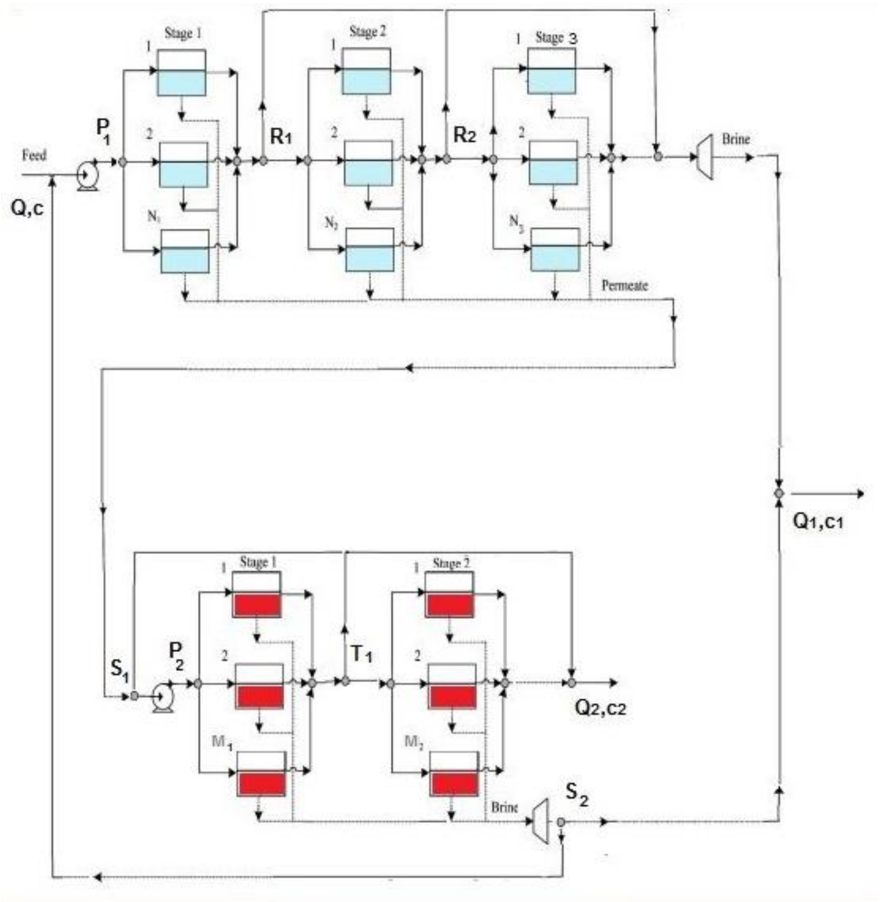


Figure 16 - RON arrangement example.

4.4 Problem formalisation and solution

BARON (Branch-And-Reduce Optimization Navigator) is an algorithm developed expressly to solve fast non-linear mixed integer non-convex problems [35].

It is possible to formalise a problem and solve it with this solver within GAMS, a commercial suite which makes available in the same environment a library of well proven and established s optimisation algorithms [36].

Considering the nature of this specific case, after a preliminary analysis based on the literature review, the BARON algorithm appeared the one best addressing the RON optimisation problem.

The more extensive is the application field of the model the higher are the associated degrees of freedom (mainly because of the number of combinatory variables required to formalise the problem through a superstructure) with the result of increasing problem complexity and, by consequence, the computational effort needed to solve it.

During the first part of the study, some trials aimed at formalising the model and solving the problem applying the BARON algorithm has been carried out.

The model foresaw combinatory variables indicating the possible existence of more successive steps for permeate purification and retentate splitting and upstream recycling, generating in this way a superstructure similar to the ones described in the literature for other applications (e.g. Saif [39], Kohr [40]).

The resulting superstructure foresaw six combinatory variables, six integer variables, eight real variables and 28 constraints.

The corresponding problem formalisation developed within the GAMS software is annexed in Appendix 8.3.

Unfortunately, maybe because of the high complexity of the specific problem, and notwithstanding several attempts, pursuing this way it was not possible to reach a feasible solution (respecting all given constraints).

Either the BARON algorithm was not able to identify a solution or the GAMS software (which does not dispose of reliable tools for problem formalisation analysis or diagnostic) was returning irreversible errors.

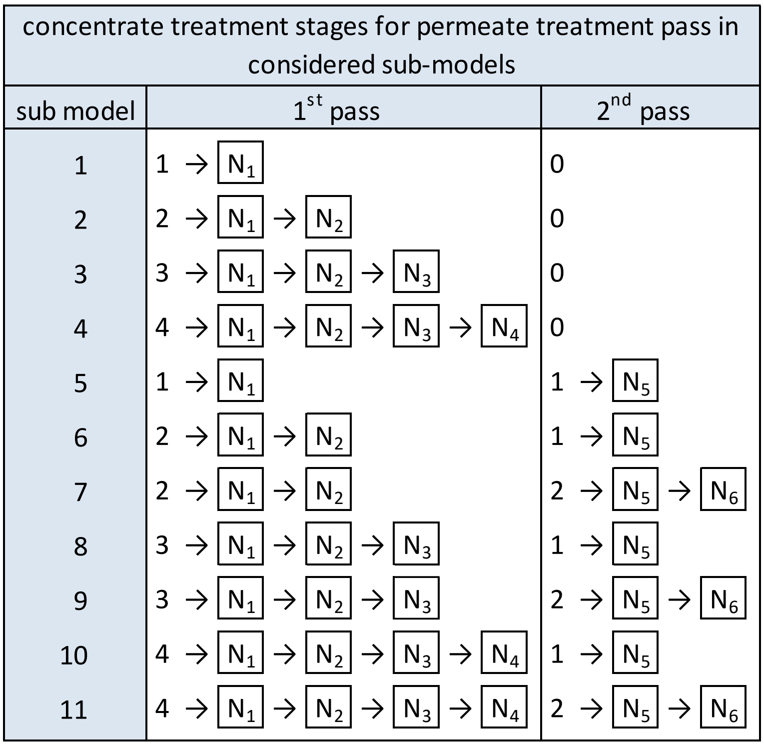
To work around this constraint, a strategy to simplify the problem has been implemented, so to facilitate the task of the solver by reducing the possible solutions domain and eliminating unreasonable and impractical options.

The following strategy was therefore adopted:

- limited to two the maximum number of treatment permeate steps (a higher number of steps is unlikely considering the real applications and investment costs due to the greater pumping needs),
- limited to four the maximum number of retentate treatment stages,
- eliminated the combinatorial variables from the problem formulation of the problem so to avoid to the solver the burden of analysing all the possible alternative combinations,
- problem split into eleven sub-cases (each one characterised by a different formalisation assuming one of the arrangements previously modelled through the combinatorial variables) to solve in parallel,
- a posteriori analysis of the results of the eleven the sub-cases and production of a ranking of results based on the economic result (objective function).

Figure 17 summarises the basic assumptions characteristic of the considered sub-cases: the model must identify for each of the cases the number of membrane elements in parallel (variables N1 ... N6) for each treatment stage.

Each sub-case assumes a fixed number of stages for each step.



concentrate treatment stages for permeate treatment pass in considered sub-models		
sub model	1^{st} pass	2^{nd} pass
1	$1 \rightarrow \boxed{N_1}$	0
2	$2 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2}$	0
3	$3 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2} \rightarrow \boxed{N_3}$	0
4	$4 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2} \rightarrow \boxed{N_3} \rightarrow \boxed{N_4}$	0
5	$1 \rightarrow \boxed{N_1}$	$1 \rightarrow \boxed{N_5}$
6	$2 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2}$	$1 \rightarrow \boxed{N_5}$
7	$2 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2}$	$2 \rightarrow \boxed{N_5} \rightarrow \boxed{N_6}$
8	$3 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2} \rightarrow \boxed{N_3}$	$1 \rightarrow \boxed{N_5}$
9	$3 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2} \rightarrow \boxed{N_3}$	$2 \rightarrow \boxed{N_5} \rightarrow \boxed{N_6}$
10	$4 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2} \rightarrow \boxed{N_3} \rightarrow \boxed{N_4}$	$1 \rightarrow \boxed{N_5}$
11	$4 \rightarrow \boxed{N_1} \rightarrow \boxed{N_2} \rightarrow \boxed{N_3} \rightarrow \boxed{N_4}$	$2 \rightarrow \boxed{N_5} \rightarrow \boxed{N_6}$

Figure 17 - RON Optimisation sub-cases.

After the revision of the strategy, the simplified sub-cases were formalised again for the BARON algorithm application: despite the considerable reduction of the computational load, also, in this case, the results were unsatisfactory.

Depending on the input, the solution was not robust, and frequently the algorithm could not find solutions satisfying the constraints within a reasonable time-frame.

Therefore, since the solution within the GAMS environment was difficult, a different type of algorithm based on a stochastic approach has been rehearsed: the “Simulated Annealing Method”, as modified by Corana [41] for functions defined in a continuous domain.

This algorithm consists of an iterative random search procedure with adaptive moves along the coordinate directions. It foresees uphill steps under the control of probabilistic criteria, so to avoid the first local minima encountered. The term Simulated Annealing is inspired by annealing in metallurgy, a technique to control the size of the crystals through cooling and heating cycles at different velocities: in the case of the algorithm the “changing temperature” controls the probability to make uphill moves.

This method enables us to explore the whole solution domain avoiding to occur in local minima of the objective function.

Figure 18 describes the steps carried out to solve the problem.

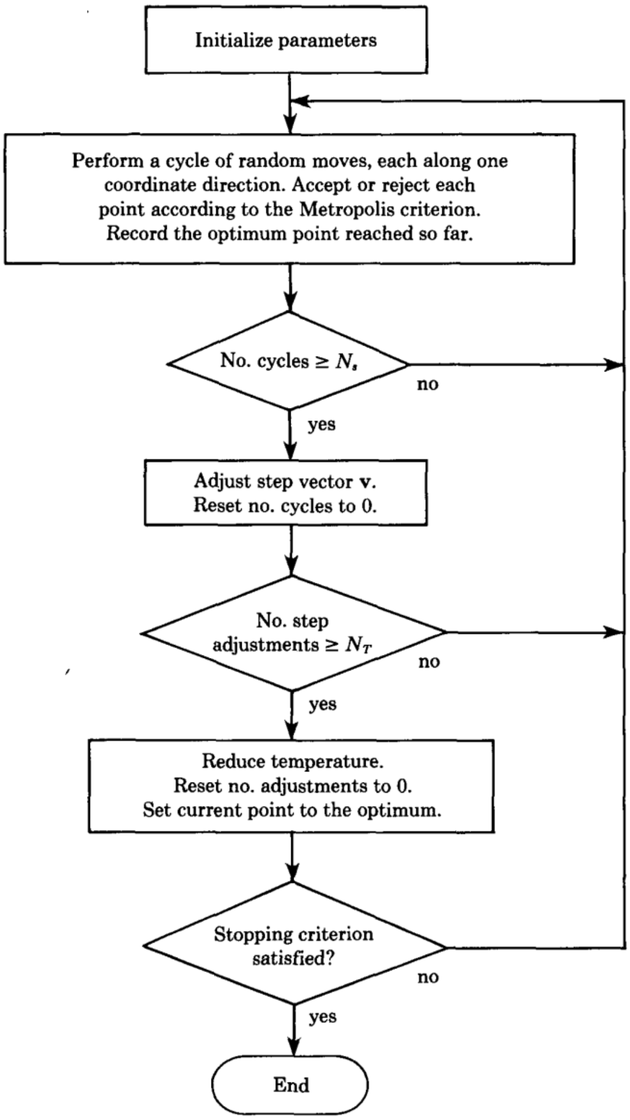


Figure 18 – The SA Optimisation algorithm [41].

The published algorithm does not manage all the types of variable required to formalise our problem, and it has been necessary to modify it to fit this specific problem.

In particular, the original algorithm did neither foresee the use of integer variables (representing in our case the number of RO modules constituting the treatment stages) nor was able to handle dynamic constraints (when the value of a constraint is not fixed but depends on the values assumed by some variables).

Therefore, the algorithm has been modified to be applied in more steps and implementing a strategy useful to transform some of the real variables into integer ones.

Furthermore, to fasten the convergence of the solving process, the economic constraints have been introduced in a second moment, following to the identification of the domain of the solutions feasible from a technical perspective.

This approach leads to satisfactory results for this application.

Based on the results of the numerical test carried out with this approach, and assuming a consistent set of input data, the modified algorithm can be effectively applied to solve this type of application.

The solution algorithm appears robust and is able, in most cases, to identify a set of feasible solutions in a reasonable time (typically less than one minute).

The possible existence of a solution for the considered subproblems depends on the values set for the calculation parameters and the associated operative constraints: in the case of inconsistent input data, it is possible that the algorithm is not able to find a feasible solution.

A software prototype (developed in the Microsoft Visual Studio environment) performing the following functions has been realised:

- Set-up of the model input parameters (listed in Table 7) through a Graphical Interface.
- The formalisation of the subproblems and resolution through the modified SA Algorithm.
- Extraction, elaboration and ranking of the solutions
- Generation of an overall report detailing the relevant results of each solution (number of models for each stage, splits and recycles, operative and investment costs, economic function).

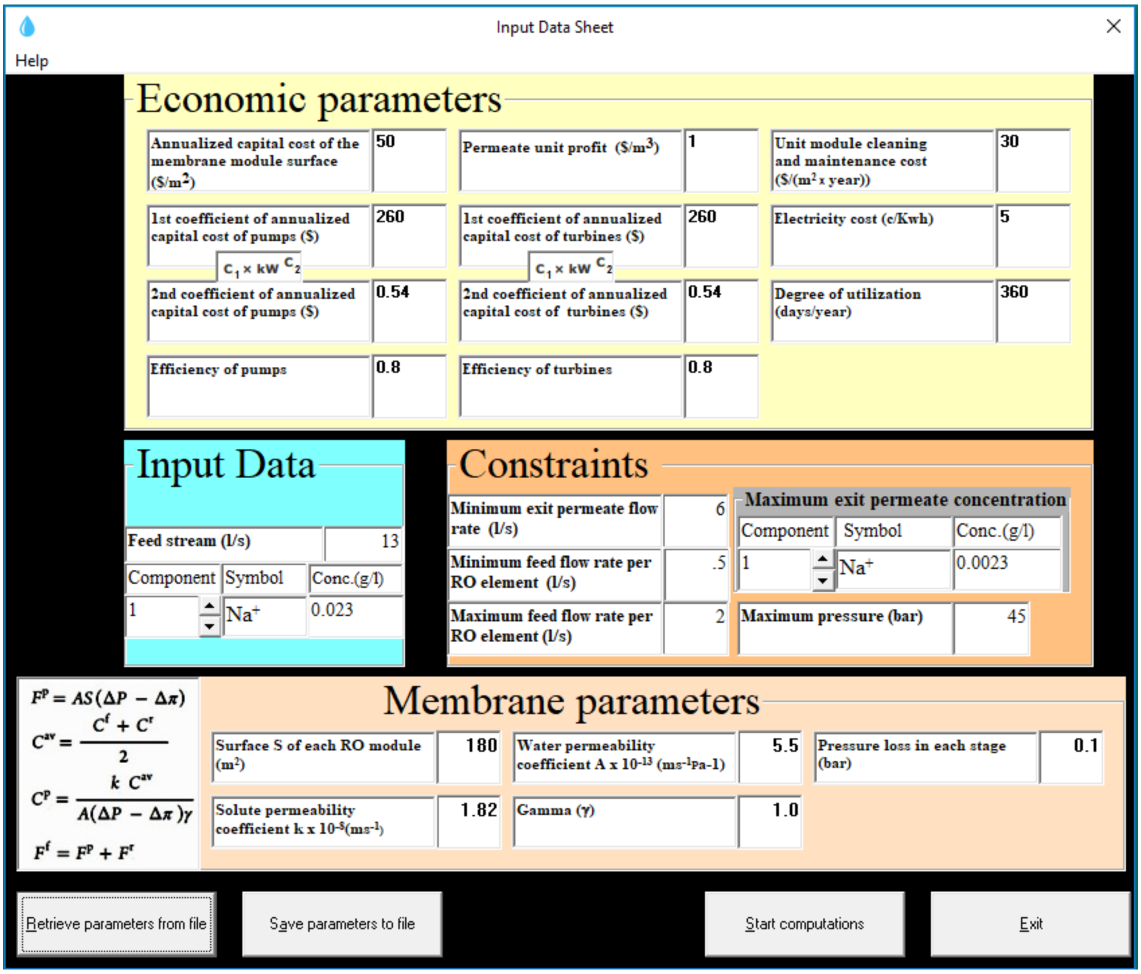
The next paragraph details the results of a run detailing the results of the three more successful configurations for this case.

4.5 Optimal RON Configuration Software – I/O Example

Figure 19 shows the input section of the developed RON Optimisation software: input parameters are grouped in:

- Economic Parameters: parameters for the calculation of capital and operative costs, maintenance costs and revenues.
- Input data: flowrate and contaminants concentration (this application can consider up to eight contaminants) of the feed stream.
- Constraints: membrane modules flowrate constraints, maximum inlet pressure, permeate contaminants concentration (same ions of the feed stream).
- Membrane parameters: information required to calculate, based on Evangelista's shortcut method [37] the separation performance of RO membrane modules.

The software enables to retrieve and store input and to run the optimisation process.



Economic parameters

Annualized capital cost of the membrane module surface ($/m²)	50	Permeate unit profit ($/m³)	1	Unit module cleaning and maintenance cost ($/(m² x year))	30
1st coefficient of annualized capital cost of pumps ($)	260	1st coefficient of annualized capital cost of turbines ($)	260	Electricity cost (c/Kwh)	5
2nd coefficient of annualized capital cost of pumps ($)	0.54	2nd coefficient of annualized capital cost of turbines ($)	0.54	Degree of utilization (days/year)	360
Efficiency of pumps	0.8	Efficiency of turbines	0.8		

$c_1 \times kW^{c_2}$

Input Data

Feed stream (l/s) 13

Component	Symbol	Conc.(g/l)
1	Na^+	0.023

Constraints

Minimum exit permeate flow rate (l/s) 6

Minimum feed flow rate per RO element (l/s) .5

Maximum feed flow rate per RO element (l/s) 2

Maximum exit permeate concentration

Component	Symbol	Conc.(g/l)
1	Na^+	0.0023

Maximum pressure (bar) 45

$$F^p = AS(\Delta P - \Delta\pi)$$

$$C^{av} = \frac{C^f + C^r}{2}$$

$$C^p = \frac{k\ C^{av}}{A(\Delta P - \Delta\pi)\gamma}$$

$$F^f = F^p + F^r$$

Membrane parameters

Surface S of each RO module (m²)	180	Water permeability coefficient A x 10^{-13} ($ms^{-1}Pa^{-1}$)	5.5	Pressure loss in each stage (bar)	0.1
Solute permeability coefficient k x 10^{-8}(ms^{-1})	1.82	Gamma (γ)	1.0		

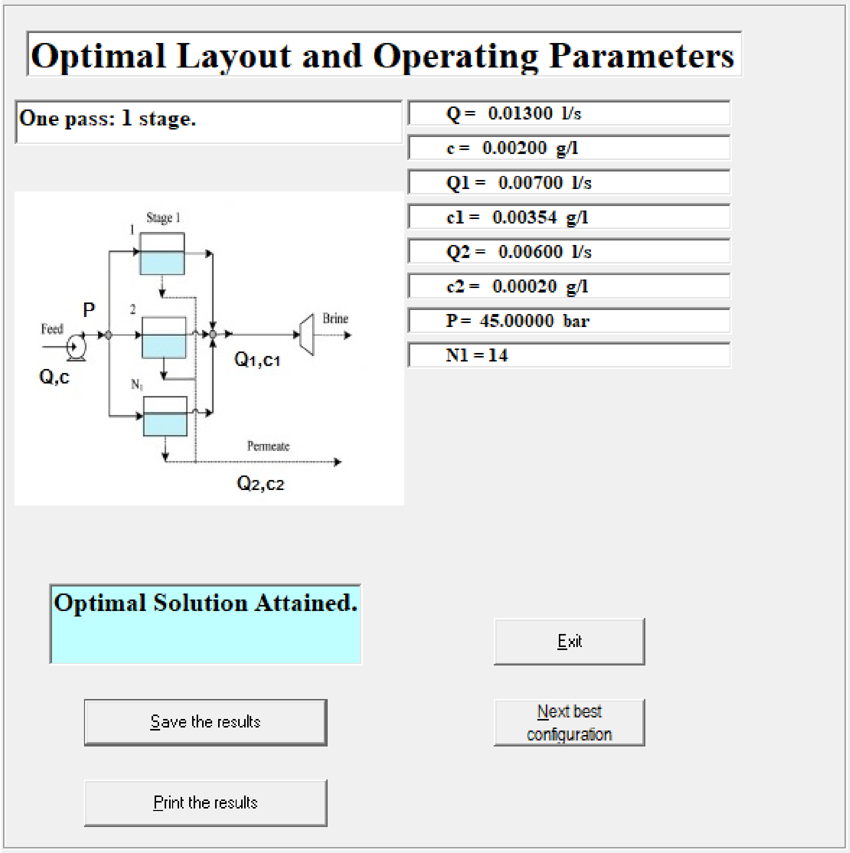
Figure 19 - RON Optimisation software Input Mask.

At the end of the Optimisation Process, the software displays a Report Screen summarising the results.

Starting from the best-ranked option, the interface indicates the corresponding arrangement, the resulting operative parameters (pressures, flow rates and concentrations) the number of modules for each treatment stage as well as the related economic result.

The interface allows to skip to the next best configuration or to save and print out the results. Figure 20 to Figure 22 shows the results of the three best-ranked arrangements for the reported numerical example.

The detailed report is available in Appendix 8.4

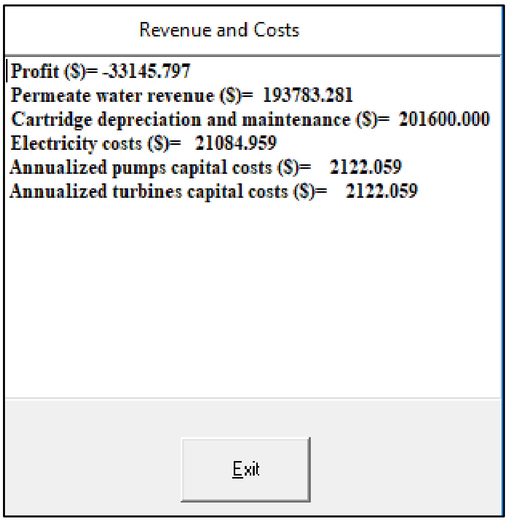


Optimal Layout and Operating Parameters

One pass: 1 stage.

Q = 0.01300 l/s
c = 0.00200 g/l
Q1 = 0.00700 l/s
c1 = 0.00354 g/l
Q2 = 0.00600 l/s
c2 = 0.00020 g/l
P = 45.00000 bar
N1 = 14

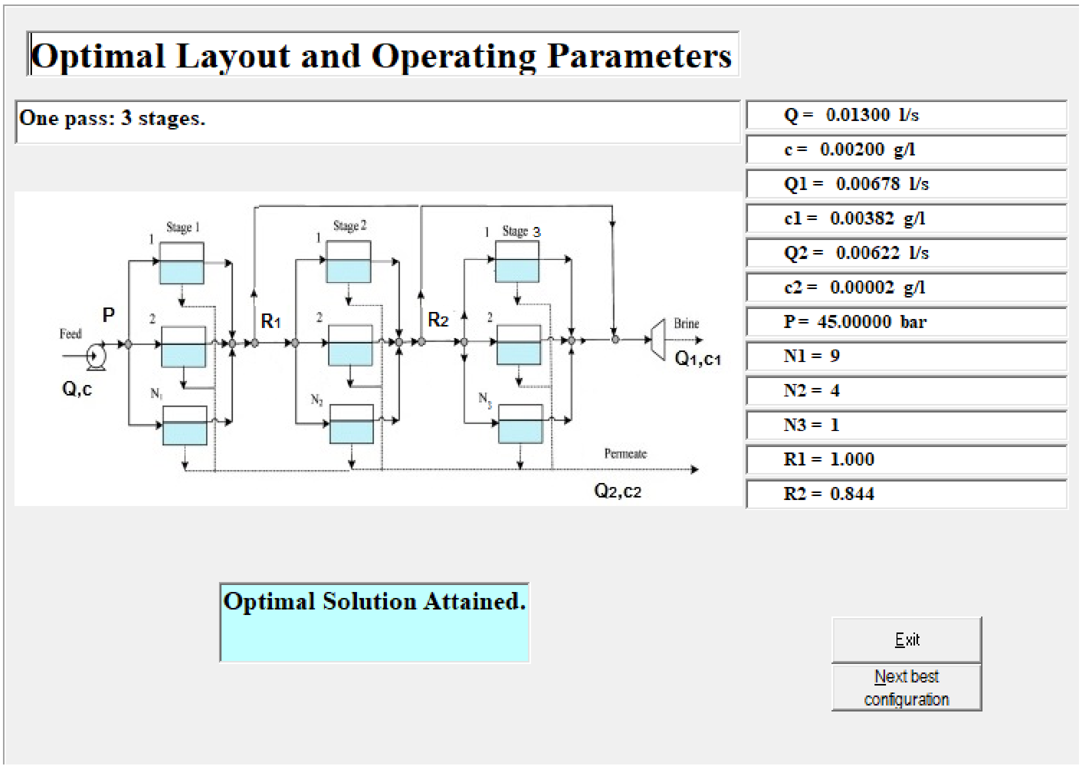
Optimal Solution Attained.



Revenue and Costs

Profit ($)= -33145.797
Permeate water revenue ($)= 193783.281
Cartridge depreciation and maintenance ($)= 201600.000
Electricity costs ($)= 21084.959
Annualized pumps capital costs ($)= 2122.059
Annualized turbines capital costs ($)= 2122.059

Figure 20 – Summary of 1st Ranked Solution Results.

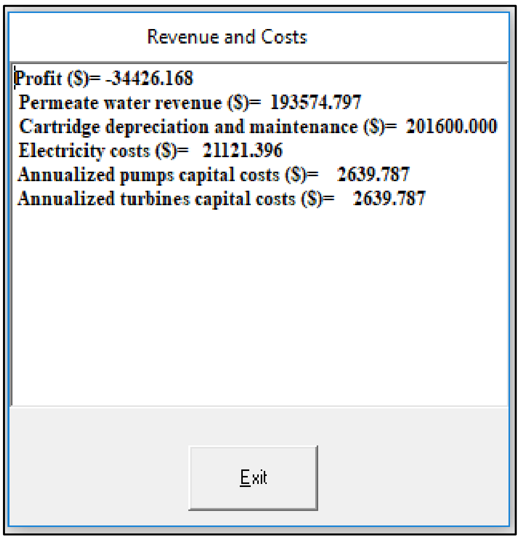


Optimal Layout and Operating Parameters

One pass: 3 stages.

Q = 0.01300 l/s
c = 0.00200 g/l
Q1 = 0.00678 l/s
c1 = 0.00382 g/l
Q2 = 0.00622 l/s
c2 = 0.00002 g/l
P = 45.00000 bar
N1 = 9
N2 = 4
N3 = 1
R1 = 1.000
R2 = 0.844

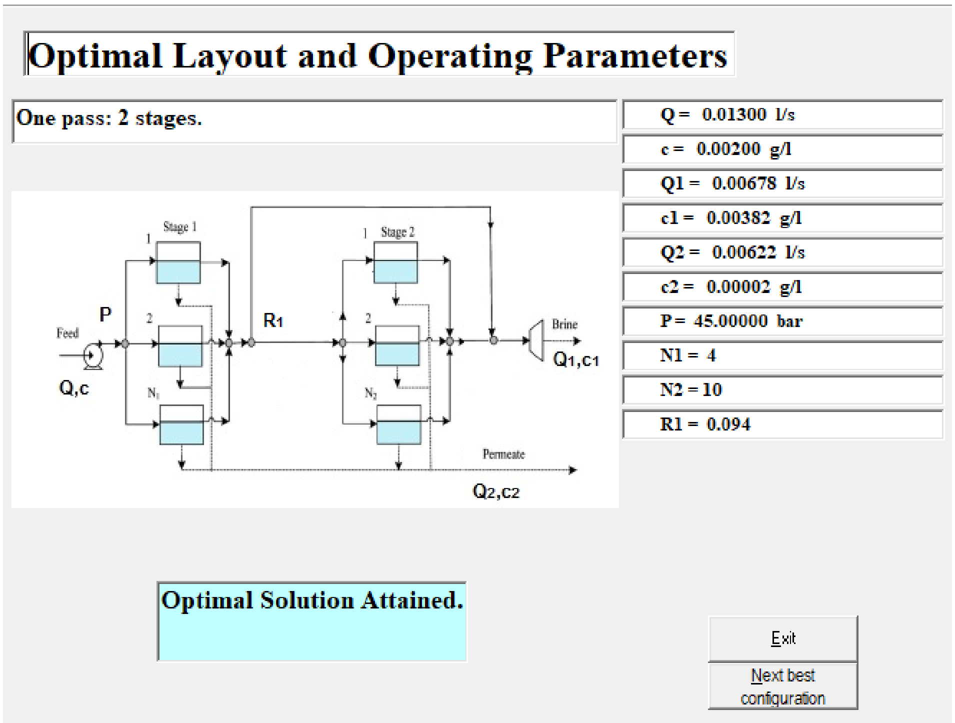
Optimal Solution Attained.



Revenue and Costs

Profit ($)= -34426.168
Permeate water revenue ($)= 193574.797
Cartridge depreciation and maintenance ($)= 201600.000
Electricity costs ($)= 21121.396
Annualized pumps capital costs ($)= 2639.787
Annualized turbines capital costs ($)= 2639.787

Figure 21 – Summary of 2nd Ranked Solution Results.

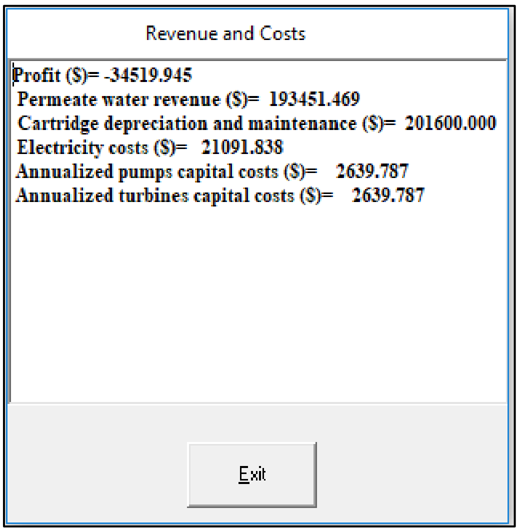


Optimal Layout and Operating Parameters

One pass: 2 stages.

Q = 0.01300 l/s
c = 0.00200 g/l
Q1 = 0.00678 l/s
c1 = 0.00382 g/l
Q2 = 0.00622 l/s
c2 = 0.00002 g/l
P = 45.00000 bar
N1 = 4
N2 = 10
R1 = 0.094

Optimal Solution Attained.



Revenue and Costs

Profit ($)= -34519.945
Permeate water revenue ($)= 193451.469
Cartridge depreciation and maintenance ($)= 201600.000
Electricity costs ($)= 21091.838
Annualized pumps capital costs ($)= 2639.787
Annualized turbines capital costs ($)= 2639.787

Figure 22 – Summary of 3rd Ranked Solution Results.

5 Conclusions

As the pressure on companies for profitability and environmental sustainability increases, advanced process design techniques are required.

In particular, process integration and intensification strategies are crucial instruments for the minimisation of energy and raw materials consumption. In the food industry, energy and water are the main utilities that need minimising.

The first step to be carried out is the correct estimation of the amounts of temperatures, water and contaminants flowrates in each stream. In the case of the food industry, the usual data reconciliation techniques are to be complemented with the information on the amount of water contained in the products. In other words, water is both a utility and a reagent.

The results obtained during the present research activity can be summarized as follows:

- the inclusion of statistical fluctuations in the composition of water in products, obtained by modifying the usual reconciliation algorithms;
- the estimate the water savings obtainable, through the application of a well-established water pinch methodology;
- the identification of the optimal arrangement of a RON (Process Synthesis problem) which involved the use of a modified Simulated Annealing algorithm (as the BARON algorithm proved to fail in the present case).

Regarding the first point, the method developed in this thesis (based on a Bayesian analysis) combines the plant measurements used in traditional reconciliation procedures with the information provided by the product quality control routinely carried out in most plants.

Indeed, it is a strategy that could be used more generally whenever mass and energy balances involve both process streams and products, and therefore it can be regarded as a significant result obtained in this dissertation work.

The increased reliability resulting from the suggested approach is particularly interesting in the case of industrial complexes like the one approached during the execution of this research, where the lack of measurement redundancy and the existence of non-measurable streams (like water losses for evaporation) risk to introduce systematic errors within the reconciliation process.

Since it is unlikely that plant owners make investments to increase the number of measurements, a practical strategy is to exploit the availability of information produced occasionally by the quality control system to improve the results of the validation process.

Once correct process data are available after the reconciliation step, pinch methodologies usually provide powerful methods for the minimisation of both energy and water consumption, as they have become standard techniques in both design and retrofitting activities. In the food plant considered in this dissertation, pinch techniques made it possible to identify the streams to be subjected to (possibly partial) purification to minimise costs while complying with the constraints set by environmental regulations.

Unfortunately, the data protection policies of the industrial operator which provided the information applied in this context did not allow to deepen the possibility to switch freshwater quality grades inside process phases which, by consequence, have forcibly been considered as black boxes with fixed demand of freshwater grades.

Notwithstanding this constraint, the analysis of the Retrofit Case highlighted the potential saving of the 8% of the fresh water supplied to the primary separation phases (Wet Milling, Dry Milling, By Products), corresponding to an overall reduction of about 140,000 tons/year.

Further savings are probably achievable entering in the detail of each processing phase and assessing the actual quality constraints and redefining the freshwater demand for each grade.

Lastly, the mathematical programming approach can conveniently complement the traditional pinch analysis, using the results provided by it as a starting point for the final optimisation. However, the resulting mixed-integer nonlinear, nonconvex problem can turn out to be too complicated even for powerful algorithms such as Baron or Couenne (the latter in the public domain).

In particular, the binary variables representing different plant configurations (the superstructure) can give rise to challenging difficulties which have been directly experienced also in the process synthesis study deepened during the last part of the research work.

The approach followed in this dissertation to overcome these limitations was to analyse different configurations separately and to compare the optimal values obtained for each one for the final selection.

This approach resulted practical and robust and permitted to identify a feasible solution in most cases: an outcome of this experience is that, notwithstanding the increasing computation availability, it is advisable to make any possible effort to control the computational burden by limiting the domain of possible solutions to the practical and feasible ones.

To this purpose, a stochastic optimisation algorithm (the simulated annealing algorithm) has been modified to deal with the presence of integer variables corresponding to the number of units and applied it to the identification of the optimal configuration of a reverse osmosis network.

The original algorithm has been modified to handle integer variables and to manage dynamic constraints. It has therefore been applied in more steps implementing a strategy useful to transform some of the real variables into integer ones.

Furthermore, to ease the convergence of the solving process, the economic constraints have been introduced in a second stage, following to the identification of the domain of the solutions feasible from a technical perspective.

The results published in this thesis do not correspond to the actual case considered because of the confidentiality requirement. The purification of production water (whose qualitative composition is well known even if the concentrations of contaminants can vary considerably) was considered instead. This example proved both robustness and efficiency of the resulting algorithm that provided the optimal solution for a wide range of concentrations.

Thus, the three main steps necessary for the optimal design of a biorefinery have been tackled in this dissertation and for both the reconciliation of data and the optimal design original algorithms have been developed.

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8 Appendices

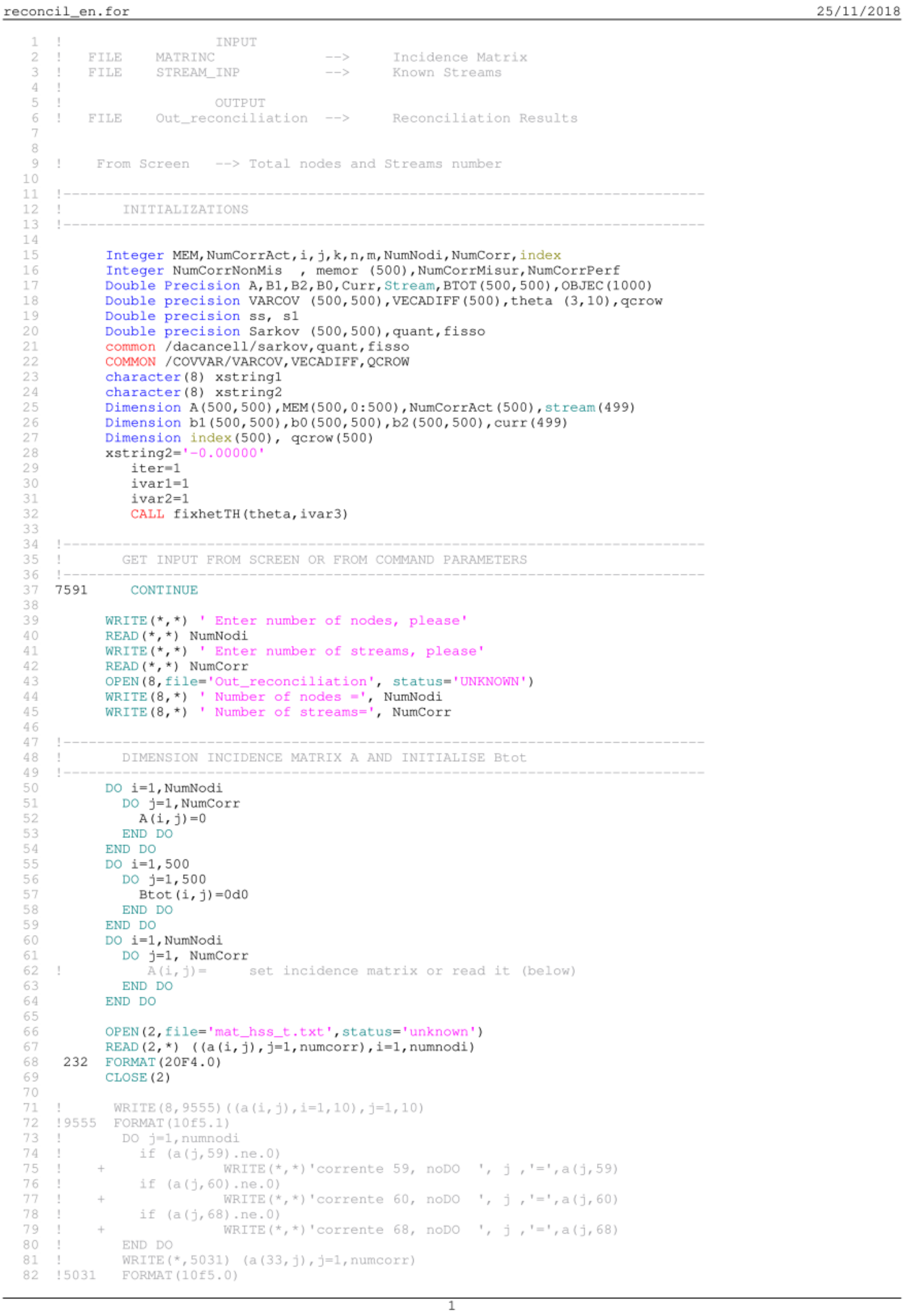
8.1. Basic Reconciliation Software Code

8.2. PCA study on water consumption seasonality

8.3. RON problem formalisation for BARON in GAMS

8.4. RON Optimisation software detailed report example

8.1 Basic Reconciliation Software Code



reconcil_en.for 25/11/2018

```
!                  INPUT
!   FILE    MATRINC             -->     Incidence Matrix
!   FILE    STREAM_INP          -->     Known Streams
!
!                  OUTPUT
!   FILE    Out_reconciliation  -->     Reconciliation Results


!    From Screen   --> Total nodes and Streams number

!----------------------------------------------------------------------------
!       INITIALIZATIONS
!----------------------------------------------------------------------------

      Integer MEM,NumCorrAct,i,j,k,n,m,NumNodi,NumCorr,index
      Integer NumCorrNonMis  , memor (500),NumCorrMisur,NumCorrPerf
      Double Precision A,B1,B2,B0,Curr,Stream,BTOT(500,500),OBJEC(1000)
      Double precision VARCOV (500,500),VECADIFF(500),theta (3,10),qcrow
      Double precision ss, s1
      Double precision Sarkov (500,500),quant,fisso
      common /dacancell/sarkov,quant,fisso
      COMMON /COVVAR/VARCOV,VECADIFF,QCROW
      character(8) xstring1
      character(8) xstring2
      Dimension A(500,500),MEM(500,0:500),NumCorrAct(500),stream(499)
      Dimension b1(500,500),b0(500,500),b2(500,500),curr(499)
      Dimension index(500), qcrow(500)
      xstring2='-0.00000'
         iter=1
         ivar1=1
         ivar2=1
         CALL fixhetTH(theta,ivar3)

!----------------------------------------------------------------------------
!       GET INPUT FROM SCREEN OR FROM COMMAND PARAMETERS
!----------------------------------------------------------------------------
7591     CONTINUE

      WRITE(*,*) ' Enter number of nodes, please'
      READ(*,*) NumNodi
      WRITE(*,*) ' Enter number of streams, please'
      READ(*,*) NumCorr
      OPEN(8,file='Out_reconciliation', status='UNKNOWN')
      WRITE(8,*) ' Number of nodes =', NumNodi
      WRITE(8,*) ' Number of streams=', NumCorr

!----------------------------------------------------------------------------
!       DIMENSION INCIDENCE MATRIX A AND INITIALISE Btot
!----------------------------------------------------------------------------
      DO i=1,NumNodi
        DO j=1,NumCorr
          A(i,j)=0
        END DO
      END DO
      DO i=1,500
        DO j=1,500
          Btot(i,j)=0d0
        END DO
      END DO
      DO i=1,NumNodi
        DO j=1, NumCorr
!          A(i,j)=     set incidence matrix or read it (below)
        END DO
      END DO

      OPEN(2,file='mat_hss_t.txt',status='unknown')
      READ(2,*) ((a(i,j),j=1,numcorr),i=1,numnodi)
 232  FORMAT(20F4.0)
      CLOSE(2)

!      WRITE(8,9555)((a(i,j),i=1,10),j=1,10)
!9555  FORMAT(10f5.1)
!       DO j=1,numnodi
!         if (a(j,59).ne.0)
!    +              WRITE(*,*)'corrente 59, noDO  ', j ,'=',a(j,59)
!         if (a(j,60).ne.0)
!    +              WRITE(*,*)'corrente 60, noDO  ', j ,'=',a(j,60)
!         if (a(j,68).ne.0)
!    +              WRITE(*,*)'corrente 68, noDO  ', j ,'=',a(j,68)
!       END DO
!       WRITE(*,5031) (a(33,j),j=1,numcorr)
!5031   FORMAT(10f5.0)
```

1

```
!       STOP
      OPEN(2,file='errlog',status='unknown')
      noerror=0
!      DO i=1,NumNodi
!        WRITE(8,*)  (a(i,j),j=1,numcorr)
!      END DO

!      Check all streams must be in at least one node
       DO k=1,Numcorr
         ij=0
         DO I=1,NumNodi
!          IF (A(I,K).NE.1.and.A(i,k).ne.-1.and.A(i,k).ne.0) then
!            WRITE (8,*)i,k
!            STOP
!          ENDIF
           IF (ABS(A(I,K)).GT.1.e-3) IJ=1
         END DO
         IF(IJ.EQ.0) THEN
           noerror=1
           WRITE(2,*) '  STREAM ',k,' IS NOT PRESENT IN INCIDENCE MATRIX'
         ENDIF
       END DO

!      Check at least 2 streams per node
       DO i=1,NumNodi
         ij=0
         DO k=1,NumCorr
           IF (ABS(A(I,K)).GT.1.e-3) IJ=IJ+1
         END DO
         IF(IJ.LT.2) THEN
           noerror=1
           WRITE(2,*) '  LESS THAN 2 STREAMS ARE PRESENT IN NODE', IJ
         ENDIF
       END DO
       IF (noerror.eq.1) then
         WRITE(8,2909)
2909     FORMAT(' The incidence matrix is not correct.'/
     +   ' See the errlog file.'/' The Programme is terminated.')
         STOP
       ENDIF
       OPEN (1,file='hss_t.txt',status='UNKNOWN',ERR=99)
       k=1
       DO J=1,NumCorr
         READ(1,*,END=99) index(k),curr(k)
!        WRITE(*,*)k, index(k),curr(k)
         km1=k-1
         DO iu=1,km1
           IF (index(k).eq.index(iu)) then
             WRITE(8,5098) index(k)
5098         FORMAT(' Value of stream ',I4,' has already been entered'/
     +            'New value ignored')
             GOTO 8111
           ENDIF
         END DO
         WRITE(xstring1,'(f8.5)') curr(k)
         IF (xstring1.ne.xstring2) then
           k=k+1
!          WRITE(*,*)k
         ENDIF
8111     CONTINUE
       END DO
99     CONTINUE
      CLOSE(1)
      NumCorrMisur=k-1
      NumCorrNonMis=NumCorr-NumCorrMisur

!----------------------------------------------------------------------------
!   For each node i memorise in MEM(I,J) the indexes of the entering (+)
!   or exiting (-) streams (J from 1 to NumCorrAct(i)) (not yet used )
!----------------------------------------------------------------------------
      DO i=1,NumNodi
        J=0
        DO k=1,NumCorr
          IF (A(i,k).NE.0) THEN
            J=J+1
            MEM(I,J)=K
            IF(A(i,k).LT.0) MEM(i,j)=-K
          ENDIF
        END DO
        NumCorrAct(i)=J
      END DO

```

```fortran
!----------------------------------------------------------------------------
!   Streams in increasing order:
!    memor(2), for example =18 > memor(1) for example =2  (streams 1 and
!       3-17 not measured) -->   memor(1)=2   memor(2)=18 ecc
!----------------------------------------------------------------------------
      j=1
      k=1
      DO while (j.ne.NumCorrMisur+1)
        DO i=1,numcorrMisur
          IF(k.eq.index(i)) then
            stream(j)=curr(i)
            memor(j)=index(i)
            j=j+1
          ENDIF
        END DO
        k=K+1
      END DO
      NumCorrPerf=0
      GOTO 9022

!----------------------------------------------------------------------------
!      matrix b0 streams with no measurement error
!----------------------------------------------------------------------------
!       Temporary Start
!       Section to be improved through direct input interpretation
       j1=5
       j2=50
       NumCorrPerf=2
       DO i=1,NumNodi
         b0(i,1)=a(i,j1)
         b0(i,2)=a(i,j2)
       END DO
!      Temporary END
!----------------------------------------------------------------------------
9022   CONTINUE

!----------------------------------------------------------------------------
!      matrices b1 streams with measurement error and b2 non measured
!----------------------------------------------------------------------------
      m=1
      k=1
      L=1
!     Btot includes b0 (no measurement error) & b1 (with measurement error)
!     Does not include b2 (not measurd) L(Btot), M(b1), K(b2)
      DO j=1,numCorr
        IF(j.eq.j1.or.j.eq.j2) then
          DO i=1,numNodi
            btot(i,L)=a(i,j)
          END DO
          L=L+1
          GOTO 34
        END IF
        DO i=1,numcorrMisur
          IF (j.eq.index(i)) goto 33
        END DO
        DO i=1,numNodi
          b2(i,k)=a(i,j)
        END DO
        k=k+1
        GOTO 34
33      CONTINUE
        DO i=1,numNodi
          b1(i,m)=a(i,j)
          btot(i,l)=a(i,j)
        END DO
        m=m+1
        L=L+1
34      CONTINUE
      END DO

      CALL FISSAVAR(NumCorrMisur,stream,memor,theta,ivar1,ivar2,ivar3)

!----------------------------------------------------------------------------
!
!                       * START MATRIX OPERATIONS *
!
!----------------------------------------------------------------------------
      CALL FINEPREPAR(b0,b1,b2,500,stream,index,NumNodi,NumCorr,
                    + numcorrMisur,NumCorrNonMis,j1,j2,NumCorrPerf,memor,BTOT,a)

!     STATISTICAL CHECKS
      Ss=0.d0
```

```
      DO j=1,NumCorrMisur
!i
!       Ss=Ss+vecadiff(j)*vecadiff(j)/qcrow(j)
        Ss=Ss+vecadiff(j)*vecadiff(j)/sarkov(j,j)
      END DO
      WRITE(*,*)ss,numcorrmisur
      STOP
      numv=10*(Ivar1-1)+Ivar2
      objec(numv)=SS
      WRITE(8,2014)SS    ,numv
2014  FORMAT(' Objective function= ',D15.5,i5)
      IF (ivar3.eq.0) THEN
        ivar2=ivar2+1
        IF (ivar2.gt.10) THEN
          ivar1=ivar1+1
          IF (ivar1.gt.10) GOTO 78
            ivar2=1
          ENDIF
          GOTO 7591
        ELSE
          ivar3=ivar3+1
          IF (ivar3.gt.10) THEN
            ivar2=ivar2+1
            ivar3=1
            IF (ivar2.gt.10) THEN
              ivar1=ivar1+1
              IF (ivar1.gt.10) GOTO 1678
              ivar2=1
            ENDIF
          ENDIF
        ENDIF
        iter=iter+1
        GOTO 7591
1678    CONTINUE
        IF (ivar3.eq.0) THEN
          DO i=1,10
            k=10*(i-1)
            DO j=1,10
              kk=k+j
              WRITE(8,*)kk, objec(kk),theta(1,i),theta(2,j)
            END DO
          END DO
        ELSE
          DO m=1,10
            k1=10*(m-1)
            DO i=1,10
              k2=k1+10*(i-1)
              DO j=1,10
                kk=k2+j
                WRITE(8,*)kk, objec(kk),theta(1,m),theta(2,i),theta(3,j)
              END DO
            END DO
          END DO
        ENDIF
        STOP
      END
```

```
      !-------------------------------------------------------------------
      SUBROUTINE fixhetTH(theta,ivar3)
            Double precision theta (3,10)
            DO i=1,10
              theta (2,i)=.111D0*DBLE(I-1)
            END DO
            theta (1,1)=.01D0
            theta (1,2)=.05D0
            theta (1,3)=.1D0
            theta (1,4)=.5D0
            theta (1,5)=1.D0
            theta (1,6)=2.D0
            theta (1,7)=5.D0
            theta (1,8)=10.D0
            theta (1,9)=20.D0
            theta (1,10)=50.D0
            ivar3=0
            RETURN
      END
      !-------------------------------------------------------------------

      !-------------------------------------------------------------------
      SUBROUTINE FISSAVAR(numCorrMisur,stream,memor,theta,iv1,iv2,iv3)
            Double precision stream ,AA, theta (3,1),qcrow(500)
            Double precision VARCOV (500,500),VECADIFF(500)
            COMMON /COVVAR/VARCOV,VECADIFF,QCROW
            dimension stream(1),memor(1)
            Double precision Sarkov (500,500),quant,fisso
            common /dacancell/sarkov,quant,fisso
            quant=.065D0
            fisso=.02D0
            DO i=1,NumCorrMisur
              DO j=1,NumCorrMisur
                VARCOV(i,j)=0d0
                sarkov(i,j)=0d0
              END DO
            END DO

            !----------------------------------------------
            DO j=1,NumCorrMisur
              VARCOV(j,j)=dabs(stream(j))*quant
              IF (dabs(varcov(j,j)).lt.1d-4)varcov(j,j)=1d-4
                sarkov(j,j)=fisso+varcov(j,j)*varcov(j,j)
            END DO
            RETURN
            !----------------------------------------------

            DO i=1,NumCorrMisur
              AA=(stream(i)*stream(i))**theta(2,iv2)
              VARCOV(i,i)=theta(1,iv1)*AA
              IF (VARCOV(i,i).lt.1.D0) VARCOV(i,i)=100.D0
                k=memor(i)
                IF(k.eq.5.or.k.eq.50) then
                  VARCOV(i,i)=VARCOV(i,i)*0.0001D0
                ENDIF
            END DO
            RETURN
      END
      !-------------------------------------------------------------------
```

```
      !--------------------------------------------------------------------
      SUBROUTINE FINEPREPAR(b0,b1,b2,NMAX,stream,index,NumNodi,NumCorr,
             +   numcorrMisur,NumCorrNonMis,j1,j2,NumCorrPerf,memor,BTOT,matnod)
            Dimension ip(500)  ,memor(500)
            Double precision b0,b1,b2,stream,YT(500,500),StreamErr(500)
            Double precision SM,TAU ,BTOT(500,500),matnod(500,500),BD(500,500)
            Double Precision StreamPrec(500),STOR(500,500),smem(500),STEX(500)
            Dimension b0(500,Numcorr),b1(500,NumCorr),b2(500,Numcorr),
             +    stream(NumcorrMisur),index(NumCorrMisur)
            Double precision Y(500,500),S(500),W(1000),B2T(500,500)

            DO i=1,NumNodi
              DO j=1,NumCorrNonMis
                B2T(j,i)=B2(i,j)
              END DO
            END DO
            CALL SVDRS (B2T, Nmax, NumCorrNonMis, NumNodi, Y, 500,0,S,W)
            ITROVA=0
            DO i=1,NumCorrNonMis
              IF (ITROVA.EQ.0) THEN
                IF (DABS(S(I)).LT.1.E-9) ITROVA=I
              ENDIF
            END DO
            IF (itrova.gt.0) then
              it=itrova-1
              ii=  NumCorrNonMis-it
              DO i=1, ii
                DO j=1,NumNodi
                  Y(j,i)=B2T(j,i+it)
                END DO
              END DO
            ENDIF

            CALL FAQR(b2,numnodi,NumCorrNonMis, ii,Btot,NumCorrMisur,stream,
                        + index,memor,matnod)
            RETURN
      END
      !--------------------------------------------------------------------

      !--------------------------------------------------------------------
      SUBROUTINE QCROWE(V,DUM3,NumCorrMisur,mminh,work)
            COMMON /COVVAR/VARCOV, VECADIFF, QCROW
            Double Precision dum3, v, work,s
            Dimension dum3(500,500),v(500,500),work(500,500)
            Double PRECISION VARCOV(500,500), VECADIFF(500), QCROW(500)

            DO i=1,mminh
              DO j=1,NumCorrMisur
                s=0.D0
                DO k=1,mminh
                !   Remind v is H-1 and must be multiplied by dum3 transposed
                !   (for this reason dum3 indexes are swapped)
                  s=s+v(i,k)*dum3(j,k)
                END DO
                work(i,j)=s
              END DO
            END DO
            DO i=1,NumCorrMisur
              DO j=1,NumCorrMisur
                s=0.D0
                DO k=1,mminh
                  s=s+dum3(i,k)*work(k,j)
                END DO
                if(i.eq.j) qcrow(j)=s
              END DO
            END DO
            RETURN
      END
      !--------------------------------------------------------------------
```

```
      !---------------------------------------------------------------------
      SUBROUTINE FAQR(A,M,N,II,BTOT,NumCorrMisur,stream,index,memor,mat)
            Double PRECISION A(500,500),qrau(5000),work(900000),H(500,500,500)
            Double PRECISION r(500,500),sss,VARCOV(500,500), VECADIFF(500)
            COMMON /COVVAR/VARCOV, VECADIFF, QCROW
            Double precision tau(5000),stream(500),mat(500,500)
            Double PRECISION v(500,500),q(500,500),DUM1(500,500),DUM2(500,500)
            Double precision DUM3(500,500) ,dum4(500,500),BTOT(500,500)
            Double precision  z(3,3) , soloprova(500,500)
            Double precision qcrow(500)
            integer jpvt(5000) ,index(500),memor(500),indnonmis(500)
            logical ridon(500)
            logical observ(500)

            nstr=n+NumCorrMisur
            k=1
            iu=1
903         DO i=1,NumCorrMisur
              IF (k.eq.index(i)) THEN
                k=k+1
                GOTO 103
              ENDIF
            END DO
            indnonmis(iu)=k
            k=k+1
            iu=iu+1
103         CONTINUE
            IF (k.le.nstr) GOTO 903
            WRITE(8,*)' UNMEASURED STREAMS'
            WRITE(8,487)  (indnonmis(iu),iu=1,N)
487         FORMAT(18i4)
587         FORMAT(30L2)
            LDA=500
            ! n  -->  NumCorrNonMis
            !         CALL perprova (m,n,z,A)
            NumCorrNonMis  =n
            DO j=1,m
              DO i=1,n
                dum4(j,i)=a(j,i)
                soloprova(j,i)=a(j,i)
              END DO
            END DO
99          FORMAT(4f15.6)
            DO i=1,n
              tau(i)=0d0
              jpvt(i)=0
            END DO
            lwork=500000
            Numnodi=m
            lda=500
            CALL DGEQP3(m,n,a,lda,jpvt,tau,work,lwork,info)
            DO j=1,m
              DO i=1,n
                r(j,i)=a(j,i)
                IF (i.lt.j) r(j,i)=0.d0
              END DO
            END DO
            it=m-1
            IF(it.gt.n)it=n
            DO num =1,it
              IF (num.gt.1) THEN
                DO j=1,num-1
                  v(num,j)=0.d0
                END DO
              ENDIF
              v(num,num)=1d0
              DO j=num+1,m
                v(num,j)=a(j,num)
              END DO
              DO k=1,m
                DO i=1,m
                  H(k,i,num)=0.d0
                END DO
                H(k,k,num)=1.d0
              END DO
              DO k=num,m
                DO i=num,m
                  H(k,i,num)=H(k,i,num)-v(num,k)*v(num,i)*tau(num)
                END DO
              END DO
            END DO
            DO k=1,m
```

```
              DO i=1,m
                dum1(k,i)=h(k,i,it)
              END DO
            END DO
            num=it- 1
            DO WHILE (NUM.GE.1)
              DO k=1,m
                DO i=1,m
                  dum2(k,i)=h(k,i,num)
                END DO
              END DO
              CALL MMUL(DUM2,lda,m,m,DUM1,lda,m,DUM3,lda)
              DO k=1,m
                DO i=1,m
                  dum1(k,i)=dum3(k,i)
                END DO
              END DO
              num=num-1
            END DO
            DO k=1,m
              DO i=1,m
                q(k,i)=dum3(k,i)
              END DO
            END DO

           !TO CHECK A=qrP     GOTO 8765
           !goto 8765
            ih=n
            DO i=1,n
              IF(dabs(r(i,i)).lt.1.d-6) then
                ih=i-1
                GOTO 79
              ENDIF
            END DO
79          CONTINUE

            nminh=n-ih
            mminh=m-ih

            DO i=1,m
              DO k=1,mminh
                dum1(i,k)=q(i,k+ih)
                dum3(k,i)=q(i,k+ih)
              END DO
              DO k=1,ih
                a(k,i)=q(i,k)
              END DO
            END DO

            !WRITE(8,*) 'Indice R1 e matrice R1'
            !WRITE(8,800)ih,((dum1(i,k),i=1,m),k=1,nminh)
800         FORMAT('   ih=',i10/(5F15.6))

            !To check ortogonality of product B2*Q2T goto 8090
            !goto 8090

            !       COMPUTATION OF ADJUSTED MEASURES    <------------>
            CALL MMUL(dum3,lda,mminh,m,btot,lda,NumCorrMisur,dum2,lda)

            DO i=1,mminh
              DO j=1,NumCorrMisur
                dum1(j,i)=dum2(i,j)
              END DO
            END DO

            !      dum2 =  F            =q2t*(b0+B1 =BTOT)
            !      dum1 =  FT

            DO j=1,NumCorrMisur
              RIDON(J)=.FALSE.
              DO i=1,mminh
                IF(dabs(dum2(i,j)).gt.1.e-6) then
                  RIDON(J)=.TRUE.
                  GOTO 56
                ENDIF
              END DO
56            CONTINUE
            END DO
            WRITE(8,965)
965         FORMAT(//' List of Redundant T and Non-Redundant F Measurements')
            WRITE(8,587)(riDOn(j),j=1,NumCorrMisur)
```

```fortran
            DO i=1,NumCorrMisur
              DO j=1,NumCorrMisur
                v(i,j)=VARCOV(I,J)
              END DO
            END DO

            CALL MMUL(v,lda,NumCorrMisur,NumCorrMisur,DUM1,lda,mminh,dum3,lda)
            !      dum2= F= q2t*(b0+B1 =BTOT)
            !      dum1 =  FT
            !      dum3 = V*FT
            CALL MMUL(dum2,lda,mminh,NumCorrMisur,dum3,lda,mminh,v,lda)
            CALL MATINV(v,lda,mminh,info)

            !--- Eteroscedasticity Optimisation ----------------------
            CALL QCROWE(V,DUM3,NumCorrMisur,mminh,work)
            CALL MATINV(VARCOV,lda,numcorrmisur,info)
            ! -------------------------------------------------------------

            CALL MMUL(dum3,lda,NumCorrMisur,mminh,v,lda,mminh,a,lda)
            CALL MMUL(a,lda,NumCorrMisur,mminh,dum2,lda,NumCorrMisur,dum4,lda)
            CALL MMUL(dum4,lda,NumCorrMisur,NumCorrMisur,stream,lda,1,work,lda)

            ! To check experimental values go to 7442
            WRITE(8,817)
817         FORMAT(/' ADJUSTMENT OF MEASURED FLOW RATES'/15X,' Stream N.',
                 +  '     Measured value', '    Reconstructed value')
            sss=0d0
            DO j=1,NumCorrMisur
              vecadiff(j)=work(j)
              work(j)=-work(j)+stream(j)
              WRITE(8,88) memor(j), stream(j),work(j)
88            FORMAT(10X,I10,2f20.6)
            END DO

            !________________________________________________________________________

            DO  i=1,ih
              DO k=1,ih
                dum1(i,k)=r(i,k)
              END DO
            END DO
            DO  i=1,ih
              DO k=1,nminh
                dum2(i,k)=r(i,k+ih)
              END DO
            END DO

            CALL MATINV(dum1,lda,ih,info)
            CALL MMUL(dum1,lda,ih,ih,dum2,lda,nminh,dum3,lda)

            DO i=ih+1,n
              lperm=jpvt(i)
              observ(lperm)=.FALSE.
            END DO

            DO i=1,ih
              lperm= jpvt(i)
              Observ(lperm)=.TRUE.
              DO j=1,nminh
                IF(dabs(dum3(i,j)).gt.1d-6) THEN
                  LPerm=jpvt(i)
                  Observ(Lperm)=.FALSE.
                  GOTO 58
                ENDIF
              END DO
58            CONTINUE
            END DO

            WRITE(8,568)
568         FORMAT(///' List of Observable T and Non-Observable F Unmeasured'
                + 1X, ' Streams')

            WRITE(8,587)(observ(j),j=1,n)
            DO i=1,m
              DO k=1,ih
                a(k,i)=q(i,k)
              END DO
            END DO

            CALL MMUL(btot,lda,m,NumCorrMisur,work,lda,1,dum2,lda)
            CALL MMUL(a,lda,ih,m,dum2,lda,1,dum3,lda)
            CALL MMUL(dum1,lda,ih,ih,dum3,lda,1,dum4,lda)
```

```

            DO j=1,n
              lperm=jpvt(j)
              IF (observ(lperm)) THEN
                work(LDA+lperm)=-dum4(j,1)
              ELSE
                work(LDA+lperm)=1.D28
              ENDIF
            END DO
            WRITE(8,1861)
1861        FORMAT (/'ESTIMATED VALUES OF UNMEASURED FLOW RATES'/)

            DO J=1,n
              IF(work(lda+j).lt.1d26) then
                WRITE (8,444)indnonmis(j),work(Lda+j)
              ELSE
                WRITE(8,445)indnonmis(j)
              ENDIF
444           FORMAT( I5, F15.6)
445           FORMAT( I5, '  is not observable')
            END DO

            GOTO 3535

            DO j=1,n
              lperm=jpvt(j)
              IF (observ(lperm)) THEN
                work(LDA+lperm)=-dum4(j,1)
                WRITE(8,44) lperm,indnonmis(lperm),work(LDA+lperm)
44              FORMAT( 2I5, F15.6)
              ELSE
                WRITE (8,45)  lperm  ,indnonmis(lperm)
45              FORMAT( 2I5, '  is not observable')
              ENDIF
            END DO

3535        CONTINUE

            ! set the values of reconstruited streams work(j) and work(j+LDA) in stream
            numcorr=NumCorrMisur+NumCorrNonMis
           !write(8,*)NUMCORR,NumCorrMisur,NumCorrNonMis,NumNodi,'  NUMCORR'
            j=1

            DO while (j.le.Numcorr)
              DO i=1,NumcorrMisur
                k=index(i)
                IF (k.eq.j) THEN
                  stream(j)=work(i)
                  GOTO 102
                ENDIF
              END DO
              DO i=1,NumcorrNonMis
                k=indnonmis(i)
                IF (k.eq.j) then
                  stream(j)=work(i+LDA)
                  GOTO 102
                ENDIF
              END DO
              WRITE(8,*)'Debug.Message: Something does not work correclty'
              STOP

102           j=j+1
            END DO

            !  Add for balance check only
            GOTO 9933

            WRITE(8,109)
109         FORMAT(//'  MASS BALANCES ARE CHECKED AT ALL NODES. '/
                  +   '   BALANCES AT NODES INCLUDING UNOBSERVABLE STREAMS '/
                  +   '   ARE NOT MEANINGFUL'/)
            DO k=1,NumNodi
              sss=0.d0
              DO j=1,NumCorr
                sss=sss+MAT(k,j)*stream(j)
               !WRITE(8,*)k,j,a(k,j),stream(j)
              END DO
              WRITE(8,*)'  NODE ',k,'   BALANCE=', sss
            END DO

9933        RETURN

```

```
            !++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
            !   Check A=QRP
            !++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
8765        CONTINUE
            CALL MMUL(q,lda,m,m,r,lda,n,a,lda)
            DO J=1,N
              K=JPVT(J)
              DO I=1,M
                DUM1(I,K)=A(I,J)
              END DO
            END DO

            WRITE(8,76)
76          FORMAT(//)
            WRITE(8,*) ' CHECK   Q*R = A ORIGINAL'

            DO i=1,m
              DO j=1,n
                IF(dabs(DUM1(i,j)-soloprova(i,j)).gt.1.d-4)
                +  write(8,*) i,j,a(i,j),soloprova(i,j)
              END DO
            END DO
            STOP

            !++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
            !
            !******************************************************************
            !           ORTOGONALITY CHECK  -   Product B2*Q2T                '
            !******************************************************************
8090        CONTINUE

            WRITE(8,76)
            WRITE(8,*)' ORTOGONALITY CHECK   -   Product B2*Q2T'

           !DO j=1,numcorrmisur
            DO j=1,n
              DO i= 1,mminh
                dum2(j,i)=0d0
                DO k=1,m
                  dum2(j,i)=dum2(j,i)+soloprova(k,j)*dum1(k,i)
                END DO
              END DO
            END DO
            DO i=1,mminh
              WRITE(8,*)i
            ! write(8,99)  (dum2(j,i),j=1,numcorrmisur)
              WRITE(8,99)  (dum2(j,i),j=1,n)
            END DO
            STOP

            !****************************************************************
            !
            !<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
            !                      EXPERIMENTAL VALUES CHECK
            !<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
7442        CONTINUE
            dum1(1,1)=0d0
            sss=0d0
            DO i=1,numcorrmisur
              work(i)=stream(i)-work(i)
              dum1(1,1)=dum1(1,1)+dum2(1,i)*work(i)
              sss=sss+dum2(1,i)*stream(i)
            END DO
            WRITE(8,*) dum1(1,1),sss
            STOP
            !>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
       END
       !----------------------------------------------------------------
```

8.2 PCA study on water consumption seasonality

An analysis of the main components (PCA) was carried out using techniques learned within the multivariate analysis course to highlight the possible influence of seasonality on the values of the measured water flows.

The analysis was performed using the free software routines developed in the dedicated R environment by the Chemometry group of the Department of Pharmacy of the University of Genoa (DIFAR)[1].

The available data are related to the monthly flows of the various water streams measured in the plant and constitute a matrix of 12 data sets and 43 variables.

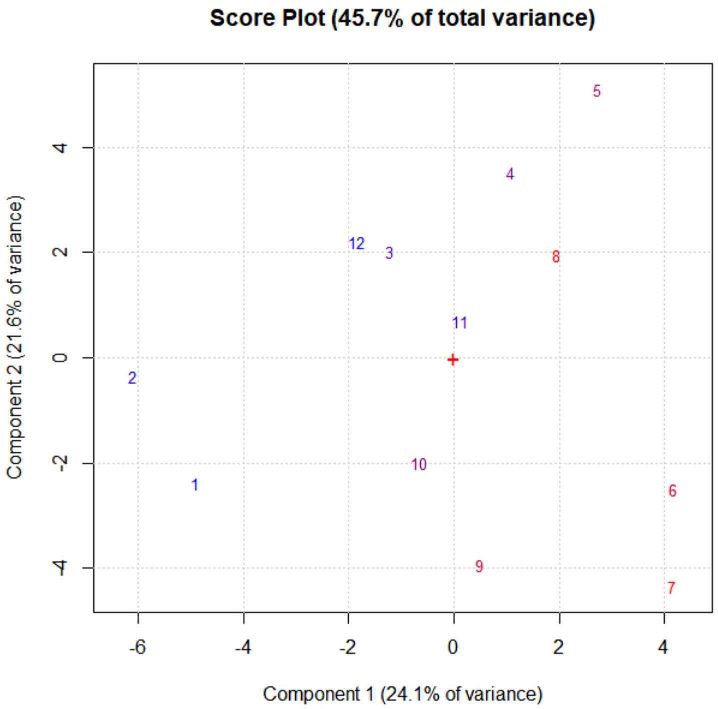
Before analysis, the centring and autoscaling data pretreatments have been applied.

The first two Principal Components (PC1 and PC2) express 45.7% of the total variance contained in the data sets.

The chart shows the resulting Score Plot (Component 2 vs Component 1). The label of each sample corresponds to the month (1 to 12 corresponding to January to December) while the chromatic scale depends on the average monthly temperature (minimum 3°C in January is blue, maximum 22.6 in July is red).

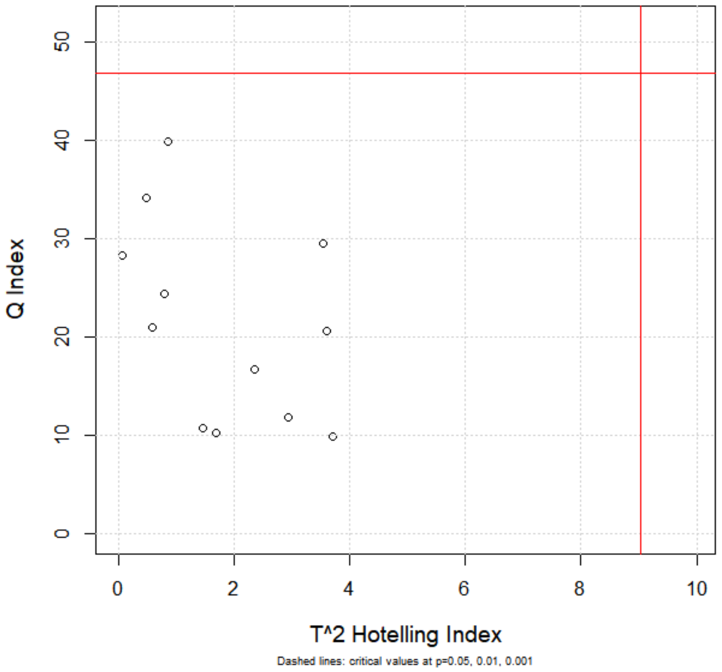
---

[1] Software available for downloading at http://gruppochemiometria.it/index.php/software (2018)



Component 1 quite clearly expresses a correlation between the datasets and the environmental conditions: the datasets associated to the colder months have low values (left-hand side of the plot) while those associated to warmer months have high values (right-hand side of the plot).

The diagnostic analysis of the model (see plot Q vs T^2 below) indicates that all the samples are within the standard confidence limits. Thus the model expresses quite well the general correlations in place between the variables.



Therefore, the PCA highlights the effect of the seasonality on freshwater consumption, even though it is not possible, based on available datasets, to understand if the trend is due to different production assets (e.g. quality of raw material or finished product demand) or changing environmental conditions.

Unfortunately, notwithstanding these interesting preliminary results, this study could not be further deepened because our counterpart did not provide the details of the monthly production (only the yearly production balance is available) corresponding to the water data already available.

This detail would have allowed highlighting any correlation between the seasonal variability of production (perhaps due to the different quality of the raw material used in different periods of the year, to different environmental conditions or different production patterns) and specific consumption of different types of water.

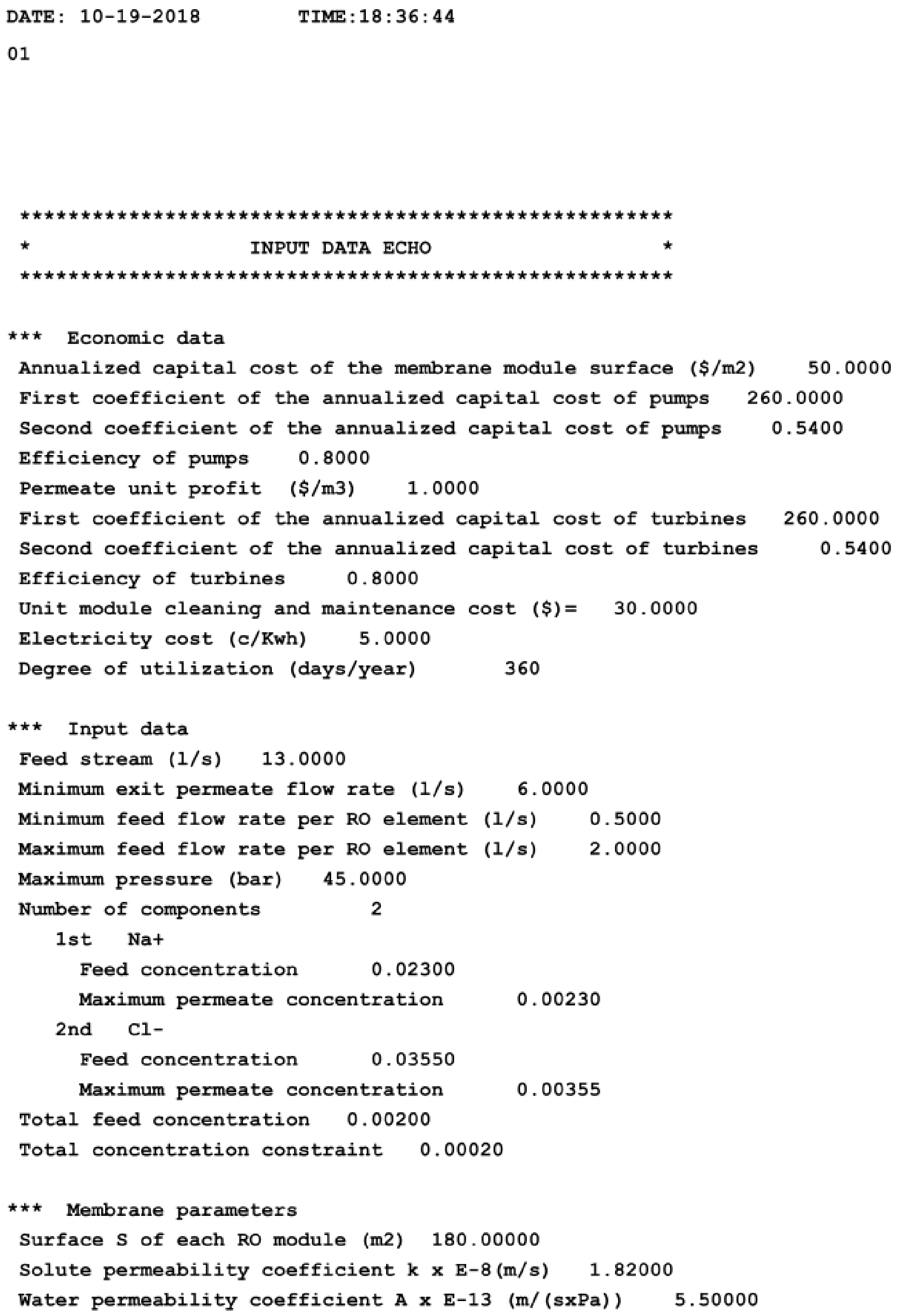
8.3 RON problem formalisation for BARON in GAMS

```
i stages /i1*i4/
*    j passes /j1*j3/

Set i stages /i1*i1/
    j passes /j1*j1/

Parameter
    Q    Feed to osmosis plant/0.013 /
    cbar Feed concentration  /.0002/

    cpr  Cost of permeate water /  1 /
    ce   Cost of electricity / 0.05 /
    cm   Annualized cost of membranes / 50 /
    cc   Cost of cleaning & maintenance /  30 /
    cp1  1st coefficient for annualized cost of pumps /260/
    ct1  1st coefficient for annualized cost of turbines /260/
    cp2  2nd coefficient for annualized cost of pumps /0.54/
    ct2  2nd coefficient for annualized cost of turbines /0.54/
    effp Pump efficiency /0.8/
    efft Turbine efficiency /0.8/
    Util Degree of utilization /360/
    k    Solute permeability coefficient  /1.82E-8/
    A    Water permeability coefficient  /5.5E-13/
    gam  Gamma /1./
    Delp Pressure loss in each stage /10000./

    sigm Surface of each RO module/180./

    MinF Minimum flowrate per module /.0005/
    MaxF Maximum flowrate per module /.002/
    MaxP Maximum pressure  /4500000./

    F1sp Minimum permeate flowrate /.009/
    c1sp Maximum permeate concentration /.00002/
    Ploss1(i)  Head loss in 1st pass;

Ploss1("i1")=0.;
loop(i, Ploss1(i+1)  = Ploss1(i) + Delp ) ;
display Ploss1;

util=util*8760/365;
effp=1000.*effp;
cpr=cpr*3600*util;
ce=ce*util;

Variable
    z           profit
    F(i,j)      Feed to i-th stage in j-th pass
    F1(i,j)     Permeate of i-th stage in j-th pass
    F2(i,j)     Retentate of i-th stage in j-th pass
    c(i,j)      Feed concentration to i-th stage in j-th pass
    c1(i,j)     Permeate concentration of i-th stage in j-th pass
    c2(i,j)     Retentate concentration of i-th stage in j-th pass
```

```
    W          Electricity consumed
    W1         Pump coefficient
    W2         Turbine coefficient
    DP         Input pressure
    DP2        Additionalhead to 2nd pass
    Pst(i,j)   Pressure at each stage
    POsm(i,j)  Osmotic pressure
    S(i,j)     Overall surface in stage i and pass j
    PermF      Permeate out of the plant
    PermC      Permeate concentration;

Positive Variables F,F1,F2,c,c1,c2,W,DP,S;
Integer Variables n(i,j);


Equation
     obj     revenue
     e0      feed distribution
     e00     feed concentration input
     e1(i,j) total surface and element surface
     e2(i,j) global mass balance
     e3(i,j) solute mass balance
     e4(i,j) solvent permeability relationship
     e5(i,j) solute permeability relationship
     e6(i)   pressure loss
*    e62(i)   pressure loss in second pass
     e7(i,j) osmotic pressure
     e8      power consumed
     eDP2    zero if one pass else DP2
     ePF     permeate flowrate
     ePc     permeate concentration
     epump   cost power coefficient
     eturb   cost power coefficient;

     obj..       z=e=cpr*Permf-(cc+cm)*sum((i,j),S(i,j))-ce*W-cp1*W1-ct1*W2;
     e0..        F("i1","j1")=e=Q/n("i1","j1")  ;
     e00..       c("i1","j1")=e=cbar;
     e1(i,j)..   S(i,j)=e= sigm*n(i,j);
     e4(i,j)..   F1(i,j)=e=A*S(i,j)*(Pst(i,j)-POsm(i,j));
     e2(i,j)..   F2(i,j)=e=F(i,j)-F1(i,j);
     e5(i,j)..   c1(i,j)=e=0.5*k*S(i,j)*(c(i,j)+c2(i,j))/(F1(i,j)*gam) ;
     e3(i,j)..   c2(i,j)=e=(F1(i,j)*c(i,j)-F1(i,j)*c1(i,j))/F2(i,j);
     e7(i,j)..    POsm(i,j)=e= 100000.*.0821*c(i,j)*300;


     eDP2..      DP2=e=0;
     ePF..        PermF=e=F1("i1","j1")*n("i1","j1");
     ePc..        PermC=e=c1("i1","j1");
     e6(i)..      Pst(i,"j1")=e= DP-Ploss1(i);
     e8..        W=e=Q*DP/effp-(Q-PermF)*(DP-Ploss1("i1"))*efft/1000.;
     epump..     W1=e=W**cp2;
     eturb..      W2=e=W**ct2;
```

```
model osmosi /all/;
option optcr=0;
F.up (i,j) = MaxF;
F.lo (i,j) = MinF;
F1.lo (i,j) = .01*MinF;
PermF.lo = F1sp;
PermC.up = c1sp;

**********************************
* Valori di tentativo
 n.l(i,j)=5;
 DP.l= 3640000;
 F.l (i,j)= .5*(MinF+MaxF);
 F1.l (i,j)= .01*MinF;
 F2.l (i,j)=  F.l(i,j)-F1.l(i,j);
**********************************

option minlp=baron;
osmosi.optfile=1;
option minlp=convert;

solve osmosi using minlp maximizing z;
display DP.l,n.l,F1.l,F2.l,z.l,S.l,Pst.l,POsm.l;
```

8.4 RON Optimisation software detailed report example



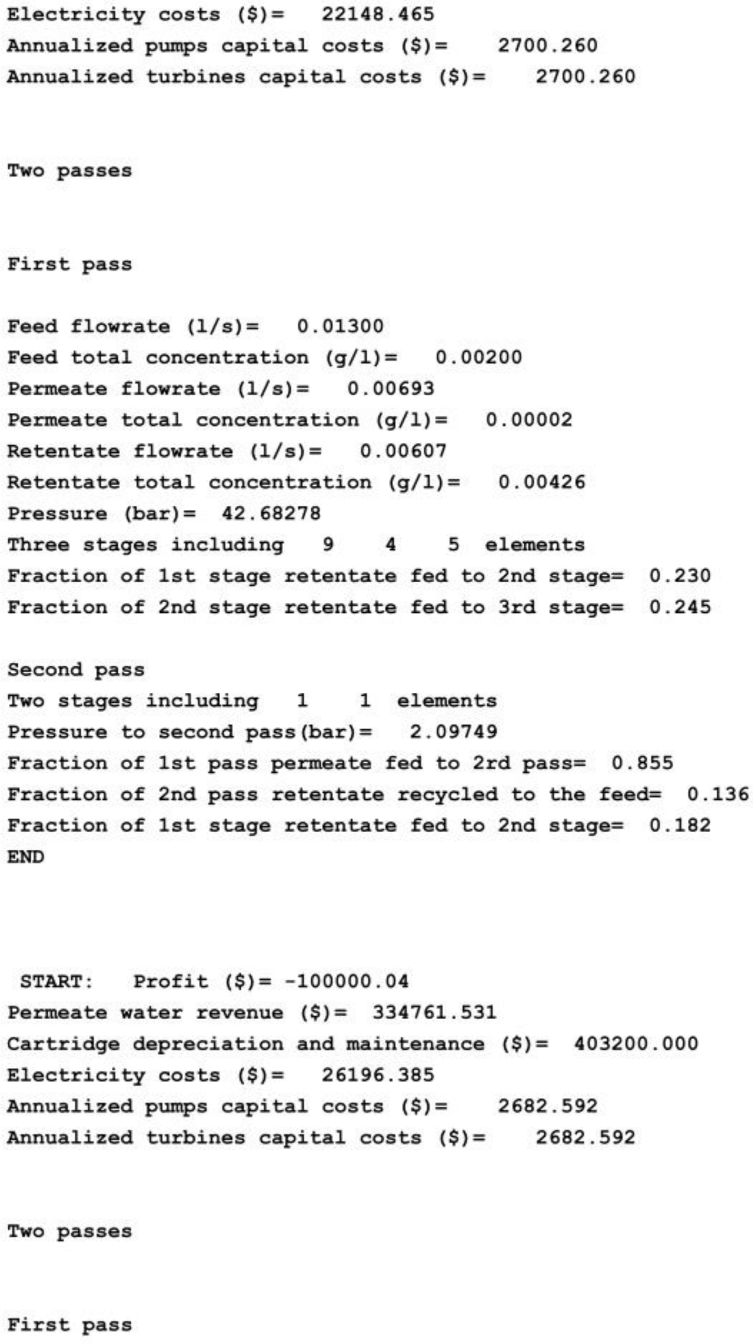
```
DATE: 10-19-2018        TIME:18:36:44

01




 *******************************************************
 *                  INPUT DATA ECHO                    *
 *******************************************************

***  Economic data
 Annualized capital cost of the membrane module surface ($/m2)    50.0000
 First coefficient of the annualized capital cost of pumps   260.0000
 Second coefficient of the annualized capital cost of pumps    0.5400
 Efficiency of pumps    0.8000
 Permeate unit profit  ($/m3)    1.0000
 First coefficient of the annualized capital cost of turbines   260.0000
 Second coefficient of the annualized capital cost of turbines     0.5400
 Efficiency of turbines     0.8000
 Unit module cleaning and maintenance cost ($)=   30.0000
 Electricity cost (c/Kwh)    5.0000
 Degree of utilization (days/year)       360

***  Input data
 Feed stream (l/s)   13.0000
 Minimum exit permeate flow rate (l/s)    6.0000
 Minimum feed flow rate per RO element (l/s)    0.5000
 Maximum feed flow rate per RO element (l/s)    2.0000
 Maximum pressure (bar)   45.0000
 Number of components         2
    1st   Na+
      Feed concentration      0.02300
      Maximum permeate concentration      0.00230
    2nd   Cl-
      Feed concentration      0.03550
      Maximum permeate concentration      0.00355
 Total feed concentration    0.00200
 Total concentration constraint    0.00020

***  Membrane parameters
 Surface S of each RO module (m2)  180.00000
 Solute permeability coefficient k x E-8(m/s)   1.82000
 Water permeability coefficient A x E-13 (m/(sxPa))    5.50000
```

```
 Pressure loss in each stage (bar)   1.00000
 Pressure loss in each stage (bar)   0.10000
 ******************************************************
 *              END OF INPUT DATA ECHO                *
 ******************************************************
 ******************************************************
  Best solution for 1 stage plant
  Number of elements ---  14
  Pressure (bar) --  45.
  Profit ($) -33145.797
 ******************************************************
  Best solution for 2 stages 1 pass plant
  Number of elements in the two stages --- 4 10
  Recycling ratio ---  Pressure(bar) 0.09379608 45.
  Profit ($)--  -34519.945
 ******************************************************
  Best solution for 3 stages 1 pass plant
  Number of elements in the three stages 9 4 1
  Recycling ratios R1,R2-- 0.99997306 0.8440336
  Pressure(bar)-- 45.
  Profit ($)-- -34426.168
 ******************************************************
  Best solution for 4 stages 1 pass plant
  Number of elements in four stages-- 4 4 1 5
  Recycling ratios R1,R2,R3---  0.999998 0.94705653 0.8309195
  Pressure(bar)--  45.
  Profit ($)-- -34835.883
 ******************************************************
  Best solution for 2 passes 1+1 stages plant
  Number of elements in three stages 18 5
  Recycling ratios -- S1,S2   0.70389634 0.8340598
  Pressures(bar) --  42.54633 2.903667
  Profit ($) -118374.92
 ******************************************************
  Best solution for 2 passes 2+1 stages plant
  Number of elements in three stages 22 1 1
  Recycling ratios R1,S1,S2--- 0.6243042 0.9433452 0.07134644
  Pressures(bar) -- P1,P2 38.832153 4.9560833
  Profit ($) -100000.05
 ******************************************************
  Best solution for 2 passes 2+2 stages plant
  Number of elements in four stages 11 6 3 1
  Recycling ratios R1,S1,S2,T1 --- 0.34842622 0.72472435 0.9999891
0.6246557
```

```
 Pressures(bar) -- P1,P2 39.374996 5.625002
 Profit ($) -122038.84
*****************************************************
 Best solution for 2 passes 3+1 stages plant
 Number of elements in four stages 8 5 1 7
 Recycling ratios R1,R2,S1,S2--- 0.10016005 0.6869468 0.4926607
0.99819183
 Pressures(bar) -- P1,P2 44.254143 0.7463055
 Profit ($) -138234.44
*****************************************************
 Best solution for 2 passes 3+2 stages plant
 Number of elements in five stages 9 4 5 1 1
 Recycling ratios R1,R2,S1,S2,T1 --- 0.2297285 0.24454837 0.85489583
0.13575593 0.18225367
 Pressures(bar) -- P1,P2 42.682777 2.0974932
 Profit ($) -100000.016
*****************************************************
 Best solution for 2 passes 4+1 stages plant
 Number of elements in five stages 12 6 7 2 1
 Recycling ratios R1,R2,R3,S1,S2--- 0.18577437 0.057076387 0.14938092
0.9349226 0.1013327
 Pressures(bar) -- P1,P2 41.406384 3.1997838
 Profit ($) -100000.04
*****************************************************
 Best solution for 2 passes 4+2 stages plant
 Number of elements in four stages 6 3 3 3 2 2
 Recycling ratios R1,R2,R3,S1,S2,T1 --- 0.12553607 0.07197241 0.18453461
0.8591422 0.9995646 0.1039122
 Pressures(bar) -- P1,P2 42.75043 2.2500067
 Profit ($) -103571.94
*****************************************************
*      VALUES FOUND BY OPTIMIZATION PROCEDURE       *
*****************************************************

Convergence attained



 START:   Profit ($)= -33145.797
Permeate water revenue ($)=  193783.281
Cartridge depreciation and maintenance ($)=  201600.000
Electricity costs ($)=   21084.959
Annualized pumps capital costs ($)=    2122.059
Annualized turbines capital costs ($)=    2122.059
```

```
One pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00600
Permeate total concentration (g/l)=   0.00020
Retentate flowrate (l/s)=   0.00700
Retentate total concentration (g/l)=   0.00354
Pressure (bar)=  45.00000
One stage including  14  elements
END



 START:   Profit ($)= -34426.168
Permeate water revenue ($)=  193574.797
Cartridge depreciation and maintenance ($)=  201600.000
Electricity costs ($)=   21121.396
Annualized pumps capital costs ($)=    2639.787
Annualized turbines capital costs ($)=    2639.787

One pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00622
Permeate total concentration (g/l)=   0.00002
Retentate flowrate (l/s)=   0.00678
Retentate total concentration (g/l)=   0.00382
Pressure (bar)=  45.00000
Three stages including   9    4    1  elements
Fraction of 1st stage retentate fed to 2nd stage=  1.000
Fraction of 2nd stage retentate fed to 3rd stage=  0.844
END



 START:   Profit ($)= -34519.945
Permeate water revenue ($)=  193451.469
Cartridge depreciation and maintenance ($)=  201600.000
Electricity costs ($)=   21091.838
Annualized pumps capital costs ($)=    2639.787
Annualized turbines capital costs ($)=    2639.787
```

```
One pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00622
Permeate total concentration (g/l)=   0.00002
Retentate flowrate (l/s)=   0.00678
Retentate total concentration (g/l)=   0.00382
Pressure (bar)=  45.00000
Two stages including   4   10  elements
Fraction of 1st stage retentate fed to 2nd stage=  0.094
END



 START:   Profit ($)= -34835.883
Permeate water revenue ($)=  193168.359
Cartridge depreciation and maintenance ($)=  201600.000
Electricity costs ($)=   21124.676
Annualized pumps capital costs ($)=    2639.787
Annualized turbines capital costs ($)=    2639.787

One pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00621
Permeate total concentration (g/l)=   0.00001
Retentate flowrate (l/s)=   0.00679
Retentate total concentration (g/l)=   0.00382
Pressure (bar)=  45.00000
Four stages including   4    4    1    5  elements
Fraction of 1st stage retentate fed to 2nd stage=  1.000
Fraction of 2nd stage retentate fed to 3rd stage=  0.947
Fraction of 3rd stage retentate fed to 4th stage=  0.831
END



 START:   Profit ($)= -100000.016
Permeate water revenue ($)=  215548.969
Cartridge depreciation and maintenance ($)=  288000.000
```



```
Electricity costs ($)=   22148.465
Annualized pumps capital costs ($)=    2700.260
Annualized turbines capital costs ($)=    2700.260


Two passes


First pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00693
Permeate total concentration (g/l)=   0.00002
Retentate flowrate (l/s)=   0.00607
Retentate total concentration (g/l)=   0.00426
Pressure (bar)=  42.68278
Three stages including   9    4    5  elements
Fraction of 1st stage retentate fed to 2nd stage=  0.230
Fraction of 2nd stage retentate fed to 3rd stage=  0.245

Second pass
Two stages including   1    1  elements
Pressure to second pass(bar)=   2.09749
Fraction of 1st pass permeate fed to 2rd pass=  0.855
Fraction of 2nd pass retentate recycled to the feed=  0.136
Fraction of 1st stage retentate fed to 2nd stage=  0.182
END



 START:   Profit ($)= -100000.04
Permeate water revenue ($)=  334761.531
Cartridge depreciation and maintenance ($)=  403200.000
Electricity costs ($)=   26196.385
Annualized pumps capital costs ($)=    2682.592
Annualized turbines capital costs ($)=    2682.592


Two passes


First pass
```

```
Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.01076
Permeate total concentration (g/l)=   0.00003
Retentate flowrate (l/s)=   0.00224
Retentate total concentration (g/l)=   0.01147
Pressure (bar)=  41.40638
Four stages including  12    6    7    2  elements
Fraction of 1st stage retentate fed to 2nd stage=  0.186
Fraction of 2nd stage retentate fed to 3rd stage=  0.057
Fraction of 3rd stage retentate fed to 4th stage=  0.149

Second pass
One stage including   1  elements
Pressure to second pass(bar)=   3.19978
Fraction of 1st pass permeate fed to 2rd pass=  0.935
Fraction of 2nd pass retentate recycled to the feed=  0.101
END



 START:   Profit ($)= -100000.05
Permeate water revenue ($)=  272537.406
Cartridge depreciation and maintenance ($)=  345600.000
Electricity costs ($)=   21772.795
Annualized pumps capital costs ($)=    2582.327
Annualized turbines capital costs ($)=    2582.327


Two passes


First pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00757
Permeate total concentration (g/l)=   0.00020
Retentate flowrate (l/s)=   0.00543
Retentate total concentration (g/l)=   0.00451
Pressure (bar)=  38.83215
Two stages including  22    1  elements
```

```
Fraction of 1st stage retentate fed to 2nd stage=  0.624

Second pass
One stage including   1  elements
Pressure to second pass(bar)=   4.95608
Fraction of 1st pass permeate fed to 2rd pass=  0.943
Fraction of 2nd pass retentate recycled to the feed=  0.071
END



 START:   Profit ($)= -103571.94
Permeate water revenue ($)=  195643.922
Cartridge depreciation and maintenance ($)=  273600.000
Electricity costs ($)=   20234.918
Annualized pumps capital costs ($)=    2690.470
Annualized turbines capital costs ($)=    2690.470


Two passes


First pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00629
Permeate total concentration (g/l)=   0.00011
Retentate flowrate (l/s)=   0.00671
Retentate total concentration (g/l)=   0.00378
Pressure (bar)=  42.75043
Four stages including   6    3    3    3  elements
Fraction of 1st stage retentate fed to 2nd stage=  0.126
Fraction of 2nd stage retentate fed to 3rd stage=  0.072
Fraction of 3rd stage retentate fed to 4th stage=  0.185

Second pass
Two stages including   2    2  elements
Pressure to second pass(bar)=   2.25001
Fraction of 1st pass permeate fed to 2rd pass=  0.859
Fraction of 2nd pass retentate recycled to the feed=  1.000
Fraction of 1st stage retentate fed to 2nd stage=  0.104
END
```

```
 START:   Profit ($)= -118374.92
Permeate water revenue ($)=  235549.906
Cartridge depreciation and maintenance ($)=  331200.000
Electricity costs ($)=   18377.076
Annualized pumps capital costs ($)=    2793.697
Annualized turbines capital costs ($)=    1554.044


Two passes


First pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00757
Permeate total concentration (g/l)=   0.00020
Retentate flowrate (l/s)=   0.00543
Retentate total concentration (g/l)=   0.00451
Pressure (bar)=  42.54633
One stage including  18  elements

Second pass
One stage including   5  elements
Pressure to second pass(bar)=   2.90367
Fraction of 1st pass permeate fed to 2rd pass=  0.704
Fraction of 2nd pass retentate recycled to the feed=  0.834
END



 START:   Profit ($)= -122038.84
Permeate water revenue ($)=  188805.734
Cartridge depreciation and maintenance ($)=  288000.000
Electricity costs ($)=   17338.025
Annualized pumps capital costs ($)=    2753.276
Annualized turbines capital costs ($)=    2753.276


Two passes
```

```
First pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00607
Permeate total concentration (g/l)=   0.00001
Retentate flowrate (l/s)=   0.00693
Retentate total concentration (g/l)=   0.00374
Pressure (bar)=  39.37500
Two stages including  11    6  elements
Fraction of 1st stage retentate fed to 2nd stage=  0.348

Second pass
Two stages including   3    1  elements
Pressure to second pass(bar)=   5.62500
Fraction of 1st pass permeate fed to 2rd pass=  0.725
Fraction of 2nd pass retentate recycled to the feed=  1.000
Fraction of 1st stage retentate fed to 2nd stage=  0.625
END



 START:   Profit ($)= -138234.44
Permeate water revenue ($)=  190407.047
Cartridge depreciation and maintenance ($)=  302400.000
Electricity costs ($)=   20742.936
Annualized pumps capital costs ($)=    2749.274
Annualized turbines capital costs ($)=    2749.274


Two passes


First pass

Feed flowrate (l/s)=   0.01300
Feed total concentration (g/l)=   0.00200
Permeate flowrate (l/s)=   0.00612
Permeate total concentration (g/l)=   0.00001
Retentate flowrate (l/s)=   0.00688
Retentate total concentration (g/l)=   0.00377
```

```
Pressure (bar)=  44.25414
Three stages including   8    5    1  elements
Fraction of 1st stage retentate fed to 2nd stage=  0.100
Fraction of 2nd stage retentate fed to 3rd stage=  0.687

Second pass
One stage including   7  elements
Pressure to second pass(bar)=   0.74631
Fraction of 1st pass permeate fed to 2rd pass=  0.493
Fraction of 2nd pass retentate recycled to the feed=  0.998
END
```

Layout of the optimal plant