Innovative design and multi-objective optimization of hybrid reverse osmosis and multi-stage flash desalination plants

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Abstract

The selection of an hybrid MSF/RO desalination plant depends on many factors, such as capital costs, electricity consumption, water conversion rate and local requirements. In order to provide the necessary information for the decision process, stand-alone reverse osmosis or multi-stage flash designs and alternative hybrid configurations must be characterized, optimized and compared on a sound basis.

The aim of this paper is to present a computer-aided method, for the design and optimization of hybrid desalination systems. The optimization is carried out on technical, economical and environmental performance indicators in a multi-objective optimization framework. The approach is based on the conceptual decomposition of the MINLP design problem into two sub-problems. The network design problem is solved using conventional MILP solvers. The master problem, which consists in generating the list of available equipments, is solved using a multi-objective evolutionary algorithm. The results of this strategy are illustrated in an industrial case study.

Key words: Hybrid desalination; Reverse osmosis (RO); Multi-Stage Flash (MSF); Superstructure; Multi-objective optimization

1. Introduction

In the next decades, the world will face a major water supply deficit. Today, already 460 millions persons suffer from water stress. This amount should rise to 2,8 billions in 2025 (almost one third of the world population) [1–3]. Considering the huge quantities of saltwater (98% of the total world water), desalination can be considered as a solution to the crisis.

At this point, two major technologies exist on the desalination market: distillation with multiple stages (multi-stage flash or MSF) and membrane filtration (reverse osmosis or RO) [4]. Their development is still restrained due to high investment costs and intensive energy consumption [5]. Operation and costs of RO depend strongly on water salinity and osmotic pressure. On the contrary, MSF operation does not vary substantially with salinity but always requires consequent heat utilities since the water has to be evaporated. Combinations between these two technologies can be carried out at different integration levels between the heat, water and salt stream flows

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(reuse of distillation waste heat to warm up the water before its filtration, blending of water stream flows of different salinity, improved load factor through adapted start-up and shut-down phases). Another possibility is to consider the heat requirements of thermal desalination and the cooling water flow rates of thermal power production: the hybrid desalination configurations as shown in Fig.1. offer significant opportunities for combined water and power production (reuse of turbine steam heat for distillation, recycling of power plant cooling water in the desalination system,...) [6–8]. Many hybrid desalination alternatives exist, which remain to be evaluated. Therefore, the advantages of most promising hybrid desalination combinations over separate water and power production need to be demonstrated systematically.

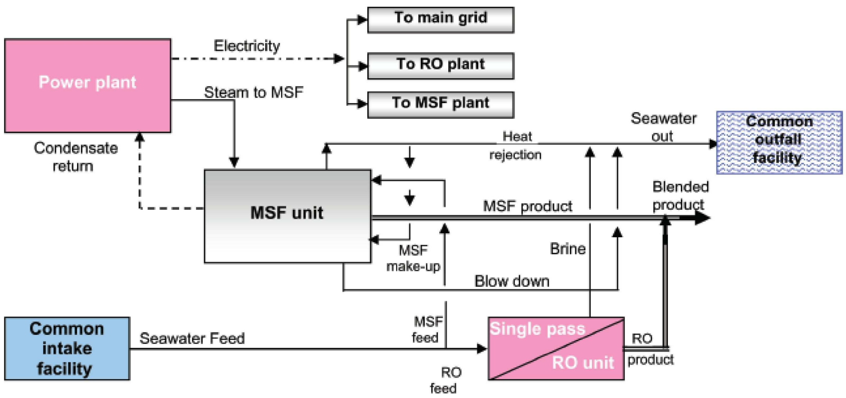

Figure 1. Example of simple hybrid desalination plant associated with power production [7]

Three successive phases are necessary to establish consistent hybrid desalination designs : the technical modelling of the process configurations, the evaluation of their performances and the optimization of both the design and the corresponding operating conditions based on the performances. Numerous authors have described the assessment of hybrid desalination concepts. However, these evaluations are developed for specific purposes (full scale modelling, design optimization, economical comparison) and do not address the process design and the selection problem.

The technical modelling of stand-alone desalination equipments has been most developed. Concerning distillation technologies, the thermo-dynamic models of MSF and multi-effect evaporation or MEE were developed by El-Dessouky and Ettouney [9]. As for RO, the transport model through the different types of reverse osmosis membranes (tubular, spiral-wound, hollow fiber) has been developed in the 70's. In the homogeneous solution diffusion model, Lonsdale et al. assumes that both the solute and solvent dissolve in the non porous homogeneous surface layer of the membrane and diffuse through in an uncoupled manner [10]. Pore based models assumes that the RO membrane is microporous [11]. The irreversible thermodynamic model was developed using phenomenological equations of transport and is useful when the molecular transport processes within the membrane are not fully understood [12]. To be extended at the scale of a real RO module, simplifying assumptions must be taken to model the total flux over the whole membrane area . The osmotic pressure and the mass transfer coefficients are approximated [13]. While the performances of individual RO modules in terms of operating conditions and module structure have been extensively studied, the modelling of RO networks has been less explored. Industrial RO plants consist in arrangements between pressure vessels containing several membrane modules. The RO pressures vessels are constituted of membranes of three types (tubular [14], hollow fiber [15], spiral wound [16]) calibrated on specific commercial membranes. In general, the RO plants are evaluated on a limited number of designs [14,15,17,18], thus leaving little room for comparison between the results. As a result, the development of a representative hybrid desalination model requires accurate models of each technology, which at the same time allow the performance comparison between each other and facilitate the modelling of new commercial products.

Numerous stand-alone or hybrid desalination configurations can fulfill the requirements of a given desalination project. The technical choices depend on the forecast of their performances. They are usually estimated by the total annual cost of the installation (TAC), that globalizes investment and operating costs. This cost function is calculated with a statistical top-down approach and may lack precision when one has to compare similar designs [19–21]. For some case studies, a bottom-up cost evaluation based on existing installations provides more precise results [22–24]. Nonetheless, these cost models have shown to be weakly transposable to other situations with different local conditions or designs. In the future, the desalination projects will probably be compared on a broader comparison grid including additional decision criteria such as environmental impact (local environmental impacts [25], life cycle impacts and GHG emissions [26], water and fuel consumption). As these various aspects cannot be taken into account through cost function weighting, a multi-objective design methodology has to be developed.

For given performance indicators, the optimization of hybrid desalination configurations is performed with two different approaches. The first approach consists in optimizing the design variables of defined hybrid MSF/RO desalination [27, 28] or dual-purpose water and power production schemes [29, 30]. However this method uses simplified RO designs with specific membranes and prevents the identification of innovative hybrid desalination configurations. The second method is to rely on a flexible superstructure approach and to optimize the definition of the piping network between the desalination equipments. This has been developed mainly for RO network. El-Halwagi proposed a design method for an fixed RO structure formulated as a mixed integer non linear programming (MINLP) model [31]. The problem can be simplified by reducing the number of variables [17, 32] or by its decomposition into two hierarchical design procedures [33]. Nevertheless, these advanced approaches still rely on implemented network designs and were not developed for the hybrid desalination evaluation. For a complete exploration of the hybrid desalination possibilities and advantages, these optimization techniques should be unified within a flexible hybrid desalination superstructure.

In the perspective of future industrial developments, the decision process must be rationalized. It is the purpose of the developed process design methodology. It will provide useful insights for sound investment decisions, by investigating and optimizing the designs of hybrid desalination plants as a function of given local water needs and resources. It is based on a computer-aided methodology, which:

(i) establishes a database of up-to-date models of desalination technologies
(ii) performs a systematic generation of integrated hybrid desalination configurations based on a flexible superstructure, with respect to given project requirements and constraints
(iii) evaluates the proposed configurations on technical, economical and environmental performances indicators
(iv) optimizes the design of these desalination configurations in a multi-objective framework
(v) applies a multi-criteria approach to select the best local technical choices among a panel of promising integrated desalination hybrid systems

This paper focusses on the problem decomposition and the methodology developed to perform the multi-objective optimization.

2. Definition of the problem

For a given project defined by water needs and resources in quantity and quality, local constraints such as price of electricity, price of steam, maximal temperature of liquid discharges in water bodies, a set of technologies (MSF, RO) and a set of objectives (investment and operating costs, GHG emissions, water conversion rate), the goal is to determine the optimal hybrid desalination process configurations among the feasible alternatives.

The mathematical modelling of this problem involves a number of state variables entirely describing the hybrid desalination configuration, i.e. :

– the choice of desalination equipments (decisions);
– the characteristics of these equipments (capacity, design, operation);
– the way the equipments are interconnected through the piping network (connections between equipments and flow rates).

The state variables can be divided into two categories. The degrees of freedom or 'decision variables' $\vec{z}$ are determined by the user within the decision space $\mathcal{D}$ (for example the number of MSF stages or the transmembrane pressure applied). Once the value of $\vec{z}$ is fixed, the dependent variables $\vec{x}$ are computed by solving the model equations (for example the global conversion rate or the energy consumption).

The hybrid desalination configuration model is defined by a set of equalities $\vec{h}(\vec{z}, \vec{x}) = 0$ (equipment model equations, energy and mass balances, unit operation models, thermodynamic equations of state), inequalities

$\vec{g}(\vec{z},\vec{x}) \leq 0$ (technical limitations) and logical equations, $\vec{L}(\vec{z},\vec{x}) = TRUE$ (decisions). In order to solve the model, a given set $\vec{z}$ must yield a $\vec{x}$ that satisfies the model equations.

Models are used to compute the desalination hybrid system performances. These performances are evaluated by the objective function $F(\vec{z},\vec{x})$, which has to be optimized. Optimizing the system with respect to the objective function means finding the set of decision variables $\vec{z_0}$ that maximizes (or minimizes) F under constraints of the model equations. This can be written as follows:

$$\min_{\vec{z}\in\mathcal{D}} F(\vec{z},\vec{x}) \ \ \text{subject to} \begin{cases} \vec{h}(\vec{z},\vec{x}) = 0 \\ \vec{g}(\vec{z},\vec{x}) \leq 0 \\ \vec{L}(\vec{z},\vec{x}) = TRUE \end{cases}$$

When combining process modelling and process integration, the model equations and $F(\vec{z},\vec{x})$ are usually non linear, the variables deciding the size and the operating conditions of the equipments are continuous and the variables deciding the existence of an equipment or a connection are boolean variable {Yes(1), No(0)}. This problem is therefore defined as a mixed integer non linear programming (MINLP) problem [34].

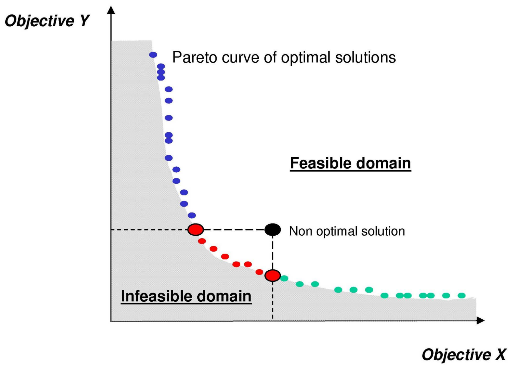

Figure 2. Pareto curve and sub-optimal solutions

Usually, optimizations are made on a one-dimensional objective function $F(\vec{z},\vec{x})$, which weights together homogenous criteria (annual operating costs and annualized investment costs for example). The multi-objective approach developed here does not require a predefined weighting philosophy and is particularly well adapted when dealing with non homogeneous criteria, which are difficult to express in financial terms, like the environmental impacts or the energy efficiency [35–37]. Consequently, $\vec{F}(\vec{z},\vec{x})$ can have more than one dimension. The solution of the problem, defined as the so-called Pareto frontier, is a set of optimal solutions $\{\vec{z_0}\}$, which represents all the technically feasible compromises between the objectives [38]. Members of this set have the characteristics of not being able to improve one objective without penalizing another at the same time (Fig.2).

3. Methodology for solving the process synthesis problem

The solving method presented in this paper is based on the decomposition of the MINLP problem into two related optimization problems, a non linear programming (NLP) master problem and a mixed integer linear programming (MILP) subproblem realizing a Benders like decomposition [39]. This method follows the principle of the outer approximation algorithm proposed by Duran [40] and is adapted for the application in a multi-objective optimization context. The resolution procedure is described in Fig.3.

The set of decision variables $\vec{z}$ is divided into two sets $\vec{z} = \{\vec{z_N}, \vec{z_I}\}$ with:
– $\vec{z_N}$ the so called complicating variables, representing the decision variables of the NLP problem and
– $\vec{z_I}$ the non complicating ones, representing the decision variables of the MILP problem.

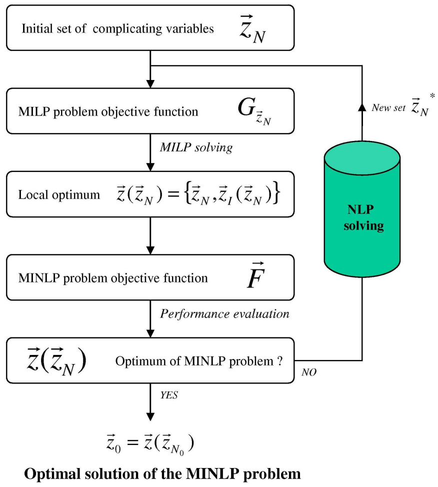

Figure 3. Resolution method of the MINLP problem

The first step of the resolution process is the definition of an initial value for the complicating variables $\vec{z_N}$. The constraints and the parameters of the MILP problem are then computed as a function of $\vec{z_N}$. For the fixed $\vec{z_N}$ and a given set of MILP variables $\vec{z_I}$, the set of decision variables $\vec{z} = \{\vec{z_N}, \vec{z_I}\}$ yields a unique set of dependent variables $\vec{x}$. For the fixed $\vec{z_N}$, the variables of the linear cost function of the MILP problem $G(\vec{z}, \vec{x})$ are consequently only the $\vec{z_I}$. As such, the linear function $G(\vec{z}, \vec{x})$ can be formalized as $G_{\vec{z_N}}(\vec{z_I})$ or $\vec{G_{\vec{z_N}}} \cdot \vec{z_I}$. The MILP problem is mathematically formulated as such:

$$\min_{\vec{z_I}} \vec{G_{\vec{z_N}}} \cdot \vec{z_I} \quad \text{subject to} \begin{cases} H_{\vec{z_N}} \cdot \vec{x} + \vec{B}_{\vec{z_N}} = 0 \\ H_{\vec{z_N}} \ \text{ constraint matrix} \\ \vec{B}_{\vec{z_N}} \ \text{ independant term} \end{cases}$$

This problem is solved with a conventional linear programming solver (CPLEX with the linear programming language AMPL) [41–43]. There is therefore one unique solution $\vec{z_I}(\vec{z_N})$. The choice of a set of $\vec{z_N}$ determines a unique set of decision variables $\vec{z}(\vec{z_N}) = \{\vec{z_N}, \vec{z_I}(\vec{z_N})\}$ as function of $\vec{z_N}$. $\vec{z}(\vec{z_N})$ is used to evaluate non linear objective functions $\vec{F}(\vec{z}(\vec{z_N}), \vec{x}(\vec{z_N}))$, which are sent to the multi-objective optimization algorithm. The NLP problem is solved by finding the optimal sets of decision variables $\vec{z_N}$, which minimizes of the objectives functions $\vec{F}$. The multi-objective optimizer used in our method (MOO) applies evolutionary algorithms, which explore the whole decision space $\mathcal{D}$ of $\vec{z_N}$, to determine the optimal sets $\vec{z_N}_0$ for the function $\vec{F}$. The evolutionary algorithms have been developed at the LENI (Industrial Energy Systems Laboratory, Swiss Federal Institute of Technology) [38].

A MINLP solution $\vec{z_0} = \vec{z}(\vec{z_N}_0)$ is optimal if the optimal solutions of the NLP objective function are always better than those of the MILP objective function (underestimation principle). To ensure that the linear $G_{\vec{z_N}}$ will not produce solutions, that are not optimal from a multi-objective point of view, relaxation variables are used as multiplicative factors for each component of the cost function $G_{\vec{z_N}}$. These relaxation variables $\vec{z}_{N,r}$ are part of the NLP decision variables $\vec{z_N}$. For a fixed $\vec{z_N} \backslash \vec{z}_{N,r}$ with $\vec{z}_{N,r}$ varying, the MILP solutions vary but the global MINLP solution remains the best. Their variation fulfill the condition of optimality.

4. Hybrid desalination process optimization

This method has been applied to the investigation and the optimization of hybrid desalination configurations. The global MINLP problem is decomposed in a master NLP problem, which tackles the generation and the characterization of equipments and a MILP subproblem, which embeds the choice of equipments and the definition of the piping network. The optimization phases follow the previous resolution procedure and are described below (Fig.4.).

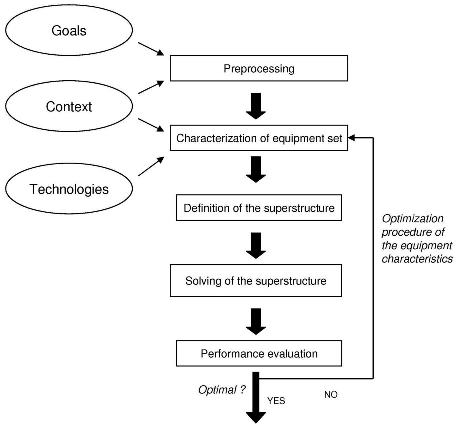

Figure 4. Hybrid configuration optimization process

4.1. *Initialization*

The first phase concerns the statement of the problem. The context and constraints are defined. The requirement are characterized as a desired capacity of desalinated water of specific quality. The water and energy resources are also characterized in terms of amount and quality. The problem constraints relating to the plant location are defined (for example the emission limits, the plant surface constraints, the localization of the water resources). From this problem specification, goals and performance indicators are defined. The list of suitable desalination equipments is then drawn from expert system rules according the resources quality.

4.2. *Characterization of equipment set*

The second step of the optimization process is to define a set of decision variables $\vec{z_N}$. These decision variables are divided in two types:

(i) the decision variables that characterize the size and the operating conditions of the equipment (desalination technology) in the model. Techno-economic models determine the feasibility of the specified equipments (respect of technical constraints such as maximal salinity, pressure, temperature,...) and their characteristics for a nominal feed flow rate (energy consumption, investment costs, operating costs, quality tolerance for the input/output water streams);

(ii) the relaxation variables of the subproblem objective function, which ensure an unbiased final optimization (see comments later).

Each desalination equipment in the database is characterized as a generic process unit u (Fig.5) with:

– 1 input stream referenced as demand $d_{u,i}$ (the feedwater: $i = 1$). Each demand d feeds one process unit u_d and is defined with a nominal mass flow rate $\dot{m}_d$ in $kg.s^{-1}$, a temperature T_d in K, a salinity X_d in ppm, and a pressure P_d in Pa.

– 2 output streams referenced as sources $s_{u,j}$ (the permeate: $j = 1$ and the concentrate: $j = 2$). Each source s comes from one process unit u_s and is defined with a nominal mass flow rate $\dot{m}_s$, temperature T_s, salinity X_s, and pressure P_s.

The characteristics of the process unit u are determined for a nominal capacity by the decision variables using the desalination equipment models. The nominal capacity depends on the technology. Besides its technical properties, the investment cost and the operating cost of the nominal process unit are defined. In order to define a linear superstructure model, performances and costs of unit u are linearized as a function of its capacity factor f^u around the nominal conditions of use. For example, the real feed flow rate $\dot{M}_d$ of the demand d feeding the process unit u_d is equal to the nominal feed flow rate $\dot{m}_d$ given by the NLP solver multiplied by the capacity factor f^{u_d} which is determined by solving the MILP problem:

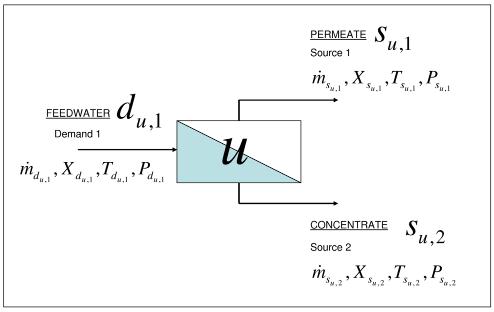

Figure 5. Desalination equipment as a process unit

$$\dot{M}_d = f^{u_d} \cdot \dot{m}_d \tag{1}$$

The pressure and the temperature of the output streams depend on the characteristics of the input stream and of the equipment. Inside the unit, the conservation of water and salts are always respected:

$$\forall \ u = 1, ..., n_u \quad \sum_{s/u_s=u} \dot{m}_s \quad = \quad \sum_{d/u_d=u} \dot{m}_d \tag{2}$$

$$\forall \ u = 1, ..., n_u \quad \sum_{s/u_s=u} \dot{m}_s \cdot X_s \quad = \quad \sum_{d/u_d=u} \dot{m}_d \cdot X_d \tag{3}$$

4.3. *Definition of the superstructure*

According to the project requirements, a superstructure is systematically generated from a given equipment set. It includes all the possible and feasible connections between sources and demands. [41].

From this superstructure, obtaining a desalination configuration consists in defining:
- the use of each equipment $y^u \in \{\text{Yes}(0), \text{No}(1)\}$
- the capacity factor of each equipment f^u
- the piping network.

The piping network is composed of pipes, water stream flows, mixers and splitters. The pipes link together sources to demands. The pipe flow rate from a source s to a demand d is labeled $\dot{m}_{s\to d}$. Each pipe introduces a temperature difference $\Delta T_{s\to d} = T_d - T_s$ and a pressure difference $\Delta P_{s\to d} = P_d - P_s$ between the input and the output, which will be used to calculate heat and power requirements. The mixer mixes the stream flows from different pipes to feed the demand. The splitter splits the stream flow from one source to feed different pipes.

The superstructure is initialized with the project local conditions:

(i) The water resource is represented as a process unit WR with a single source s_{WR}. s_{WR} is characterized with a maximum production flow rate $\dot{m}_{s_{WR}}$, a temperature $T_{s_{WR}}$ corresponding to the water resource temperature, a salinity $X_{s_{WR}}$ corresponding to the water resource salinity, and a given pressure $P_{s_{WR}}$ as well as a cost per cubic meter (Fig.6).

(ii) The permeate production $PROD$ and the water discharges are represented as a process unit with a single demand d_{PROD}. This demand is characterized with a potable water flow requirement $\dot{m}_{d_{PROD}}$ corresponding to the project capacity, a maximal temperature $T_{d_{PROD}}$, a maximal salinity $X_{d_{PROD}}$ corresponding to the potable water quality, and a pressure $P_{d_{PROD}} = P_{network}$ with $P_{network}$ the feed pressure of the distribution network (Fig.6).

(iii) The water discharges DIS is represented as a process unit with a single demand d_{DIS}. It is characterized with a maximal flow rate $\dot{m}_{d_{DIS}}$, a maximal discharge temperature $T_{d_{DIS}}$, a maximal salinity $X_{s_{DIS}}$, a maximal pressure $P_{s_{DIS}}$ and a cost per cubic meter (Fig.6).

The generated configurations must fulfill the potable water requirements and respect the following constraints.

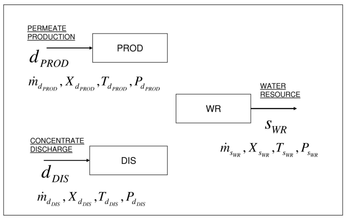

Figure 6. Desalination equipment as a process unit

When used, each equipment must be used within a specified capacity range depending on the technology.

$$\forall \;\; u = 1, .., n_u \quad f^u_{min} \cdot y^u \leq \;\; f^u \;\; \leq f^u_{max} \cdot y^u \quad \text{with } y^u \in \{0, 1\} \tag{4}$$

The potable water requirements d_{PROD} are respected by forcing the permeate production $\dot{m}_{d_{PROD}} = \dot{M}_{d_{PROD}}$:

$$\begin{cases} y^{PROD} = 1 \\ f^{PROD}_{min} = f^{PROD}_{max} = f^{PROD} = 1 \end{cases} \tag{5}$$

For each demand, the sum of the transferred flow rates from the sources must be equal to the corresponding need (water mass conservation).

$$\forall \;\; d = 1, ..., n_{demands} \;\; \sum_s \dot{m}_{s \to d} \;\; = \;\; f^{u_d} \cdot \dot{m}_d \tag{6}$$

For each source, the sum of the transferred flow rates to the demands must be equal to the produced flow rate (water mass conservation).

$$\forall \;\; s = 1, ..., n_{sources} \;\; \sum_d \dot{m}_{s \to d} \;\; = \;\; f^{u_s} \cdot \dot{m}_s \tag{7}$$

For each demand, the salinity tolerated by the demand must be superior to the total salinity of the transferred flow rates (mass conservation of the salts).

$$\forall \;\; d = 1, ..., n_{demands} \;\; \sum_s (\dot{m}_{s \to d} \cdot X^s) \;\; \leq \;\; f^{u_d} \cdot \dot{m}_d \cdot X^d \tag{8}$$

The power required $\dot{E}^+_d$ by demand d for the compression of the feedwater and for internal use in the equipment is defined in W by:

$$\dot{E}^+_d = \sum_s^{u_s} \frac{max(0, \Delta P_{s \to d}) \cdot \dot{m}_{s \to d}}{\mathcal{V}_{s \to d} \cdot \eta_p} + \dot{E}^+_{d,int} \tag{9}$$

with $\eta_p = 0.75$ the pump efficiency,
$\Delta P_{s \to d}$ the pressure difference between s and d in Pa,
$\dot{m}_{s \to d}$ the water flow rate from s to d in $kg.s^{-1}$,
$\mathcal{V}_{s \to d}$ the average water density between s and d in $kg.m^{-3}$,
$\dot{E}^+_{d,int}$ the electrical power used in the process unit u_d for other purposes than compression in W .

The total power $\dot{E}^-_s$ which can be recovered from the water streams leaving the source s is defined in W by:

$$\dot{E}^-_s = \sum_d^{u_d} max(0, -\Delta P_{s \to d}) \cdot \frac{\dot{m}_{s \to d}}{\mathcal{V}_{s \to d} \cdot \eta_e} \tag{10}$$

with $\eta_e = 0.85$ the efficiency of the energy recovery equipment.

In the model, energy recovery equipments are systematically installed on the water streams being discharged. The recovered power $\dot{E}^{-}_{ERI}$ is equal to:

$$\dot{E}^{-}_{ERI} = \sum_{s}^{u_s} max(0, -\Delta P_{s\rightarrow DIS}) \cdot \dot{m}_{s\rightarrow DIS} \cdot \eta_e \tag{11}$$

The heat requirement $\dot{Q}^{+}_{d,H}$ of demand d is defined in W by:

$$\dot{Q}^{+}_{d,H} = max(0, \sum_{s}^{u_s} \Delta T_{s\rightarrow d} \cdot \dot{m}_{s\rightarrow d} \cdot c_{p_{s\rightarrow d}}) + \dot{Q}^{+}_{d,H,int} \tag{12}$$

with $c_{p_{s\rightarrow d}}$ the average specific heat capacity between s and d in $J.kg^{-1}.K^{-1}$,
$\dot{Q}^{+}_{d,H,int}$ the intern heating requirement of process unit u_d .

The cooling requirement $\dot{Q}^{-}_{d,C}$ of demand d is defined in W by:

$$\dot{Q}^{-}_{d,C} = max(0, -\sum_{s}^{u_s} \Delta T_{s\rightarrow d} \cdot \dot{m}_{s\rightarrow d} \cdot c_{p_{s\rightarrow d}}) + \dot{Q}^{-}_{d,C,int} \tag{13}$$

with $\dot{Q}^{-}_{d,C,int}$ the intern cooling requirement of process unit u_d .

At this point, the energy requirements are calculated without considering the enthalpy temperature profile. Further developments of the model will integrate the heat cascade constraints [44].

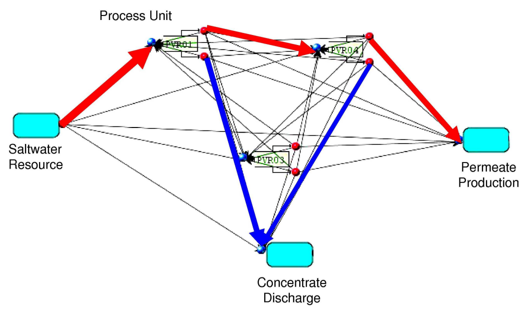

Figure 7. Superstructure with one feasible configuration

4.4. *Resolution of the superstructure*

The next step is to identify the most promising hybrid desalination configuration among the solutions developed in the superstructure. The superstructure is modeled as a MILP problem. For a given linear objective function, there will be one unique solution defining the best hybrid desalination configuration feasible for the set of equipments generated by $\vec{z_N}$. The linear objective function $G_{\vec{z_N}}$ used for the resolution is the total annual cost TAC.

The total annual cost TAC is the sum of the annualized investment cost $\mathcal{C}_{inv,ann}$ and the annual operating cost $\mathcal{C}_{op,ann}$. The function TAC is based on fixed cost models. Its minimization introduces bias in the global optimization procedure by favoring solutions adapted to the linear cost models but not necessarily optimal in the non linear multi-objective framework. To guarantee the optimality of the final MINLP solutions, a relaxed objective function TAC^{*} is used for the MILP problem resolution:

$TAC^{*} = \mathcal{C}^{*}_{inv,ann} + \mathcal{C}^{*}_{op,ann}$
with $\mathcal{C}^{*}_{inv,ann}$ the relaxed annualized investment cost in euros and

$\mathcal{C}^*_{op,ann}$ the relaxed annual operating cost in euros.

Relaxation variables $\vec{r}$ with $r_i \in$[0,1] are used as multiplicative factors for each major cost component of TAC. The approach is equivalent to use a weighting strategy for the MILP problem. As such, $\vec{r}$ is added in the decision set $\vec{z_N}$. The definition of r_i decides of the relative importance of the cost component $\mathcal{C}_i$. Depending on the set of $\vec{r}$, cheap, energy efficient or environmentally friendly solutions will be favored.

The relaxed annualized investment cost is equal to :

$$\mathcal{C}^*_{inv,ann} = \frac{i(1+i)^L}{(1+i)^L-1} \cdot \sum_{u=1}^{n_u} r_u(y^u \cdot \mathcal{C}^1_{inv} + f^u \cdot \mathcal{C}^2_{inv})$$

with $\mathcal{C}^1_{inv}$ the fixed component of investment cost for unit u independent of capacity in euros,
$\mathcal{C}^2_{inv}$ the variable component of investment cost for unit u depending on capacity in euros,
i the interest rate in percent,
L the life time of the plant in years.

Relaxation factors are also applied on the operating cost:
$\mathcal{C}^*_{op,ann} = r_{el} \cdot \mathcal{C}_{el} + r_{th} \cdot \mathcal{C}_{th} + r_{O\&M} \cdot \mathcal{C}_{O\&M}$

with $\mathcal{C}_{el}$ the annual electrical power cost in euros,
r_el the relaxation variable of power cost,
$\mathcal{C}_{th}$ the annual heating and cooling cost in euros,
r_th the relaxation variable of heating and cooling cost,
$\mathcal{C}_{O\&M}$ the O&M cost in euros,
$r_{O\&M}$ the relaxation variable of the O&M cost.

The annual electrical power cost $\mathcal{C}_{el}$ is estimated with:

$$\mathcal{C}_{el} = (\sum_d \dot{E}^+_d - \dot{E}^-_{ERI}) \cdot 24 \cdot 365 \cdot l \cdot p_{Wh_{el}}$$

with l the load factor of the plant,
$p_{Wh_{el}}$ the price of a electrical Wh in $euros$.

The annual heating and cooling cost $\mathcal{C}_{th}$ is estimated with:
$\mathcal{C}_{th} = \sum_d(\dot{Q}^+_{d,H} \cdot p_{Wh_H} + \dot{Q}^-_{d,C} \cdot p_{Wh_C}) \cdot 24 \cdot 365 \cdot l$

with l the load factor of the plant,
p_{Wh_H} the price of a Wh for heating purpose in $euros$,
p_{Wh_C} the price of a Wh for cooling purpose in $euros$.

4.5. *Multi-objective optimization*

Once the piping network and the equipments are defined by solving the MILP problem, the global hybrid desalination system can be characterized in details. Pumps, boilers, energy recovery devices, pipes, RO trains, heat exchangers are designed according to the flow rates, temperatures and pressures. The investment cost is calculated by summing the investment costs of the equipments and the additional costs related to their installation on the plant (bottom-up approach [45]). The operating cost is composed of the electricity, heat, chemical, labor and maintenance costs and is evaluated with non linear equations on the basis of the calculated flow rates. The environmental impacts are expressed in terms of GHG emissions (calculated from the total energy consumption) and in terms of water resource consumption depending on the conversion rate.

The performances evaluated are associated to a unique hybrid desalination system optimized for a unique set of equipments. The Multi-objective optimizer (MOO) searches for the sets of equipments, which produce the best hybrid desalination configurations with regard to the objectives chosen. The Pareto frontier, which represents

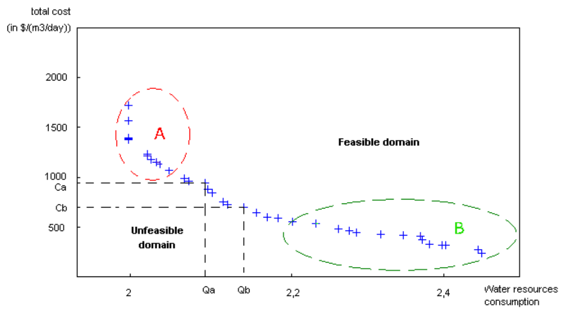

Figure 8. Pareto curve of the multi-objective optimization

the whole ensemble of optimal hybrid desalination solutions, can be interpreted as a materialization of technical, economical or environmental constraints applied to the hybrid desalination configuration.

For two chosen objectives (for example, the annual costs per m^3/day of potable water produced and the water resource consumption per m^3 of potable water produced), the Pareto frontier is :

(i) the set of non dominated solutions such that for any given water resource consumption Q_a, it is not possible to achieve a lower cost of water C_a; or

(ii) the set of non dominated solutions such that for any cost of water C_b, it is not possible to achieve lower water resource consumption Q_b

These optimal configurations can then be compared considering different criteria. The optimal solutions in the circle A are environmental friendly configurations with low water consumption but high investment costs. On the contrary, the solutions in the circle B represent the less expensive solutions consuming more water resources. This panel of optimal solutions coupled with multi-criteria analysis provides technology developers with various design alternatives and comparison elements, which will help in the decision process.

5. Case study

The goal of the case study is to demonstrate the application of the water network design. The project considered in this case study aims at producing 30000 m^3/day of potable water with a maximum salinity of 100 ppm. The unique water resource is the sea with a salinity of 35000 ppm. The technologies proposed are the reverse osmosis (RO) and the multi-stage flash distillation with brine recirculation (MSF-BR).

5.1. *Mathematical models of technologies*

For more flexible designs, the heat recovery section and the heat rejection section of the MSF installation are modeled separately.

The pressure losses in the pipes, mixers and splitters are neglected.

5.1.1. *Reverse Osmosis*

One objective of the project has been to develop a flexible and updated membrane database, which incorporates the technological development of desalination equipments. Accurate models of membranes require the definition of numerous membrane-specific parameters [16, 18]. In order to conserve a limited number of specific parameters for each membrane and to facilitate the insertion of new membranes in the database, the choice was made to use simple homogeneous solution-diffusion models of spiral-wound membranes [10]. The concentration polarization is neglected and constant pressure drop is assumed.

The model is based on the general equations of conservation of the solvent and of the solute through the membrane to define the flow rate and the salinity of the input and output streams.

The water flux through the membrane $\dot{J}_e$ is defined as the permeate mass flow rate divided by the membrane surface. $\dot{J}_e$ is modeled by Fick's law:

$$\dot{J}_e = \mathcal{F} \cdot A_T \cdot (\Delta P_{tm} - \Delta \pi_{tm}) \tag{14}$$

with $\dot{J}_e$ water mass flux in $kg.m^{-2}.s^{-1}$
A_T membrane water permeability in $kg.m^{-2}.s^{-1}.Pa^{-1}$
ΔP_{tm} transmembrane pressure in Pa
$\Delta \pi_{tm}$ transmembrane osmotic pressure in Pa

The fouling factor $\mathcal{F}$ is introduced to represent the effects of membrane fouling on flux reduction. $\mathcal{F}$ is fixed by hypothesis at $\mathcal{F} = 0.85$.

A_T depends on the water viscosity, which varies with temperature. A_T is related to the temperature T by an Arrhenius-type correlation:

$$A_T = A_0 \cdot e^{\frac{E_i}{\mathcal{R}}(\frac{1}{298} - \frac{1}{T})} \tag{15}$$

with T temperature of the feedwater in K
A_0 membrane water permeability at $T_0 = 298\ K$
E_i the apparent activation energy in $kJ.kmol^{-1}$
$\mathcal{R}$ the universal gas constant $\mathcal{R} = 8.314\ J.mol^{-1}.K^{-1}$

For reverse osmosis membranes, the apparent activation energy E_i varies between 15000 and 25000 $kJ.kmol^{-1}$ depending on the water temperature [46]. By hypothesis, it will be considered constant: $E_i = 20000\ kJ.kmol^{-1}$.

On the other hand, the salt mass flux $\dot{J}_s$, defined as the salt flow rate through the membrane divided by the surface of the membrane, is given by:

$$\dot{J}_s = B \cdot (X_f - X_p) \tag{16}$$

with $\dot{J}_s$ salt mass flux in $kg.m^{-2}.s^{-1}$
B membrane salt permeability in $kg.m^{-2}.s^{-1}$
X_f, X_p respectively the salinity of feedwater and permeate in ppm

B is also called the solute transport parameter and is assumed to be independent of temperature and constant for both monovalent and divalent ions.

The membrane flux is totally characterized by A_0 and B, when assuming that the mass flux of solute is equal to the volume solvent flux multiplied by the mass concentration of solute in the permeate:

$$\dot{J}_s = \dot{J}_e \cdot X_p \tag{17}$$

The retention rate R is obtained by the following expression:

$$R = \frac{1}{1 + \frac{B}{\dot{J}_e}} \tag{18}$$

The transmembrane osmotic pressure is defined by the following equation:

$$\Delta \pi_{tm} = \frac{\pi_f + \pi_b}{2} - \pi_p \tag{19}$$

with π_f, π_p, π_b the osmotic pressures of the feedwater, the permeate and the concentrate in Pa.

Considering that the saltwater contains only NaCl, the osmotic pressure π_i can be calculated with the Van't Hoff formula

$$\pi_i = M_i \cdot \mathcal{R} \cdot T_i = \frac{2 \cdot X_i \cdot \mathcal{V}_i}{\mathcal{M}_{NaCl}} \cdot \mathcal{R} \cdot T_i \tag{20}$$

with $i \in \{f, p, b\}$ water stream
π_i osmotic pressure in Pa
X_i mass concentration of salts in ppm
M_i molar concentration of salts in $mol.m^{-3}$

T_i temperature in K
$\mathcal{V}_i$ water density at T_i in $g.m^{-3}$
$\mathcal{M}_{NaCl} = 58.5\ g.mol^{-1}$ molar mass of NaCl

In the example, two different membranes have been characterized, one specialized for brackish water and another dedicated to seawater. Their characteristics are estimated from the data and calculations performed using the design software ROSA® on two commercial membranes SW30-HR380 and BW30LE-440i from Filmtec^{TM} (Tab.1).

Table 1
Membrane Database

Commercial name	**SW30**	**BW30**
Membrane area $\mathcal{A}$ in m^2	35.3	40.9
Solvent permeability A_0 in $10^{-9}.kg.m^{-2}.s^{-1}.Pa^{-1}$	2.4	12
Solute permeability B in $10^{-9}.kg.m^{-2}.s^{-1}$	7.1	15
Maximum Pressure P_{max} in bar	70	40
Minimum Pressure P_{min} in bar	20	10
Max permeate flow rate $\dot{m}_{e_{max}}$ in m^3/j	25	40
Max feed flow rate $\dot{m}_{f_{max}}$ in m^3/h	14	30
Min concentrate blowdown $\dot{m}_{b_{min}}$ in m^3/h	3	3
Pressure drop ΔP_{drop} in bar	0.2	0.2
Max brine salinity $X_{b_{max}}$ in ppm	65000	30000

A pressure vessel with n_e membrane elements is equivalent to n_e serial membranes, the concentrate of membrane n being the feedwater of membrane $n+1$. It is modeled as a global system of n_e successive interconnected membrane models. The system has only 5 degrees of freedom:
– T_f the temperature of water feeding the pressure vessel
– X_f the salinity of water feeding the pressure vessel
– $\dot{m}_f$ the flow rate of water feeding the pressure vessel
– r the total recovery rate of the pressure vessel
– ΔP_{tm} the transmembrane pressure applied on the first membrane of the pressure vessel

The definition of these 5 decision variables explicitly determines the model. The Newton-Raphson algorithm is used to solve the model and to characterize the unique solution. The solving of the system characterizes each membrane with a specific recovery rate, flux and retention rate. If each membrane does not fit to the constructor good practices tests (minimum concentrate flow rate, maximum feed flow rate,...), the pressure vessel is discarded.

At the scale of the pressure vessel, the conversion rate r and the global retention rate R determine the costs of the pressure vessel and the characteristics of the water streams leaving the equipment, which are then used to build the process unit u (Fig.6).

The demand is characterized by:
$\dot{m}_{d_u} = \dot{m}_f$
$X_{d_u} = X_f$
$T_{d_u} = T_f$
$P_{d_u} = \Delta P_{tm} + P_{s_{u,1}}$

The source 1 (the permeate) is characterized by:
$\dot{m}_{s_{u,1}} = \dot{m}_f \cdot r$
$X_{s_{u,1}} = X_f \cdot (1 - R)$
$T_{s_{u,1}} = T_f$
$P_{s_{u,1}} = 0.5\ \ bar$

The source 2 (the concentrate) is characterized by:
$\dot{m}_{s_{u,2}} = \dot{m}_f \cdot (1 - r)$

$\dot{X}_{s_{u,2}} = \frac{X_f - X_f(1-R)r}{1-r}$
$T_{s_{u,2}} = T_f$
$P_{s_{u,2}} = \Delta P_{tm} - n_e \Delta P_{drop}$

There are no power, heating or cooling requirements for RO other than high pressure compression needs for the membrane filtration.

5.1.2. *Multi-stage Flash: Heat Recovery Section*

An advanced steady-state model of MSF-BR at high temperature (HT) and cross tube configuration as described in [9] has been implemented. Without heat rejection, the MSF-BR heat recovery section is equivalent to a MSF Once-Through installation. For a given quality of feedwater (temperature T_f, salinity X_f, flow rate $\dot{m}_f$), the model is totally characterized by fixing the 6 decision variables, which are:
– T_f the temperature of water feeding the equipment
– X_f the salinity of water feeding the equipment
– $\dot{m}_f$ the flow rate of water feeding the equipment
– N_{rec} the number of distillation stages
– TBT the top brine temperature
– T_{b_n} the temperature of the rejected brine.

The heat consumed in the boiler is an intern heat requirement and is calculated in the total annual heating cost.

5.1.3. *Multi-stage Flash: Heat Rejection Section*

The heat rejection section is based on the model described by El-Dessouky and Ettouney [9]. The model has 8 decision variables:
– T_f the temperature of water feeding the equipment
– X_f the salinity of water feeding the equipment
– $\dot{m}_f$ the flow rate of water feeding the equipment of cooling water (temperature
– T_{cw} the temperature of the cooling water
– X_{cw} the salinity of the cooling water
– K_{cw} the ratio of the flow rate of cooling water divided by the feed water
– N_{rej} the number of rejection stages
– T_{b_n} the temperature of the rejected brine

The heat rejection section has two feed streams (the cooling water and the water to be distilled). Its process unit in the equipment database is different. The cooling water is considered as a water stream as well. It has 3 sources (the distillate, the concentrate and the rejected cooling water $j = 3$) and 2 demands (the feedwater and the cooling water $i = 2$).

5.2. *Results*

This method is applied to the following project:
– Objectives: minimize the total annual cost (TAC) and the water consumption per cubic meter of water desalinated
– Available desalination technologies: MSF and RO
– Available quantity of local water resource: $\dot{m}_{s_{WR}}$ = Infinite (Seawater)
– Salinity of the resource: $X_{s_{WR}}$=35000 ppm
– Desired capacity of desalinated water: The desired capacity of 30000 m^3/day at 298 K corresponds to $\dot{m}_{d_{PROD}}$ =30.10^6 kg/day
– Desired quality of the desalinated water: $X_{d_{PROD}}$ =100 ppm

The research of hybrid configuration solutions is carried out with a database of equipments composed of 4 RO different pressure vessels, 2 MSF recovery section and 1 MSF rejection section. These equipments are characterized by the decision variables listed in Tab.2. Depending on the set chosen, they will be feasible or not.

Table 2
Decision variables of the multi-objective optimization

Type	Unit	Variation bounds	Quantity
Relaxation factors			
r_{el} relaxation factor of electricity cost		[0,1]	1
r_{th} relaxation factor of heating cost		[0,1]	1
r_{pre} relaxation factor of pretreatment cost		[0,1]	1
r_u relaxation factor of investment cost of unit u		[0,1]	7
Pressure vessel			
choice of membrane		SW, BW	4
n_e number of membranes composing the pressure vessel		[5 , 8]	4
X_f salinity of feedwater	*ppm*	[100 , 60000]	4
T_f temperature of feedwater	*K*	[280 , 310]	4
r recovery rate		[0.2 , 0.6]	4
ΔP_{tm} applied transmembrane pressure on the first membrane	*bar*	[10 , 70]	4
MSF-BR heat recovery section			
N_{rec} number of stages		[18 , 26]	2
X_f salinity of feedwater	*ppm*	[100 , 60000]	2
T_f temperature of feedwater	*K*	[280 , 310]	2
TBT top brine temperature	*K*	[365 , 375]	2
T_{b_n} rejected brine temperature	*K*	[300 , 350]	2
MSF-BR heat rejection section			
N_{rej} number of stages		[2 , 4]	1
X_f salinity of feedwater	*ppm*	[100 , 60000]	1
T_f temperature of feedwater	*K*	[280 , 310]	1
X_{cw} salinity of cooling water	*ppm*	[0.01 , 60]	1
T_{cw} temperature of cooling water	*K*	[280 , 300]	1
K_{cw} ratio cooling water/feed water		[0 , 2]	1
T_{b_n} rejected brine temperature	*K*	[300 , 350]	1

The two objectives are the minimization of the total annual cost (calculated with non linear functions) and the maximization of the conversion rate $r = \frac{\dot{M}_{d_{PROD}}}{\dot{M}_{s_{WR}}}$. The multi-objective optimization is performed using 20000 evaluations with a starting population of 2000 individuals in the space of decision variables. The resulting optimal points form the Pareto curve displayed in Fig.9.

In order to avoid salt precipitation, a maximum salinity X_{max} has been fixed as a technical limitation for the leaving streams of each equipment. Its value is set to 65000 *ppm* for both RO and MSF equipments. The maximum conversion rate r_{max} is defined by:
$\frac{X_{wr}}{1-r_{max}} \leq X_{max}$.

This corresponds to a r_{max} equal to 0.46.

The proposed desalination solutions have minimum and maximum limits of conversion whatever the costs. By mixing concentrate with water of lower salinity, some of the proposed configurations achieve conversion rates higher than r_{max}. These advanced configurations are however more expensive.

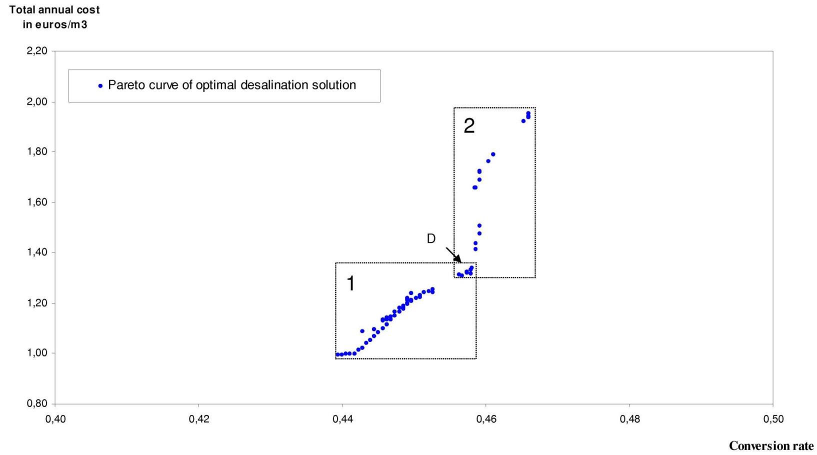

Figure 9. Pareto curve of the multi-objective optimization

The minimum conversion rate illustrates the trade-off between two phenomena. By operating at a small conversion rate, the osmotic pressure and the applied transmembrane pressure decrease. But the smaller the conversion rate, the more feedwater needs to be pre-treated and pumped at high pressure. This increases the energy consumption and the costs. Consequently, there is a minimum conversion rate, corresponding to the cheapest available solution.

2 clusters of solutions are identified in the Pareto curve. At high cost and high conversion rate, the hybrid solutions are chosen because the mixing of water fluxes allows a better management of salt precipitation (cluster 2). At low price and lower conversion rate, the pure membrane technologies are selected (cluster 1). The point D, where the slope of the Pareto curve increases, corresponds to the technological switch between pure membrane designs and advanced hybrids. This repartition depends strongly on the comparative prize of vapor and electricity. Each point of the Pareto curve corresponds to a desalination configuration. An example of a generated desalination configuration is shown in Fig.10 with an optimized RO design with two passes, two stages and recirculation of the concentrate.

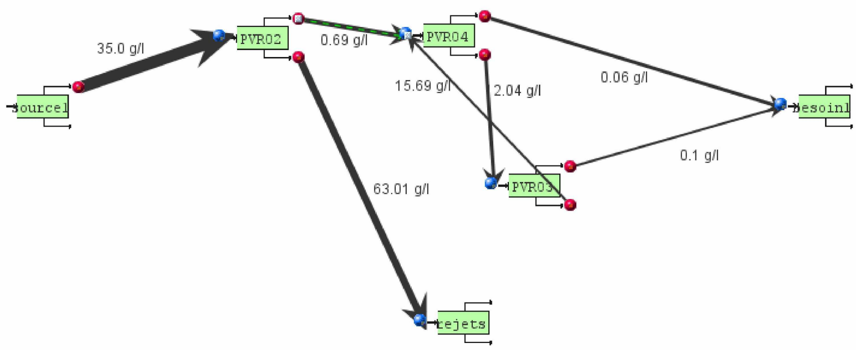

Figure 10. Example of generated desalination configuration: RO with 2 stages

6. Discussion

A multi-objective MINLP optimization strategy, for the synthesis of optimal hybrid desalination configurations, has been presented. This method combines process modelling and process integration techniques (the superstructure principle) and advanced mathematical solving tools to optimize simultaneously the design and the operation of integrated desalination systems. It identifies promising hybrid desalination configurations, which are fully characterized and optimized. The Pareto curves resulting from the multi-objective approach allow more transparent negotiation and weighting procedure between decision criteria. As such, the proposed approach is particularly suitable for process engineers. It helps them to explore at an early stage of development the whole technical possibilities and to identify the non-intuitive solutions, which they can quickly assess relying on the generated design and on their own expertise.

Besides an accurate technical modelling of desalination technologies, the optimization method rely strongly on the quality of the performances indicators (equipment cost models, operating cost, GHG emissions calculations) and on the working hypothesis (steam/electricity prize, heat transfer coefficient, fouling factor,...). These key parameters and a detailed sensitivity analysis will be presented in the next article.

The flexibility of the method is an outstanding advantage, which will be used in further developments by upgrading the equipment database with additional desalination technologies (Nanofiltration, MEE, MEE-TVC) and different energy conversion options (Gas turbine, Combined Cycle, Rankine Cycle). The combination of power conversion and desalination techniques will then be investigated using the process integration techniques.

This optimization strategy can be globalized to dual-purpose water and power production schemes but may also be applied to simpler configurations such as single membrane or distillation plant. The database of commercial membranes can be extended with membranes from all producers, allowing the design and the optimization of schemes between various membranes from different constructors.

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