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PROCESS INTEGRATION FOR SIMULTANEOUS ENERGY AND WATER MINIMIZATION

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Abstract

The minimization of water and energy has become an imperative constraint in the process industries. The two objective (i.e. water and energy minimization) are often highly correlated and should not be dealt with as disjointed problems.

In view of the above, the purpose of this study is to carry on an integration of two existing programs for the optimization of energy and wastewater consumption respectively. An example from the literature was used as a benchmark. Results show that it is possible to combine the two programs and achieve the best energy and wastewater saving for a generic process. For the adopted case study, the final process network was designed, showing that it is feasible to achieve a wastewater reduction of 20%, a hot utility reduction of 86,39% and a cold utility reduction of 100%.

An interface was designed and implemented in Visual Basic to make the two programs exchange key information and consumption, to allow the user to perform a generic process integration.

Riassunto

L'acqua e l'energia termica sono delle risorse essenziali nell'ambito dei processi industriali. Una grande quantità d'acqua è usata in molti settori importanti come cartiere, raffinerie, industria alimentare e, in generale, per varie operazioni come lavaggi, estrazioni e reazioni. L'energia termica è necessaria soprattutto per far raggiungere le temperature richieste ai vari flussi materiali presenti nelle operazioni dell'industria di processo.

L'aumento delle attività industriali avvenuto negli ultimi decenni, grazie al quale si è potuto registrare un importante sviluppo tecnologico con conseguente miglioramento della qualità della vita, ha provocato però anche un allarmante incremento per quanto riguarda il consumo delle risorse naturali, ed ha portato in primo piano nel panorama internazionale, il problema dell'esaurimento di tali risorse. Come risposta a ciò, grandi sforzi sono stati effettuati nella ricerca di processi più sostenibili e norme ambientali sempre più stringenti sono state applicate alle emissioni acquose, atmosferiche ed ai gas ad effetto serra. Negli ultimi anni tali problemi sono diventati così importanti per l'opinione pubblica che le politiche di sostenibilità nelle aziende sono diventate uno standard essenziale nel mercato globale.

L'integrazione di processo si è dimostrata una metodologia molto efficiente a riguardo, permettendo la minimizzazione dei consumi di acqua ed energia nelle attività industriali anche se, molti degli studi svolti fino ad ora si concentrano di più sul minimizzare queste due risorse in maniera separata anziché congiunta.

La scelta di una minimizzazione simultanea del consumo di energia e delle risorse idriche non è in realtà casuale; questo perché l'acqua usata come solvente nelle operazioni di estrazione, non viene utilizzata alle condizioni di sorgente, ma è scaldata alla temperatura richiesta dall'operazione e, prima di essere scaricata, viene raffreddata nel rispetto delle norme ambientali vigenti.

Lo scopo di questo lavoro è stato la ricerca di un approccio per la minimizzazione simultanea del consumo energetico e di risorse idriche per un generico processo che utilizza acqua per la rimozione di contaminanti, attraverso la combinazione di due programmi esistenti, *FI²EPI* e *AquoMin* sviluppati presso il Centro di Processi Chimici (CPQ) dell'Istituto Superiore Tecnico dell'Univerità di Lisbona

AquoMin è un programma sviluppato in Visual Basic che effettua la minimizzazione del consumo di acqua fresca e della produzione di acqua di scarico, in un generico processo che utilizza l'acqua per la rimozione di contaminanti. FI²EPI è un programma sviluppato

in Java che effettua l'integrazione energetica fra le streams di un generico processo, in modo da ottenere il minimo consumo di utilities.

Lo studio è stato diviso in due parti: nella prima parte è stato definito l'approccio per la combinazione ottimale dei due programmi, mentre la seconda parte ha compreso lo sviluppo in Visual Basic di un terzo software, AFI, che funge da interfaccia grafica fra AquoMin e FI^{2}EPI per l'ottenimento, mediante l'utilizzo dei software in modo sequenziale, della minimizzazione dei consumi energetici ed idrici in un generico processo. È stato scelto, come approccio all'integrazione di processo, di sviluppare un interfaccia fra AquoMin e FI^{2}EPI piuttosto che un singolo programma, in quanto questo lavoro è alla base di un progetto futuro il cui fine ultimo è quello di unire AquoMin e FI^{2}EPI in un unico software.

Per definire il metodo di integrazione dei due programmi e ottenere l'integrazione di processo, è stato utilizzato un esempio numerico di un processo composto da quattro operazioni, proposto da Savulescu, et al., (2005).

È stato possibile calcolare che, senza l'applicazione di alcun tipo di integrazione, il processo produce 112.5 kg/h di acqua di scarico e necessita rispettivamente di 27687 kW e di 22976 kW per il riscaldamento ed il raffreddamento delle streams. L'esempio indica inoltre che, applicando la simultanea minimizzazione del consumo energetico e di risorse idriche al processo, si ottiene una produzione di acqua di scarico di 90 kg/h ed un fabbisogno energetico rispettivamente di 3780 kW e 0 kW per il riscaldamento ed il raffreddamento delle streams.

Sono stati innanzitutto effettuati dei primi tentativi di integrazione, combinando AquoMin e FI^{2}EPI direttamente, cioè senza nessuna rilevante interfaccia fra i due. I migliori risultati ottenuti con questo approccio mostrano una produzione di acqua di scarico di 90 kg/h ed un fabbisogno energetico rispettivamente di 4845 kW e 1075 kW per il riscaldamento ed il raffreddamento delle streams. Come è stato possibile osservare, il valore minimo di produzione di acqua di scarico è già raggiunto senza l'utilizzo di migliorie nell'unione dei due programmi, mentre i consumi energetici, pur mostrando una rilevante riduzione, non raggiungono il target indicato dall'esempio. È opportuno specificare che l'unico approccio possibile per combinare i due programmi è quello di utilizzare prima AquoMin e in seguito FI^{2}EPI; questo perché l'integrazione di massa, per minimizzare il consumo idrico va a modificare le streams di processo, mentre l'integrazione energetica utilizza i dati delle streams esistenti per ricavare i Minimum Energy Requirements (MER). Grazie ai primi tentativi di integrazione è stato possibile recepire i punti chiave su cui si è concentrato il lavoro nel miglioramento dell'integrazione energetica:

i. Massimizzare il numero di streams coinvolte nello scambio termico in modo da avere un range più ampio di temperature da poter sfruttare nell'integrazione energetica

ii. Prevenire le perdite di calore che avvengono quando ad esempio una stream viene raffreddata per poi essere riutilizzata e scaldata nuovamente

iii. Tenere in considerazione la qualità delle streams; cioè non mescolare stream ad alta temperatura con stream a bassa temperatura.

La prima miglioria effettuata interessa un particolare comportamento di AquoMin per cui, nella costruzione del Mass Exchange Network (MEN), combina tutte le streams in uscita con la stessa concentrazione di contaminante, prima del riutilizzo. Dato che non è stato possibile modificare direttamente AquoMin, in base ai valori di portata restituiti dallo stesso, il software AFI è stato programmato per sviluppare un nuovo network in cui le streams in uscita rimanessero divise. Con questo miglioramento tuttavia è stata introdotta una nuova variabile processuale, ossia la quantità di portata che deve essere riutilizzata, per ognuna delle streams che precedentemente erano mescolate fra loro. In questo studio, tale nuova variabile è stata chiamata split ratio.

Il secondo miglioramento effettuato ha interessato il calcolo della posizione ottimale in cui era possibile installare gli scambiatori di calore nelle streams in ingresso. Assumendo che le possibili posizioni fossero due (prima o dopo il mixing point) l'opzione migliore, per una stream che necessita di riscaldamento, coincide con l'installare lo scambiatore di calore nel punto in cui la stream è più fredda. La scelta opposta, invece, se la stream necessita di raffreddamento. Il software AFI è stato programmato per selezionare automaticamente la posizione ottimale degli scambiatori di calore nelle streams in ingresso.

Con l'implementazione di queste migliorie, è stato possibile raggiungere gli stessi risultati indicati nell'esempio di Savulescu, Kim et al., 2005.

L'alto aspetto importante di questo lavoro, riguarda lo sviluppo di un terzo software (chiamato AFI) che funge da interfaccia grafica per la risoluzione di un processo contenente un massimo di quattro operazioni. Il limite maggiore del software realizzato, è rappresentato dal fatto che l'integrazione di processo non è effettuata tramite un singolo programma, ma è necessario utilizzare tutti e tre i software (AquoMin, AFI e FI^{2}EPI) in maniera sequenziale. Sono state inoltre riscontrate ulteriori difficoltà nella ricerca del valore ottimale di split ratio (ossia il valore che restituisse i minimi consumi energetici e idrici) in quanto non è stato possibile sviluppare un programma di ottimizzazione attraverso i tre differenti programmi. Al momento, il valore ottimale di split ratio, deve essere trovato a tentativi.

Un ulteriore limite di questo studio è rappresentato dal massimo di quattro operazioni che attualmente può contenere il processo in esame. Tale limite è stato inserito in quanto la

quantità di calcoli e programmazione necessaria per aggiungere ulteriori operazioni non sarebbe stata fattibile.

Come accennato in precedenza, questo lavoro rappresenta la base per un progetto futuro il cui scopo finale è quello di fondere AquoMin e FI^{2}EPI in un unico programma. Si consiglia quindi, una volta uniti i due software, l'implementazione di tutti i miglioramenti sviluppati in questo lavoro. In particolare l'implementazione nel software AquoMin del primo miglioramento discusso, sarebbe sufficiente a rimuovere il limite sul numero di operazioni presente nel processo. Si suggerisce oltretutto di sviluppare una funzione per l'ottimizzazione dello split ratio nel Mass Exchange Network.

La tesi è strutturata come segue:

Nel Capitolo 1 è descritta la teoria e le tecnologie che stanno alla base dello studio effettuato. Nel dettaglio sono descritte le linee generali dell'integrazione di processo, l'integrazione di massa e gli approcci principali dell'integrazione energetica.

Il Capitolo 2 presenta AquoMin, uno dei due software utilizzati per questo lavoro. In particolare AquoMin è il programma che effettua la minimizzazione del consumo idrico, in un generico processo che utilizza acqua per la rimozione di contaminanti.

Nel Capitolo 3 è descritto FI^{2}EPI, il secondo programma utilizzato in questo lavoro. Nel dettaglio FI^{2}EPI è il software che effettua l'integrazione energetica fra le streams di un generico processo, con lo scopo di ottenere il valore del consumo minimo di utilities.

Il capitolo 4 descrive lo sviluppo del software AFI, l'approccio ed i calcoli effettuati per combinare AquoMin e FI^{2}EPI e la guida per l'utilizzo dell'interfaccia grafica sviluppata in Visual Basic.

Alcuni commenti conclusivi e una discussione sui possibili sviluppi futuri concludono la tesi.

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Introduction

Water and energy are two essential resources for process industries. A massive amount of water is needed for many important fields such as pulp and paper mills, refineries or food processing and, in general process industry, for various unit operations like washing, extractions or reactions. Energy, in the other hand, is mostly used for heating and cooling purposes in order to reach the operation temperatures required for the industrial processes. The increasing industrial activities that took place in the last decades has led to an alarming consumption of natural resources and raised the international attention on the problem of resource depletion. As response of this problem, significant efforts have been made to seek more sustainable processes and more stringent environmental regulations have been imposed on the aqueous, atmospheric and greenhouse gas emissions. In the last years, the public concern for the environment has so increased in importance that the sustainability policies in the industries have become an essential standard to stay competitive in the market.

Process integration techniques have shown to be very efficient to minimize water and energy consumptions; however, most of the studies are focused on water and energy minimization separately, rather than simultaneously. The choice of a simultaneous minimization of the water and energy consumption is not casual; in fact, the two aspect of water and utilities minimization are actually very much related. That because the water used in the process as an extractive agent, is not merely used at the source conditions, but it is usually heated to match the requirements of the operation, and before being discharge, the wastewater is generally cooled to comply with the environmental constraints.

This dissertation has been made during an Erasmus program at the Instituto Superior Técnico (IST) of the University of Lisbon; under the supervision of Prof. Henrique A. Matos.

The goal of this study is the simultaneous minimization of wastewater and energy consumption, through a combination of two existing programs, FI^2EPI and *AquoMin* developed at the Center for Chemical Processes of the Instituto Superior Técnico (IST) of the University of Lisbon. AquoMin is a program coded in Visual Basic (VBA) that performs the minimization of the fresh water consumption and wastewater production in a generic process using water as a contaminant remover. FI^2EPI is a tool coded in Java that performs energy integration between hot streams and cold streams in a generic process to obtain the minimum utilities consumption.

Namely, this work aims at reproducing the results of an example taken from the literature. The study made in this thesis also aims at finding the improvements needed to combine

the two software, so as to lay down the foundations for a future project, whose final goal is to merge AquoMin and FI^{2}EPI in one single program. The work also includes the development of a third program, AFI (AquoMin FI^{2}EPI interface), coded in VBA, that proposes to be an user friendly interface between FI^{2}EPI and AquoMin.

The dissertation is structured as follows:

The first chapter aims at discussing the theory and technology that lie behind the subject of this thesis. The basics of process integration, the theory of wastewater minimization and the main approaches for energy integration will be introduced and explained.

The second chapter presents in detail AquoMin, one of the two programs used for this work; in particular, the one that performs the minimization of the fresh water consumption and wastewater production in a generic process that use water as a contaminant remover. The third chapter describes in detail FI^{2}EPI, the second program used for this work; FI^{2}EPI performs the energy integration between hot streams and cold streams in a generic process, to obtain the minimum utilities consumption.

The fourth and last chapter shows the development of the AFI software: the approach and calculations made to combine AquoMin and FI^{2}EPI; and the walkthrough of the user-frendly interface coded in Visual basic.

Some final remarks and a discussion on future possible developments will conclude the work.

Chapter 1

State of the art, motivations and objective

This chapter focus on the theory and technology that lie behind the subject of this thesis. In particular, on the first part, it will be explained the basics of the process integration, the theory of the wastewater minimization and the main approaches of the energy integration.

In the second part of this chapter will be exposed the motivations that support this study and the goals to which this work aims.

1.1 Process integration

Process Integration is a term to indicate an holistic approach to achieve process improvements by the optimization of different operations all together, rather than separately (El-Halwagi, 1997).

The purposes of the Process integration could be identified by the seven themes of Keller and Bryan, 2000:

- Reduction in raw material cost
- Reduction in capital investment
- Reduction in energy use
- Increase in process flexibility and reduction in inventory
- Ever greater emphasis on process safety
- Increased attention to quality
- Better environmental performance

In this study, it will be take in account the aspect of energy integration and the wastewater minimization, that concerns the aspects of material cost, capital investment, energy use and environmental performance.

The steps required to perform process integration are the following:

1. Task Identification: it represents the goal that the study aims to achieve, described as an actionable task; for this thesis, the task identification could be the energy and water reduction in a generic process.

2. Targeting: refers to the identification of performance benchmarks ahead of detailed design (El-Halwagi, 2006).

3. Generation of alternatives: usually there are almost infinite possible solutions to reach the target. Therefore is important to have a framework that shows all the different possibilities, or at least the ones of interest. In our study there are many different solutions given by the different possible positions of the heat exchangers and of the streams to reutilize.

4. Selection of Alternatives: refers to the choice of the alternative that gives the optimum solution among all the others; typically to select the right choice are necessary some mathematical/graphical/algebraic techniques.

5. Analysis of Selected Alternatives: refers to analysis technique to evaluate the selected alternative. In this study, it is only possible to perform this kind of evaluation by trial and error.

1.2 Mass integration

Water is a very important component for the chemical process industries; it could be used, other than as a raw material, as a thermal agent and/or as a separation agent.

If used to extract or in general separate different components, water is contaminated; with the unlimited fresh water source capacities and the permissive limits of pollutant for the water discharge, there were not many incentives for the companies to reduce water consumption in the past. Now, because of the increasingly stringent environmental regulations and the public concern for the environment, many industries have started seeking ways to reduce water consumption and to modify the process so as to achieve that reduction.

Cleaning the wastewater is indeed an important step, but before that, it is necessary to use an approach to minimize the wastewater generation.

The concept of pinch analysis was originally proposed by Hohmann, 1971; Linnhoff and Flower, 1982 for the Heat Exchangers Network Synthesis (HENS). Based on analogies between mass and heat transfer (Table 1.1), the pinch method was further extended into Mass Exchange Network Synthesis (MENS) by El-Halwagi and Manousiouthakis, 1989. This allowed the development of various mass integration techniques (El-Halwagi, 1997; El-Halwagi, 2006) and subsequently Wang and Smith, 1994; Mann, 1999 list the approaches to minimize the wastewater generation:

- Regeneration-reuse, when the wastewater is purified and reused in another operation of the process. It is usually mixed with freshwater or wastewater from other operations.

Table 1.1. *Analogy between MENS and HENS*

	MENS	HENS
Transported property	Mass	Energy
Driving Force	Difference of Concentration	Difference of Temperature
Source	Rich Streams	Hot Streams
Sink	Lean Streams	Cold Streams

- Regeneration-recycling, when pollutants from wastewater are partly eliminated and the wastewater is returned to the same process afterwards.
- Process change, the water consumption is reduced due to modification for instance in the number of stages of extractions, change the water used in the cooling towers or exchangers with other fluids, etc.
- Reuse, when wastewater is reused in another operation or process: Generally, the wastewater could be mixed with freshwater or other wastewater to decrease the concentration of contaminant.

One of the first systematic approaches for evaluating water reuse in chemical process industrial plan was proposed by Rosain, 1993 followed by Bagajewicz, 2000 with a review of recent design procedures for water networks in refineries and process plants that analyze a conceptual approach and a mathematical programming to obtain an optimal wastewater design.

One of the most used systematic approaches was developed by the Centre for Waste Reduction Technologies (CWRT) that can be resumed in five steps (Byers, 1995):

1. Establishing boundary limits
2. Identify and evaluating water reuse issues
3. Evaluating technical opportunities and water reuse techniques
4. Implementing a new water reuse model
5. Reviewing and updating the approach

1.2.1 Mass Exchange Network Synthesis (MENS)

It is possible to define a mass exchanger as an unit that perform a direct-contact mass transfer and use mass separating agents (MSAs). The most common industrial operations that performs mass exchange are for instance: absorptions, adsorptions, ion exchange, solvent extractions, leaching and stripping, while the most common MSAs are: solvents, adsorbents, ion exchange resins and stripping agents.

El-Halwagi, 1997 gives a detailed definition of the MENs synthesizing problem:

"Given a number N_R of waste (rich) streams (sources) and a number N_S of MSAs (lean streams), it is desired to synthesize a cost-effective network of mass exchangers that can preferentially transfer certain undesirable species from the waste streams to the MSAs. Given also are the flowrate of each waste stream, G_i, its supply (inlet) composition y_i^s, and its target (outlet) composition y_i^t, where $i = 1,2,\ldots,N_R$. In addition, the supply and target compositions, x_j^s and x_j^t, are given for each MSA, where $j = 1,2,\ldots, N_S$. The flowrate of each MSA is unknown and is to be determined so as to minimize the network cost. Figure 1.1 is a schematic representation of the problem statement.

The candidate lean streams can be classified into N_{SP} process MSAs and N_{SE} external MSAs (where $N_{SP} + N_{SE} = N_S$). The process MSAs already exist on plant site and can be used for the removal of the undesirable species at a very low cost (virtually free). The flowrate of each process MSA, L_j, that can be used for mass exchange is bounded by its availability in the plant:

$$L_j \leq L_j^c \quad j = 1,2, \ldots, N_{SP} , \tag{1.1}$$

Where L_j^c is the flowrate of the jth MSA that is available on the plant. On the other hand, the external MSAs can be purchased from the market. Their flowrates are to be determined according to the overall economic considerations of the MEN"
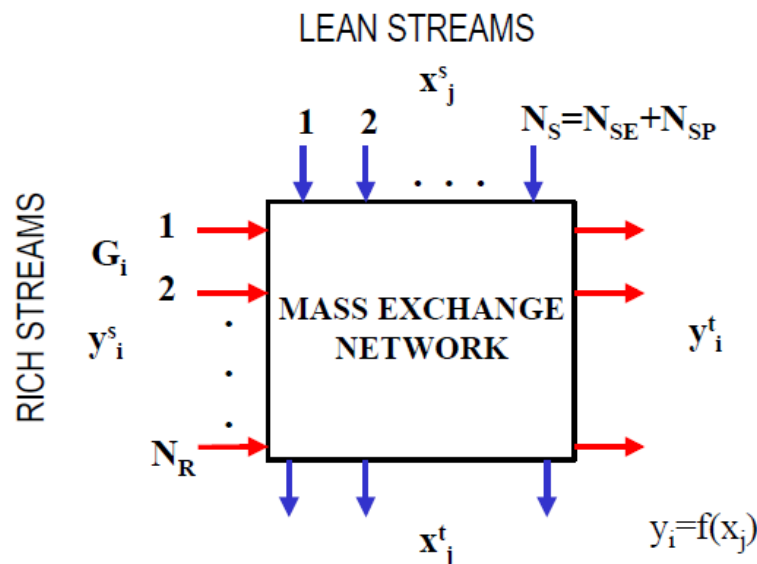

Figure 1.1. *Schematic representation of MEN synthesis problem*

1.2.2 The pinch diagram

The pinch diagram is a graphical approach, developed by El-Halwagi and Manousiouthakis, 1989 that aims at the minimization of the cost of MSAs, i.e. to make the maximum use of process MSAs before considering the application of external MSAs.

The steps for the construction of the diagram are the following:

1. Plot the composition of each rich stream versus the mass exchanged as in Figure 1.2. Each rich stream is represented as an arrow whose head corresponds to its target composition and the tail to its supply composition. The slope of each arrow is equal to the stream flowrate and the horizontal distance between the head and the tail of each arrow corresponds to the mass pollutant that is lost by the rich stream, MR_i, according to:

$$MR_i = G_i(y_i^s - y_i^t), \quad i = 1, 2, \dots, N_R, \tag{1.2}$$

Where, for each ith rich stream:
G_i is the flowrate;
y_i^s is the supply composition;
y_i^t is the target composition:
N_R is the total number of rich streams.

Any stream can be moved left or right while preserving the same horizontal distance between the arrow head and tail, so as to maintain the same supply and target composition.
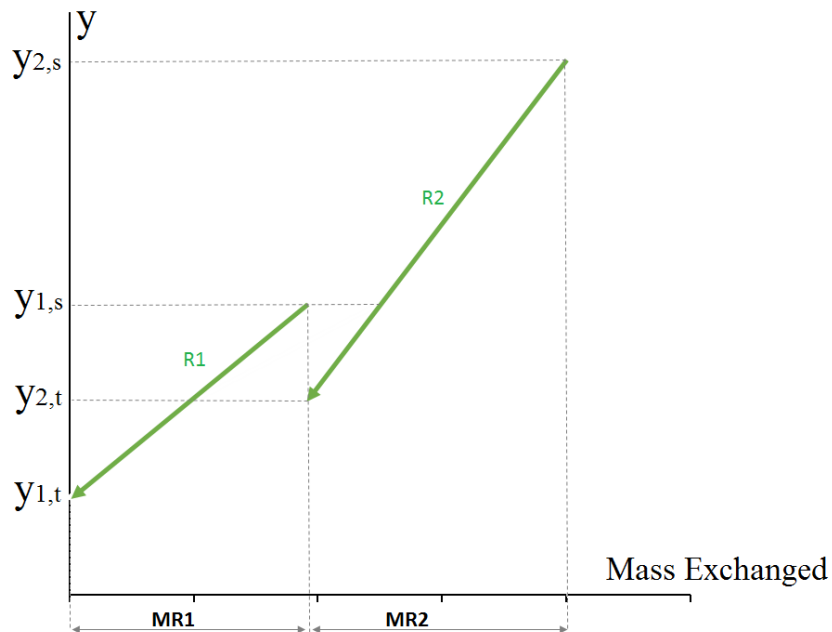

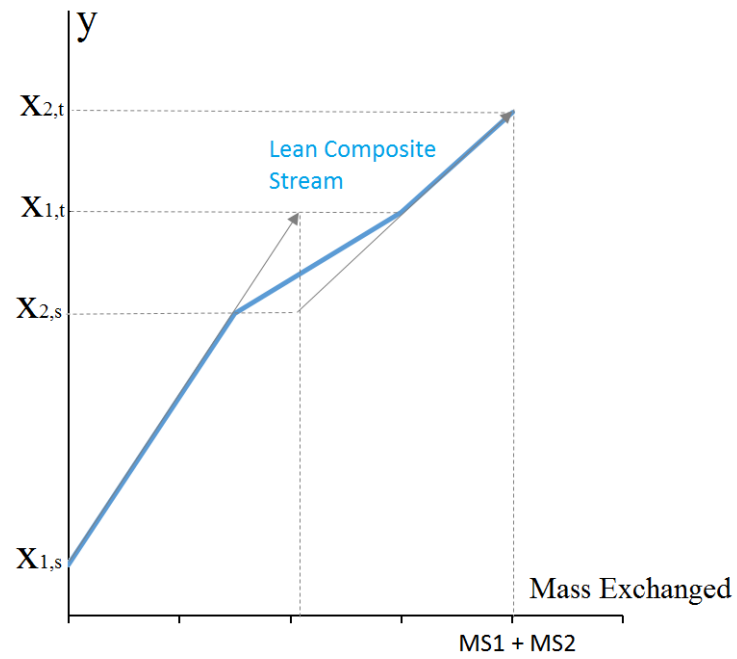**Figure 1.2.** *Representation of mass exchange by two rich streams*

2. Construct the rich composite stream as in Figure 1.3. The stream is obtained by using the diagonal rule for superposition and correspond to the cumulative mass of the pollutant lost by all the rich streams altogether.

Figure 1.3. *Rich Composite Stream abstained for superposition*

3. It is possible to do the same thing with the lean streams so as in Figure 1.4; where the horizontal distance between the arrow head and the tail is given by:

$$MS_j = L_j^c\left(x_j^s - x_j^t\right), \quad j = 1, 2, \dots, N_{SP}, \tag{1.3}$$

Where, for each jth MSA:
L_j^c is the flowrate;
x_i^s is the supply composition;
x_i^t is the target composition:
N_{SP} is the total number of lean streams.

4. Next, both composite streams are plotted on the same diagram (Figure 1.5). On this diagram, thermodynamic feasibility of mass exchange is guaranteed when at any mass-exchange level (which corresponds to a vertical line), the composition of the lean composite stream is located under the rich composite stream.

Figure 1.4. *Lean Composite Stream abstained for superposition*
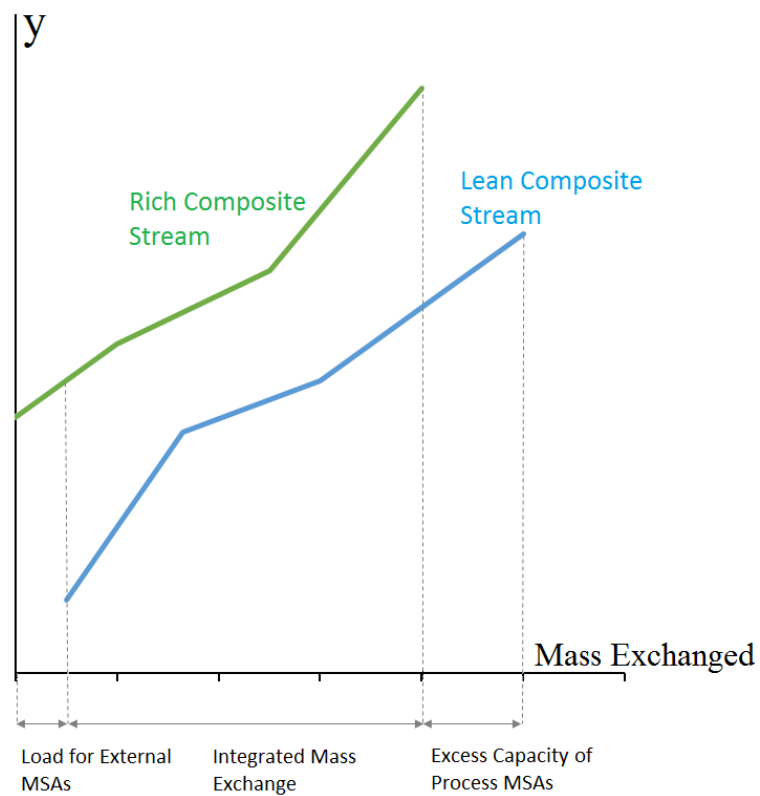
Figure 1.5. *Partial integration of rich and lean streams*

The lean composite stream can be moved left and right which implies different mass exchange decisions:

- If we move the lean composite stream on the right in a way that leaves no vertical overlap with the rich composite stream, then there is no integrated mass exchange between the rich composite stream and the process MSAs (Figure 1.6)
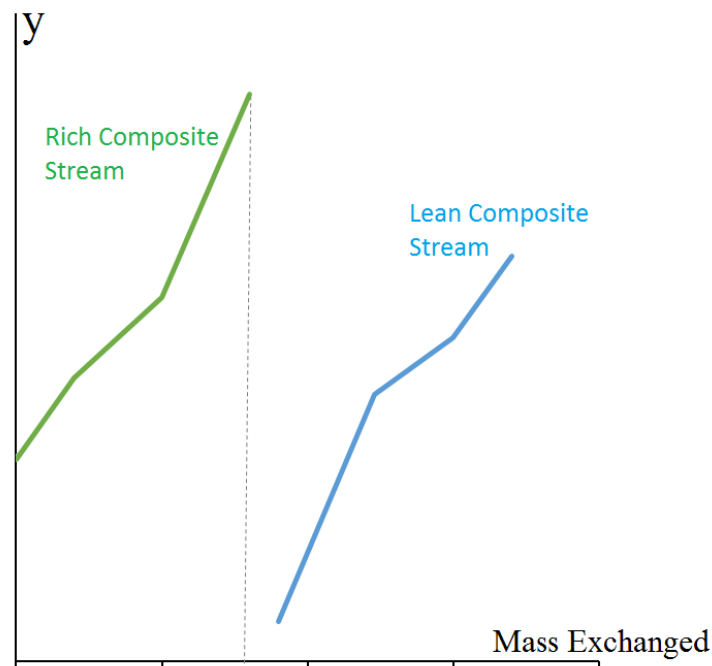
Figure 1.6. *No integration of rich and lean streams*

- If the lean composite stream is moved left, such that a portion of the lean is placed above the rich composite stream, creating thermodynamically infeasibility (Figure 1.7)
- The optimal situation is constructed when the lean composite stream is slid horizontally until it touches the rich composite stream while lying completely under the rich composite stream at any vertical level. The point where the two composite streams touch is called the "mass-exchange pinch point" (Figure 1.8)
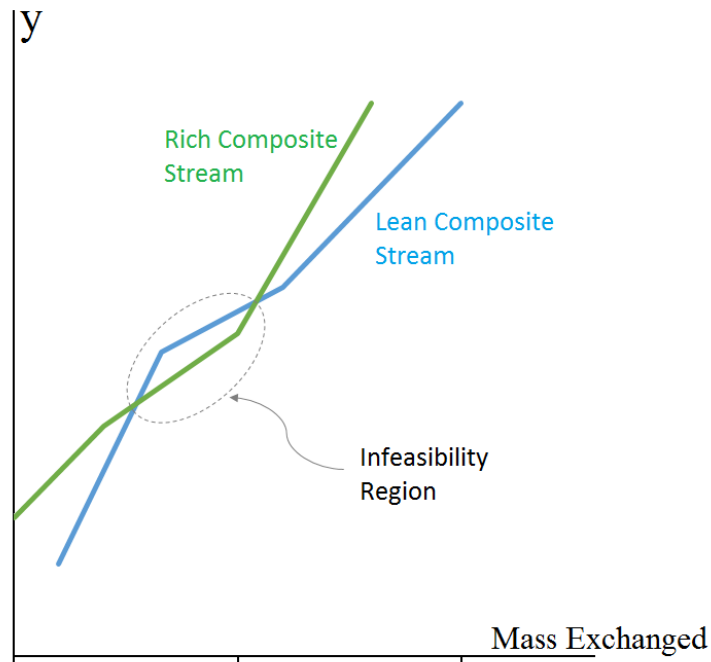
Figure 1.7. *Infeasibility situation*
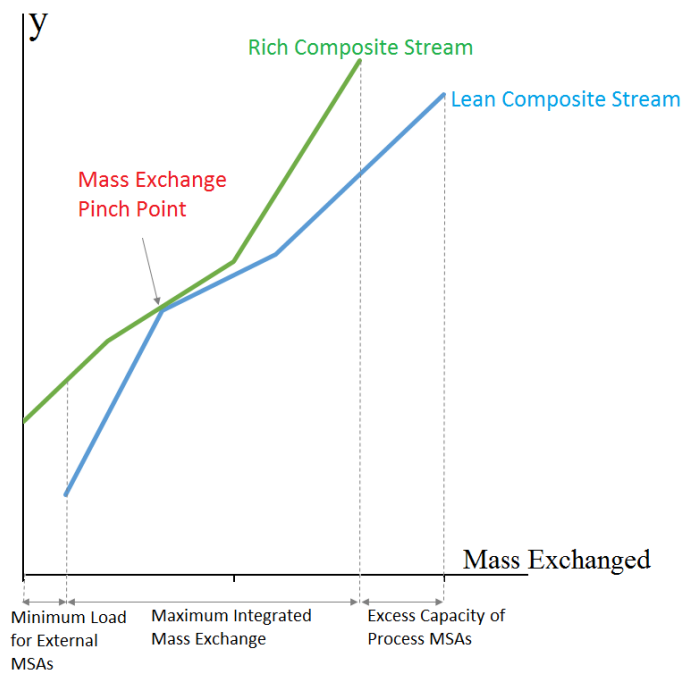
Figure 1.8. *Mass exchange pinch point*

On the pinch diagram, the horizontal overlap between the two composite streams represents the maximum amount of the targeted species that can be transferred from the rich streams to the process MSAs. It is referred to as the "integrated mass exchange." The horizontal distance of the lean composite stream, which lies right to the upper end of the rich composite stream, is referred to as "excess process MSAs." It corresponds to that

capacity of the process MSAs to remove the targeted species that cannot be used because of thermodynamic infeasibility. According to the designer's preference or to the specific circumstances of the process such excess can be eliminated from service by lowering the flowrate and/or the outlet composition of one or more of the process MSAs. Finally, the horizontal distance of the waste composite stream which lies left to the lower end of the lean composite stream corresponds to the mass of the targeted species to be removed by external MSAs.

These targets have been identified rigorously using little data and without detailing the design of the MEN. Above the pinch, exchange between the rich and the lean process streams takes place. External MSAs are not required. Using an external MSA above the pinch will incur a penalty eliminating an equivalent amount of process lean streams from service. On the other hand, below the pinch, both the process and the external lean streams should be used. If any mass is transferred across the pinch, the composite lean stream will move right and, consequently, external MSAs in excess of the minimum requirement will be used. Therefore, to minimize the cost of external MSAs, mass should not be transferred across the pinch.

Said that, for sake of consistency, all the future pinch diagrams will be plotted with concentration instead of composition, in line with Wang and Smith, 1994.

1.2.3 Wastewater minimization

After the exposition of the basics of the mass integration and the construction on the pinch diagram, it is now possible to explain how the wastewater minimization process actually works.

Given a number of operations each of all requiring an MSAs; the principle is that, if it is allowed for the inlet streams to have some degree of contamination, it is possible to reusing the outlet MSAs from an operation as an inlet MSAs for another operation.

For sake of simplicity consider the example in Table 1.2, that can be found in Smith, 2005; Savulescu, Kim et al., 2005.

Table 12. *Data of the example problem*

Operations	Mass of Contaminant (g/h)	C_{in} (ppm)	C_{out} (ppm)	Limiting water flowrate (t/h)
1	2000	0	100	20
2	5000	50	100	100
3	30000	50	800	40
4	4000	400	800	10

As can be seen, in the first column it is shown the number of the operations; the second column contains the mass of contaminant (or mass load), Δm_c; the third column contains respectively the maximum inlet, C^{in}, and outlet, C^{out}, limiting concentrations for a single contaminant. Note that the concentrations are specified on the basis of mass flowrate of water only:

$$\Delta C = C^{out} - C^{in} = \Delta m_c / m_w , \qquad (1.4)$$

Where m_w is the limiting water flowrate.

The last column shows the limiting water flowrate, m_w, that is the flowrate required if the specified mass of contaminant is picked up by the MSAs between the maximum inlet and outlet concentrations. If an operation has a value of C^{in} greater than the concentration of the feeding water, then for the specified mass load, it is used a lower flowrate of water than the limiting one.

The first step is to calculate, using (1.4), the flowrate required. Each operation is fed by pure water (with $C^{in} = 0$); that for this example is equal to 112.5 t/h.

Considering now the possibility of reusing the streams, it is possible to construct the pinch diagram (Figure 1.9) as shown in §1.2.2.

Note that in this case rich streams are not present so, instead, a line is drawn to represent the water supply. For this case the line starts at zero concentration (to satisfy the requirements), but it is not necessary always the case.

To achieve the minimum water flowrate, the water supply line have to be the steepest possible, and that correspond with the water supply line touching the lean composite curve at the pinch point.

Knowing the mass load from zero to pinch point (9000 g/h) and the concentration of the pinch (100 ppm), the flowrate of the system can be calculated from (1.4) to be 90 t/h; and that represent the minimum water consumption.

Once the target of minimum water consumption is achieved, the next task is to seek a design strategy of the problem.
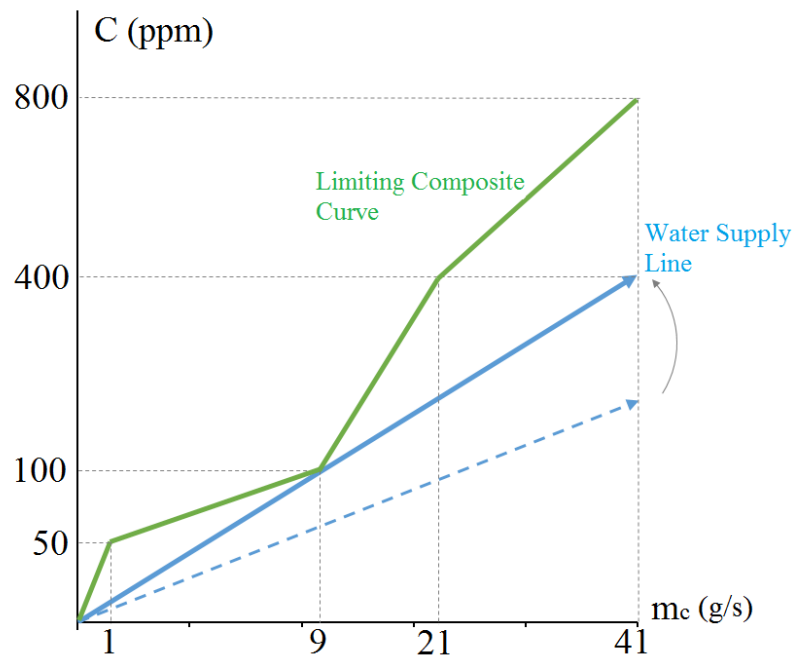
Figure 1.9. *Pinch diagram for wastewater minimization*

The first step is to define the design regions and the water requirements in each of them; in our case it is possible to define two regions:

1. Below the pinch; where, by definition, the full amount of the target minimum flowrate is needed (90t/h);
2. Above the pinch; where is possible to operate with a lower flowrate than the target, defined by a mass balance (45.7 t/h).

The goal of the design strategy is to use the target water flowrate below the pinch, while, above the pinch, using only the required amount of flowrate, with the balance going to effluent.

To set up the strategy, the first step is to construct a design grid as in Figure 1.10 that, for this example, will contain three water mains, corresponding to freshwater concentration (0 ppm), pinch concentration (100 ppm) and the maximum concentration (800 ppm).

Streams representing the individual operation requirements are drawn as arrows in the grid, with the tail and the head being respectively the maximum inlet concentration and the maximum outlet concentration. Note that the stream of Operation 3 is divided in two streams as it features both below and above the pinch point.

The operations are then connected to the appropriate water mains and as shown in Figure 1.11, for this example it involves the water from Operations 1 and 2 to be reused in the Operations 3 and 4 via a water main at the pinch concentration.
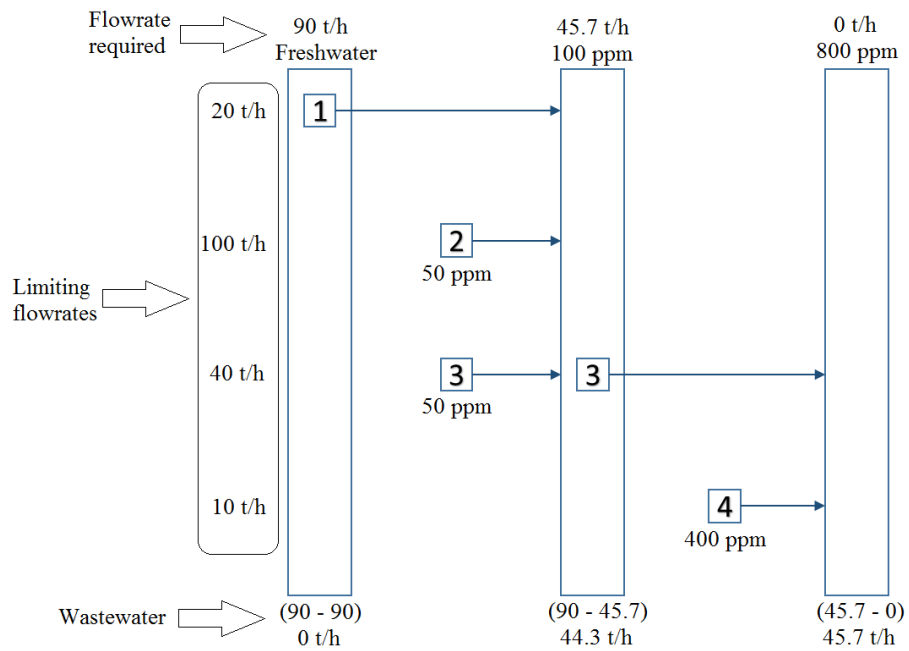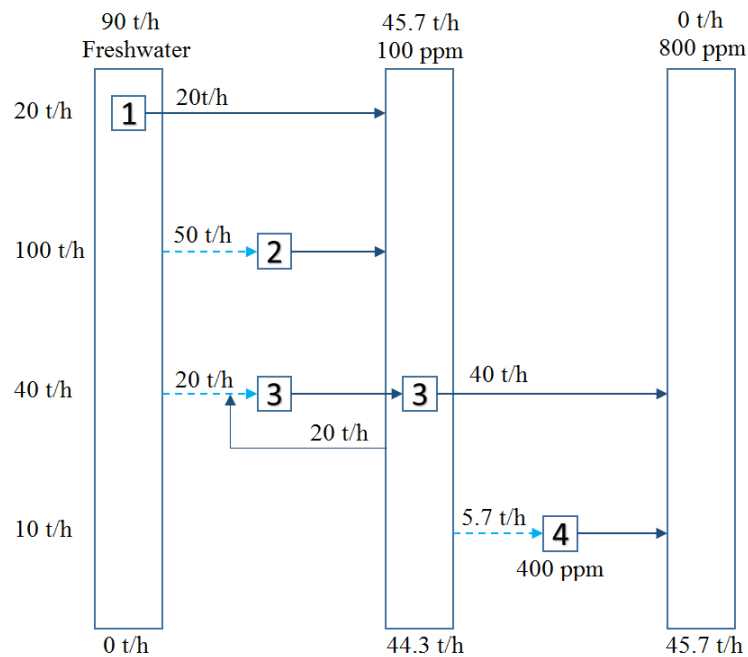
Figure 1.10. *Design grid for water system*

Figure 1.11. *Final design grid*

A possible design alternative is to not use the pinch main, and make the connections directly. That leaves with two water source at 100 ppm, being Operation 1 and 2; and two sinks at 100 ppm, being Operation 3 and 4.

As can be seen, in Figure 1.12 it is shown a case with a direct connection from Operation 1 to Operation 3 and another from Operation 2 to Operation 4, with 44.3 t/h going to

wastewater from Operation 2. The design shown in Figure 1.12, however, it is only one of possible networks available for this case.
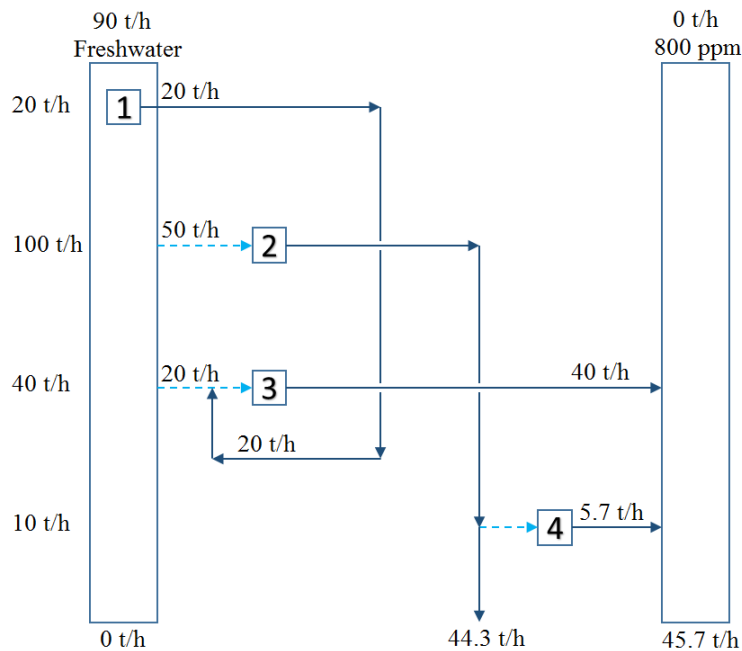
Figure 1.12. *Water network without the intermediate water main*

1.3 Energy integration

Energy or more specifically heat integration is an important aspect of all the process. That because the utilities used in a typical process to heat cold streams or contrary to cool hot streams, are a relevant part of the operating cost (El-Halwagi 2006).

The approach used to reduce that cost is to utilize the hot streams of the process to heat the cold streams and obtain a heat exchangers network (HEN); but when we are in presence of multiple hot and cold streams, the challenge is to combine the streams in the highest energy saving way.

For a given system, the synthesis of HENs entails answering several questions:

- Which heating/cooling utilities should be employed?
- What is the optimal heat load to be removed/added by each utility?
- How should the hot and cold streams be matched?
- What is the optimal system configuration?

1.3.1 Pinch approach

Considered a ΔT_{min} as the driving force of the heat exchange, the thermal equilibrium of the heat transfer from a hot stream (at temperature T_h) to a cold stream (at temperature t_c) is the following:

$$T_h = t_c + \Delta T_{min} , \tag{1.5}$$

So for given values of T_h and t_c, it is possible, both practically and thermodynamically, to transfer heat from any hot stream whose temperature $T \geq T_h$ with any cold stream with temperature $t \leq t_c$.

The goal is to minimize the usage of utilities by maximize the heat exchange among process streams, and one approach to do that is called "thermal pinch diagram": a graphical technique developed by Linnhoff and Hindmarsh, 1983.

The steps for the construction of the diagram are the following:

1. Given a number N_h of hot streams; for every hot stream in the process, plot the enthalpy exchanged versus the temperature; the result is an arrow whose tail corresponds to its supply temperature, T_i^s, and its head corresponds to its target temperature, T_i^t, where $i = 1...N_h$; (Figure 1.13). Note that HH_i is the heat exchanged from the ith hot stream; and any stream can be moved left or right while preserving the same horizontal distance between the arrow head and tail to maintain the same supply and target temperature.

2. It is possible now to create a hot composite stream using the diagonal rule (Figure 1.14)
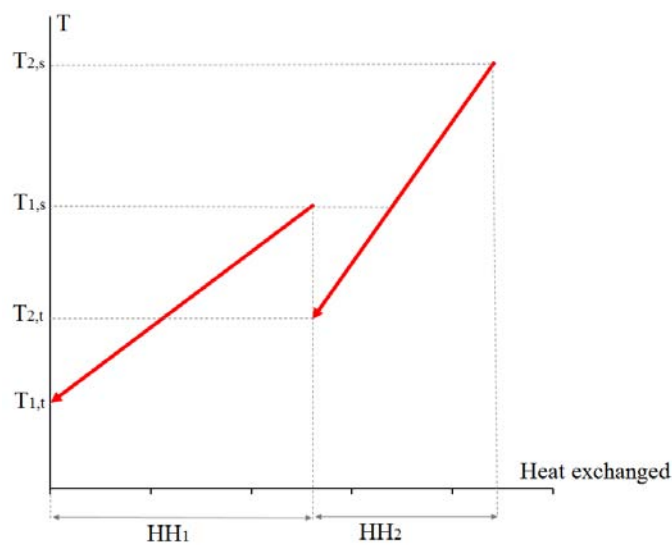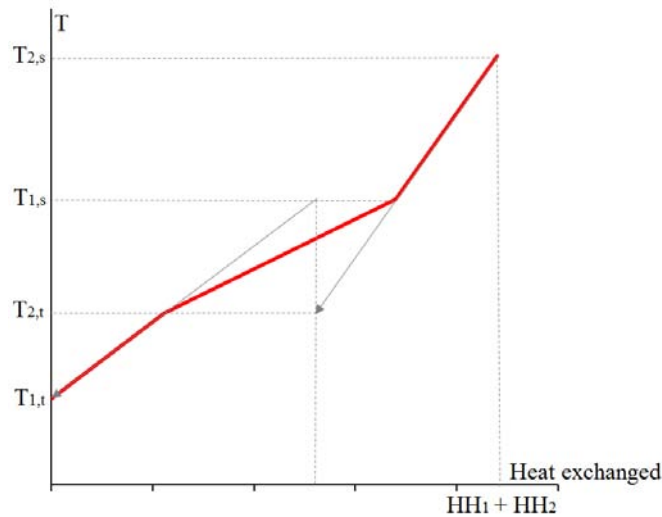

Figure 1.13. *Hot streams*

Figure 1.14. *Constructing a hot composite stream using superposition*

3. In the same way plot the composite line for the cold streams
4. Represent both the hot composite line and the cold composite line on the same diagram as in Figure 1.15
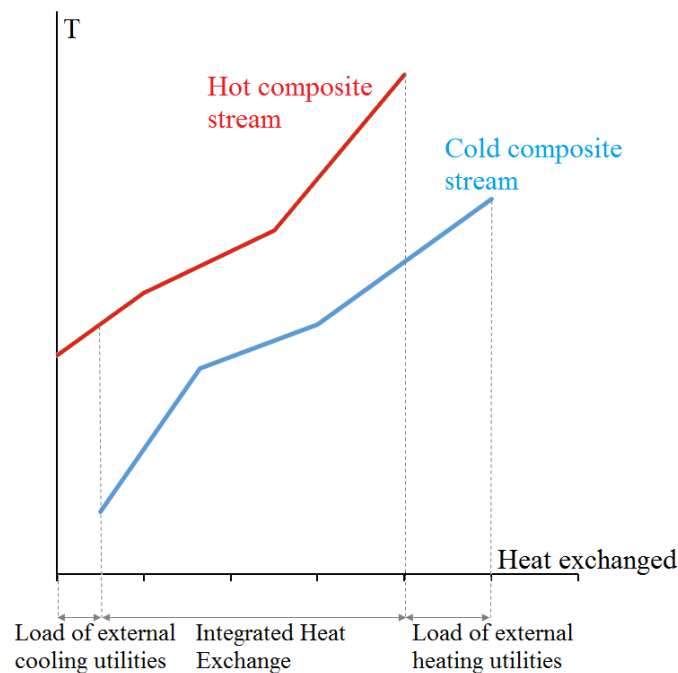

Figure 1.15. *Thermal pinch diagram*

Thermodynamically the heat exchange can be performed for the range of the diagram delimitated by two vertical lines (which corresponds to a heat exchange level) that contain both the hot composite line and the cold composite line, as shown in Figure 1.15

Since the cold composite line can be freely moved left and right, there are many possibilities that can be summarized at following:

a) If the cold composite stream lies or is moved right than the vertical line that represents the tail of the hot composite stream, in that case there is no integrated heat exchange between the two streams. Figure 1.16
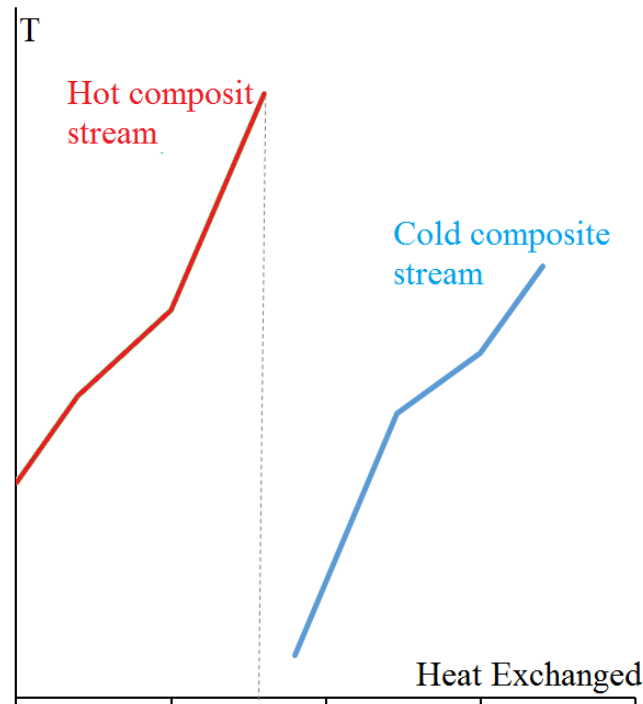
Figure 1.16. *Placement of composite streams with no heat integration*

b) If the cold composite stream lies or is moved in a isenthalpic space of the diagram that contains also part of the hot composite stream, but the two streams do not touch each other, in that case there is integrated heat exchange, but it is not the best achievable (Figure 1.15).

c) When the cold composite stream is moved until it touches the hot composite stream, we have the optimal solution that corresponds to the minimum heating and cooling utility requirements. The point where the two composite streams touch is called "thermal pinch point" (Figure 1.17). Note that, when considering a value ΔT_{min} between hot and cold streams, the two composite curves cannot touch, and the thermal pinch point is reached when the vertical distance between the two composite curves, is equal to the value of the ΔT_{min}.

d) If the cold composite stream is moved even more to the left, so that it crosses the thermal pinch point, then it creates a region of thermodynamic infeasibility because the cold stream (the heat) becomes hotter than the hot stream itself (Figure 1.18). When a value of ΔT_{min} is considered, the

thermodynamic infeasibility is achieved even if the vertical distance between the two composite curves become lower than the value of the $\Delta T_{min.}$
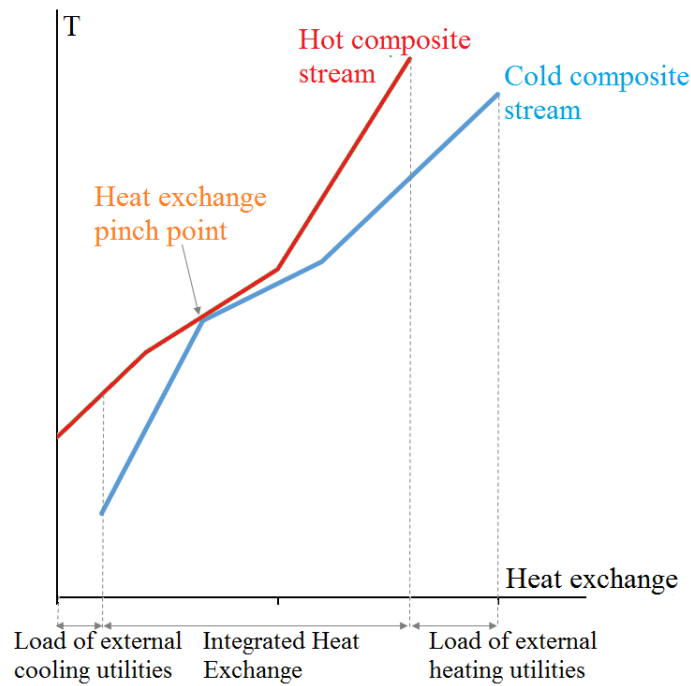

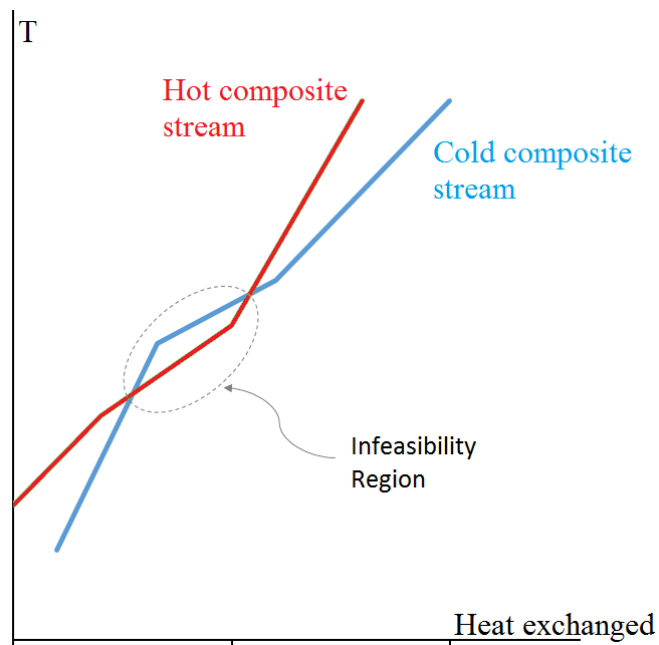**Figure 1.17.** *Optimum solution of thermal pinch diagram*

Figure 1.18. *Infeasible heat integration*

As shown in Figure 1.19, the thermal pinch diagram also helps giving an idea the number of heat exchangers needed; that because the dotted boxes, that represent the vertical heat transfer, also may represent the actual number of heat exchangers (one box correspond to one heat exchanger, or more in case of multiple streams in the box)
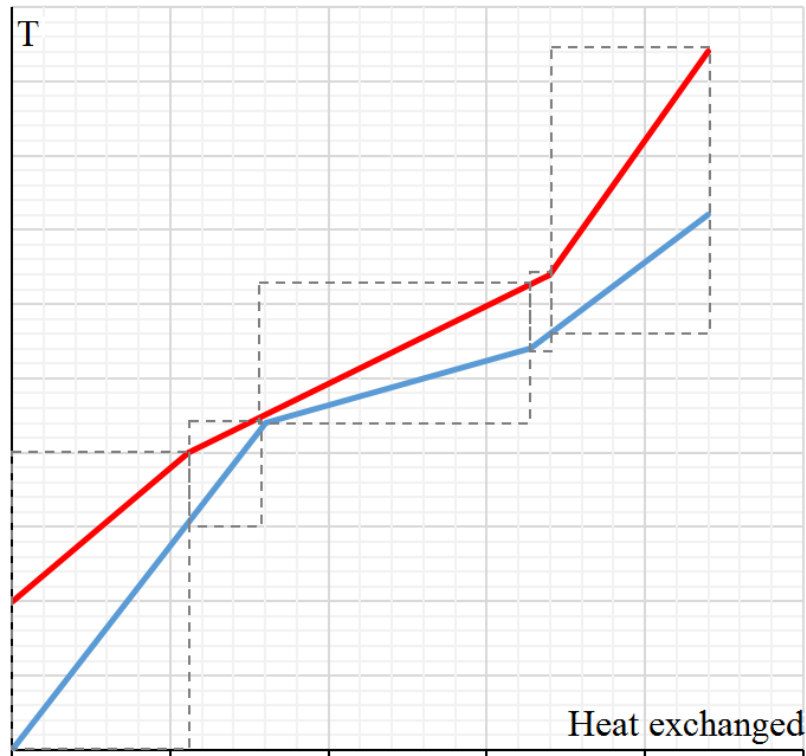
Figure 1.19. *Matching of hot and cold streams*

1.3.2 Algebraic approach (problem table algorithm)

The approach concerns solving a heat balance around a number of temperature intervals, n_{int} (as shown in Figure 1.21); the scale correspondence for the intervals is determined using (1.5).

The series of temperature interval is defined with $z = 1, 2 \dots n_{int}$.

For purposes of constructions, the hot streams are shifted to be $\Delta T_{min}/2$ colder than it is in practice and the cold streams are shifted to be $\Delta T_{min}/2$ hotter than it is in practice. This allow the heat transfer to be feasible within each shifted interval, since the hot streams are in reality hotter than the cold streams by ΔT_{min}.

The first step is to construct a table of exchangeable heat loads with the exchange loads of the process streams in each temperature interval. For a generic i^{th} hot stream which passes throng the zth interval, the exchangeable load, $HH_{i,z}$, is defined as:

$$HH_{i,z} = F_i \cdot C_{P,I} \cdot (T_{z-1} - T_z),$$ (1.6)

Where T_{z-1} and T_z are the shifted hot temperatures respectively at the top and bottom of the zth interval, F_i is the flowrate and $C_{P,I}$ is the heat capacity of the ith hot stream.

It is now possible to do the same thing for the cold streams and calculate the exchangeable capacity, $HC_{j,z}$, of the jth cold stream that passes through the zth interval:

$$HC_{j,z} = F_j \cdot C_{P,J} \cdot (t_{z-1} - t_z), \tag{1.7}$$

With t_{z-1} and t_z as the shifted cold temperatures respectively at the top and bottom of the zth interval, F_j is the flowrate and $C_{P,J}$ is the heat capacity of the jth cold stream.

At this point it can be obtained the collective load of the hot streams, HH_z^{Tot}, and cold streams, HC_z^{Tot}, within the zth interval:

$$HH_z^{Tot} = \sum_{z=1}^{n_{int}} HH_{i,z} \tag{1.8}$$

$$HC_z^{Tot} = \sum_{z=1}^{n_{int}} HC_{j,z} \tag{1.9}$$

It is now possible to write the heat-balance equation for the zth temperature interval, as shown in Figure 1.20:

$$r_z = HH_z^{Tot} - HC_z^{Tot} + r_{z-1}, \tag{1.10}$$

Where r_{z-1} and r_z are the residual entering and leaving the zth interval.
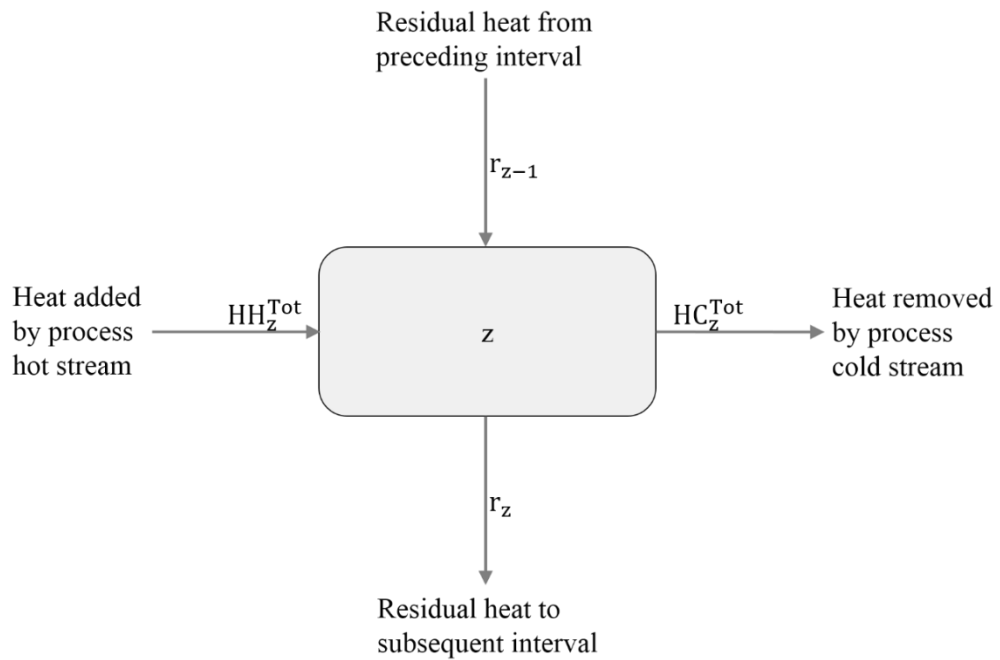
Figure 1.20. *Heat balance around temperature interval*

Note that residual r_0 is zero due to the fact that there are no process streams above the first interval and thermodynamically it is not possible to have negative values of r_z. For that reason, all negative residual must be made non-negative by adding at every residual a value equal to the most negative residual.

The goal of the algebraic approach is to obtain a heat cascade diagram as in Figure 1.21. The results given by the cascade, are identical to those obtained using the graphical pinch approach.

Figure 1.21. *Heat cascade diagram*

1.4 Motivations

The simultaneous integration of both mass and energy in chemical process, is a much more complex task due to interaction between mass and energy (Figure 1.22). For instance the equilibrium relation that can be found during an extraction operation is very influenced by the variation of the temperature. Srinivas and El-Halwagi, 1994 developed a lineal programming formulation to select the optimal temperature and flowrate of each sub-stream, considering the trade-off between the utilities costs and the costs of the separation agents. After that the heat exchanger tasks were subject to the synthesis of the HEN (El-Halwagi, 1997).

It should be remembered that the goal of the minimization of water is not only for the environment but also it is really important in the economical aspect (reduction of water consumption and improvement of energy integration).

For that reason all the studies combining mass and energy integration, developed in the past can be categorized according to two general approaches:

1. Consider a set of reach and lean streams for which it is possible to define a minimum concentration difference in order to set the targets of minimum cost of separation agent and minimum number of mass exchange units. When also temperature issues are taken into account, it should be possible to determine the optimum operating temperature of mass-exchange (El-Halwagi and Manousiouthakis, 1989; Savulescu, Kim et al., 2005)

2. From the beginning it is considered a set of mass-exchange units defined by limiting conditions (contaminant concentration levels, flowrate requirements). Then, it is possible to set up targets to identify the minimum separation agent flowrate and design the mass exchanger network to achieves the flowrate target (Wang and Smith, 1994; Savulescu, Kim et al., 2005)
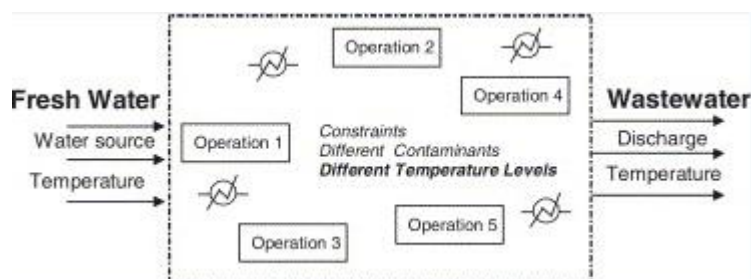

Figure 1.22. *Features of the problem of simultaneous energy and water minimization (Savulescu, Kim et al., 2005)*

Some of the past studies worth mentioning are the following: Srinivas and El-Halwagi, 1994 introduce the problem of synthesizing combined heat and reactive mass exchange networks "CHARMENs"; the work involves the preferential transfer of a certain species

from a set of rich streams to a set of lean streams and at the same time accomplish a specified heat transfer task in a cost effective manner. Savulescu, Kim et al., 2005 focus on developing a separate systems approach and a two dimensional grid diagram for the simultaneous minimization of energy and water. Savulescu, Sorin et al., 2002 addresses direct/indirect heat recovery network design for water network systems and propose a new systematic heat recovery design approach, for water stream sets leading to energy pinch problems, based on thermodynamics. Manan, Tea et al., 2009 propose a three steps technique for simultaneous minimization of water and energy in process plants through a combination of numerical and graphical tools. Liu et al.,2013 propose a simultaneous method, based on the mass pinch technology and the pseudo-T-H diagram approach, for synthesizing heat and mass exchanger networks

1.5 Objectives

The main goal of this thesis is the simultaneous minimization of wastewater and energy consumption, through a combination of two existing programs, FI^{2}EPI and AquoMin.

AquoMin is a program coded in Visual Basic (VBA) that perform a minimization of the fresh water consumption and wastewater production in a generic process that use water as a contaminant remover.

FI^{2}EPI is a tool coded in Java that perform energy integration between hot streams and cold streams in a generic process, to obtain the minimum utilities consumption.

In detail, this work aims to combine the two programs and reproduce a known example from the literature, to seek and solve the issues that could emerge combining the two program and, in the end, to try to achieve the same results of the example. All this to confirm that an integration of the two programs is actually possible; and to lay the foundations for a future union of FI^{2}EPI and AquoMin in one single program. The work also includes the development of a third program, AFI (AquoMin FI^{2}EPI interface), coded in VBA, that proposes to be an user friendly interface between FI^{2}EPI and AquoMin and it is programmed to perform the simultaneous energy and wastewater minimization in the most general way possible, with respect of the limitations given by the two programs.

Chapter 2

AquoMin

In this chapter it is presented in detail AquoMin, one of the two programs used for this work; in particular the one that performs the minimization of the fresh water consumption and wastewater production in a generic process that use water as a contaminant remover. In details, it will be exposed the approaches and the methods of calculation that the program uses to execute the target and design of the wastewater minimization.

2.1 General approach

AquoMin is a software tool, developed at Process Integration Group of CPQ, that concerns with the Mass-Exchange Networks (MEN) targeting and design in the area of pollution prevention.

AquoMin can analyze different options to reduce fresh water consumption and minimize wastewater production; these options are analyzed in two stages: first the targeting and then the design. The former stage uses algorithms based on pinch analysis to obtain the minimum consumption of external water and also the minimum wastewater production. These targets are then used in the second stage, the MEN design.

The alternatives to reduce wastewater production and water consumption are the following:

- Reuse/Reutilization : Wastewater from some operations can be used as feed to other operations, wastewater can be also mixed with fresh water (Figure 2.1a);
- Regeneration reuse: Contaminants in the wastewater are partially/totally removed by regeneration, before the wastewater itself is used in other operations (Figure 2.1b);
- Regeneration recycle: Wastewater is redirected to the same operation where was previously used (Figure 2.1c); this option is not implemented in AquoMin yet.

In a chemical process it is not rare to find an operation that requires water, and usually it is used to remove a specific amount of a certain contaminant; for that reason the pinch analysis focus on the idea of reusing wastewater from other operations instead of fresh water, to remove the contaminant. For this purpose and to analyze each process, the water using operations are characterized by their limiting data that comprise maximum inlet and outlet concentrations of contaminant in water.
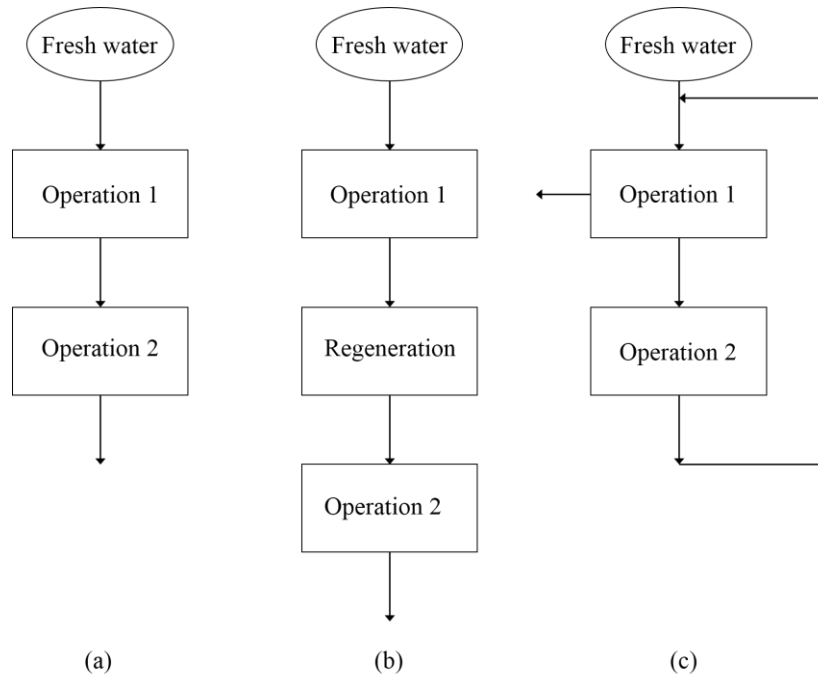
Figure. 2.1. *Alternatives to reduce wastewater production and fresh water consumption when applying process integration: (a) reuse; (b) regeneration reuse; (c) regeneration recycle.*

The current version of Aquomin is limited to five operations and two external water sources, a single contaminant and a single regeneration process (Castro, et al., 1999). The minimum water source flowrate is targeted and the design of the corresponding MEN is established for each of the following strategies: without water reutilization, with water reutilization (or reuse) and regeneration reuse. All the current features and interconnections among them are given in Figure 2.2

2.2 Input data

The first thing necessary to use correctly AquoMin, is to input the right data. As can be seen in Figure 2.3a, 2.3b the program start with an introduction window followed by the first box that request the user to choose the approach used for the study and the type of contaminant to be extracted in the mass transfer operation. The alternatives available in this version are:

- Without reutilization;
- With reutilization;
- Regeneration reuse.

For this work only the cases with and without reutilization are taken into account because the reuse is not developed enough to give the MEN, that it is necessary for the following integration with FI^2EPI. In addition, the type of contaminant is not relevant for this study.
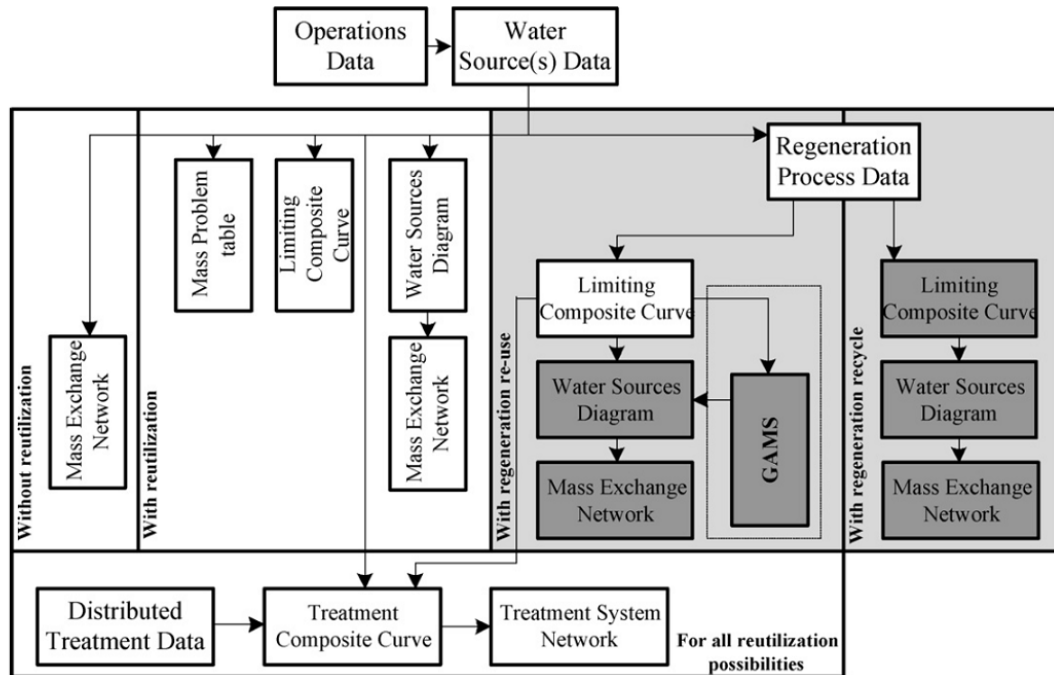
Figure 2.2. *AquoMin program map, showing menus interdependence (the light-grey area is currently under implementation in AquoMin), from (Relvas, Matos et al. 2008)*

The first box shown to the user is the input one: first of all the user is call to insert, for each operation, the values of the maximum inlet and outlet concentrations and the limiting flowrates (Figure 2.4a).
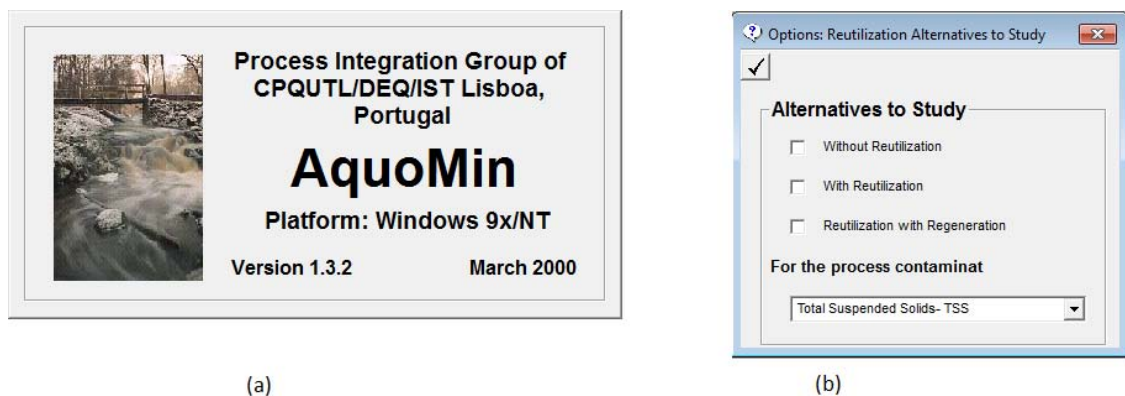

Figure 2.3. *(a) Introduction window; (b) reutilization alternatives.*

The second dialog box requires the values of the concentration of contaminant and the maximum available value of concentration of the external water source (EWS), as shown in Figure 2.4b. The third input box concerns the regeneration process input data (Figure 2.4c).

As said previously the regeneration was not taken in account in this study, so for this aspect of the program it is possible to use the explanation given by Relvas, Matos et al., 2008.

(a)   (b)   (c)

Figure 2.4. *Data input boxes: (a) limiting data; (b) EWS data; (c) regeneration process data.*

2.3 Approach

The calculation methods that AquoMin take in account are discussed in the following paragraphs.

2.3.1 Without reutilization

It is a typical process when all sort of reutilization is forbidden or not yet explored. Each operation is feed with external water sources (EWS). This scenario corresponds to the maximum EWS consumption; that is determined through a mass balance. AquoMin displays the calculated values in the only analysis tool available for this alternative, which is the Mass-Exchange Network (MEN).

Figure 2.5 displays an example of MEN without reutilization and as can be seen, there is no connection between operations.

The right side of the MEN window indicates each of the characteristics (targets), which are the total EWS flowrate, F_{min}, at C_{WS} (external water source concentration) and the mass of contaminant exchanged in each process operation.
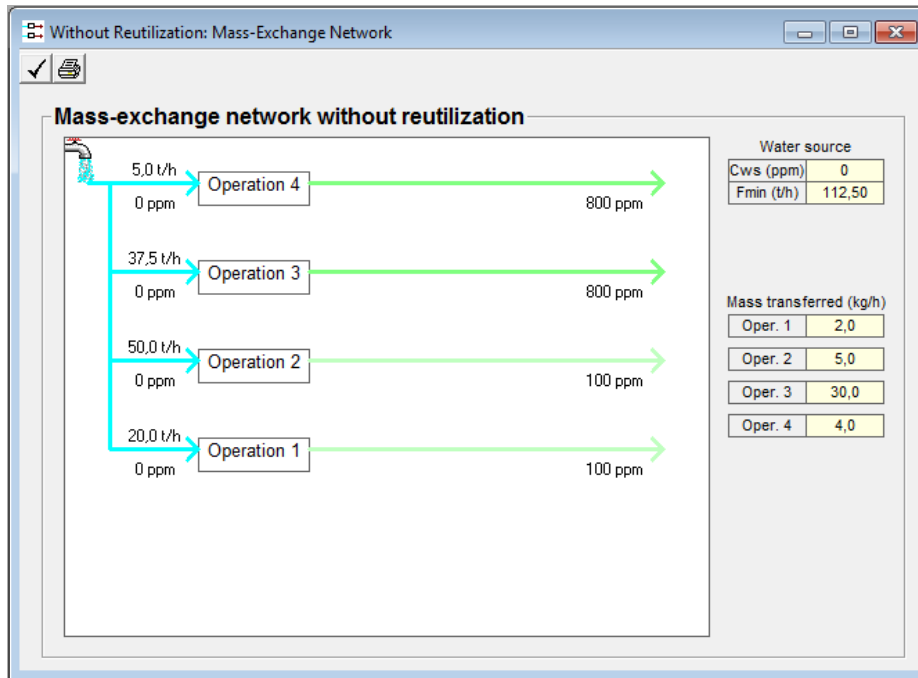
Figure 2.5. *Water consumption without reutilization*

2.3.2 With reutilization

AquoMin decomposes the reutilization targeting analysis in three different tools (Castro, Matos et al., 1999):

- The Mass Problem Table (MPT);
- The Limiting Composite Curve (LCC);
- The Water Sources Diagram (WSD).

The Mass Problem Table (MPT) was introduced by Castro, Matos et al., 1999 and it is an evolution of the Composition Interval Table (CIT) first present by El-Halwagi and Manousiouthakis, 1989 where the target was the minimum requirement of external mass separating agents to promote the separation of a contaminant from the rich streams to the lean streams. In the MPT, given a number N_{OP} of operations, a set of ascending concentrations is built including inlet and outlet concentrations of all the operations of the process; giving birth of a set of N_{IN} intervals (Figure 2.6). The second step is to represent as arrows each operation. Each arrow starts at $C_{max,i}^{in}$ (maximum inlet concentration of ith operation) and ends at $C_{max,i}^{out}$ (maximum outlet concentration of ith operation), where $i = 1, 2…N_{OP}$.

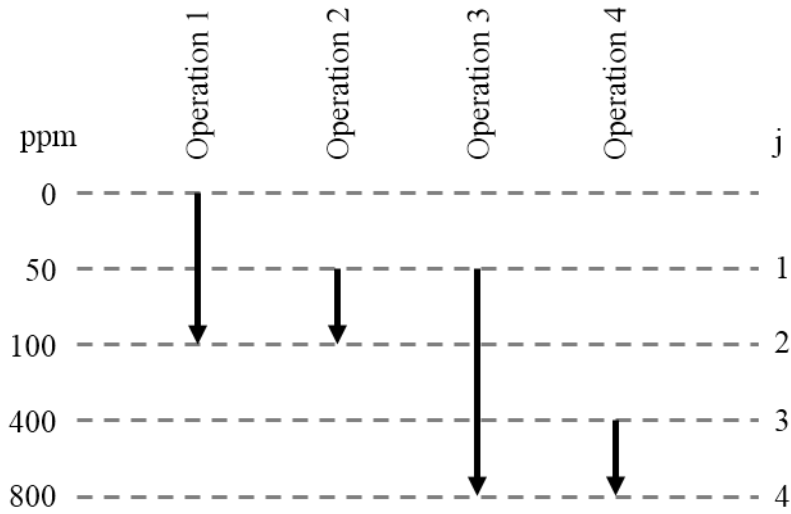**Figure 2.6.** *Concentration intervals distribution employed in the MPT*

Figure 2.7. *Mass Problem Table (MPT)*

Figure 2.7 shows the MPT built through AquoMin.

Each concentration interval, C_j, has its boundaries represented in the first column. The second column indicates which operations are present in each concentration interval. For the remaining columns, simple calculations are required. The third column displays the sum of the limiting flowrates, $\sum F_{lim,i}$, of the operations present at the jth concentration interval; where $j = 1,2\ldots N_{IN}$ and $F_{lim,i}$ as the limiting flowrate of the ith operation. The fourth column indicates the amount of mass of contaminant, $\Delta m_{c,j}$, transferred in the jth mass interval;

$$\Delta m_{c,j} = \left(\sum F_{lim,i} \right)_j (C_j - C_{j-1}) \tag{2.1}$$

With $C_0 = \min_i (C_{max,i}^{in})$

The fifth column shows the cumulated mass of contaminant exchanged until the present concentration interval, $\Delta m_{c,j}^{cumilative}$. The last column includes the calculations of the required external water source flowrate at each interval and also the remaining water source needed after the pinch point. In mass exchange problems, the pinch point concentration is identified when the problem achieves the maximum water flowrate, which is the minimum fresh water consumption target, F_{min}, for this strategy:

$$F_{min} = \max_j \left\{ \frac{\Delta m_{c,j}^{cumulative}}{C_j - C_{WS}} \right\} \tag{2.2}$$

Where C_{WS} is the external water source concentration.

The LCC is an alternative graphical targeting strategy, which generates the same information obtained in the MPT. This was first provided by El-Halwagi and Manousiouthakis, 1989 and developed later by Wang and Smith, 1994.This targeting tool is very important to determine targets for all possible mass exchange alternatives, once all the feasible water profile lines are below the LCC line. The optimal solutions, i.e.water profile lines that lead to minimum values of the targets, are the ones that touch the LCC in, at least, one point (the pinch). The LCC is constructed using the concentration intervals boundaries, C_j, and cumulative exchanged mass along them, $\Delta m_{c,j}^{cumulative}$,. For a single water source, it is necessary to increase the water profile line slope (minimizing flowrate), until it touches the LCC, and starting at (0, C_{WS}). Figure 2.8 presents an example of LCC, with the corresponding water profile featuring reutilization. F_{min} and the multiple pinch points are shown on the right side.

The third tool is the WSD, introduced by Castro, Matos, et al. 1999.This methodology is an improvement of the Grid Diagram of Kuo and Smith, 1998. It can be used to obtain the same targets as the MPT and the LCC, but it is essentially a tool to support design decisions to obtain the final MEN structure. Thus, the targeting and the design can be developed simultaneously in this tool. Another advantage is that it is not limited to only one EWS. The key idea is to represent all the available water sources in a decreasing quality set of depths. Water sources can be external water sources; internal water sources produced by wastewater from previous operations and internal water sources produced

by regeneration (when this option is available) and they are represented on the main window of Figure 2.9 as rectangles.
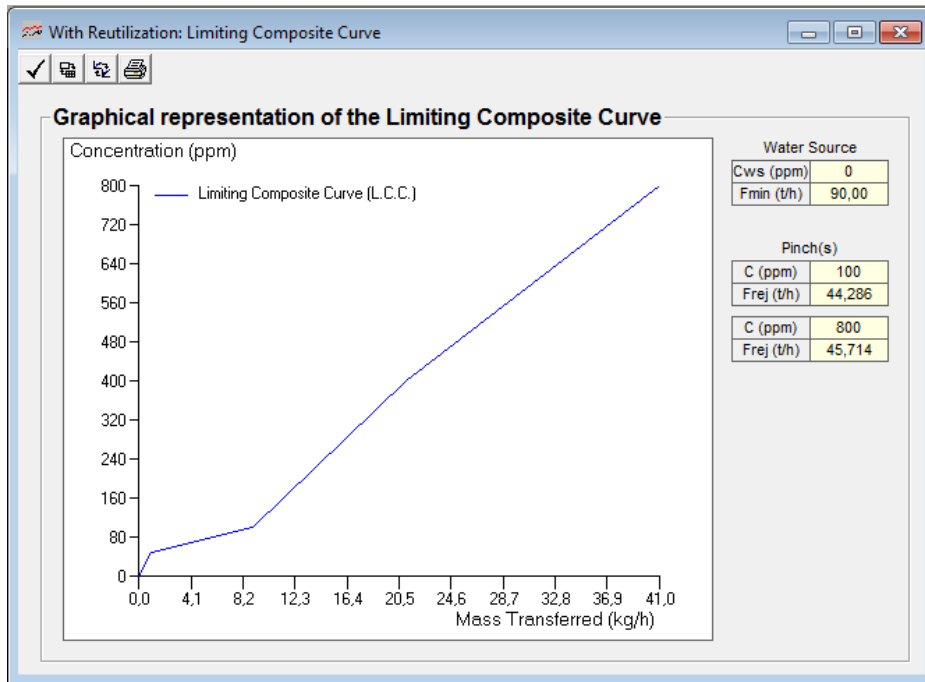

Figure 2.8. *Limiting Composite Curve (LCC) and water supply line*
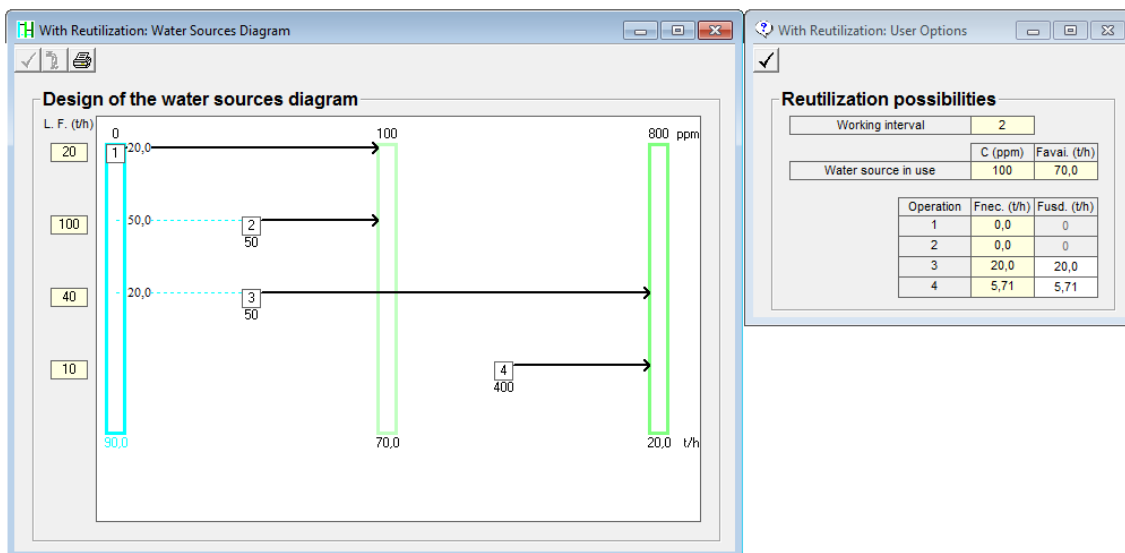

Figure 2.9. *Construction of a concentration interval of the Water Sources Diagram (WSD)*

In the top of each rectangle, it is indicated the concentration at which the respective water source is available. Operations are represented as arrows. Note that while the end of each arrow matches with one of the depths, the beginning of each arrow can lie between two depths. On the left side of the WSD it is indicated the value of F_{lim} for each operation.

The construction of the WSD starts from the least to the most contaminated concentration interval. This procedure ensures that no water source is used prior to be generated. At each interval, the right sequence to use the water sources is from the most contaminated to the least contaminated, since the first are, in general, cheaper. Castro, Matos et al., 1999 indicated two rules to guarantee minimum flowrate:

- **Rule 1.** Use external water sources only when internal water sources are not available, in either quality or quantity.
- **Rule 2.** For each operation, the water source(s) used in a specific concentration interval, must transfer exactly the amount of mass that is needed (this ensures that the maximum inlet concentration is not exceeded).

AquoMin allows the user to follow the calculations for each of the WSD concentration intervals. On the right side of Figure 2.9, it is represented a user interactive box, which is displayed whenever different options of mass-exchange operations are possible. This box indicates on the top the current concentration interval and below the available flowrate of the current water source. In the bottom, there is an interactive table allowing the user to allocate a certain amount of the current water source to each operation, F_{usd}. The water source flowrate needed for each of the operations, F_{nec}, is indicated on the left side of this table. The complete WSD is represented in Figure 2.10.
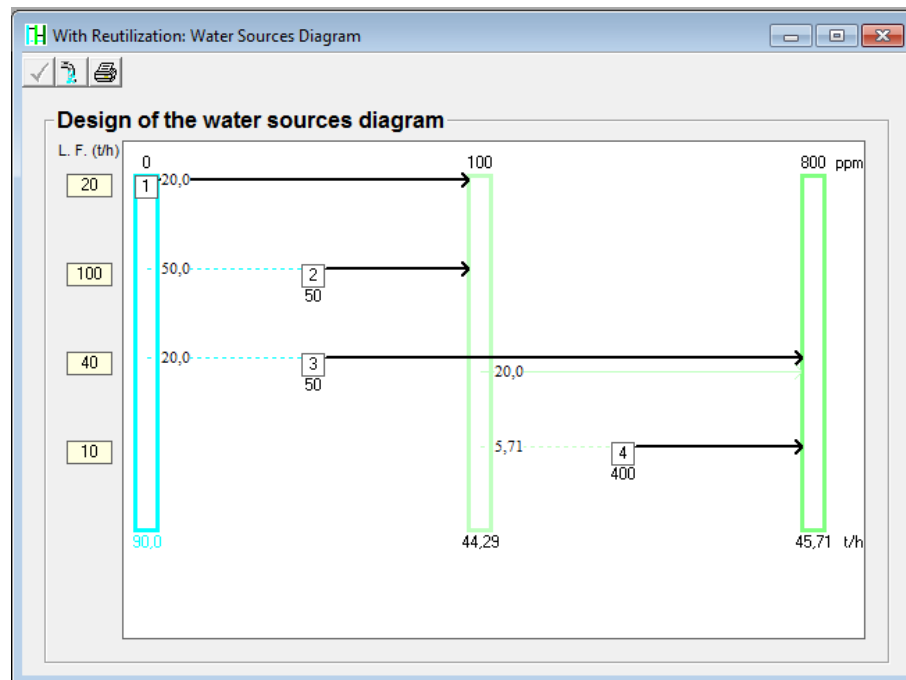

Figure 2.9. *CompleteWater Sources Diagram for the reutilisation strategy*

Each arrow represents a water source flowrate allocation at one of the concentration intervals. The final WSD contains all the information needed to build an optimized MEN. There is one more procedure before the WSD is converted to a MEN: the loop

elimination. AquoMin does this simplification process automatically. Each extra arrow at one operation of the WSD corresponds to a loop. The loops are eliminated by stream mixing generating a single feed stream (Castro et al., 1999a).

In the final MEN design (Figure 2.11) it can be easily identified the reutilization options considered by the user as well as the rejected flowrates.
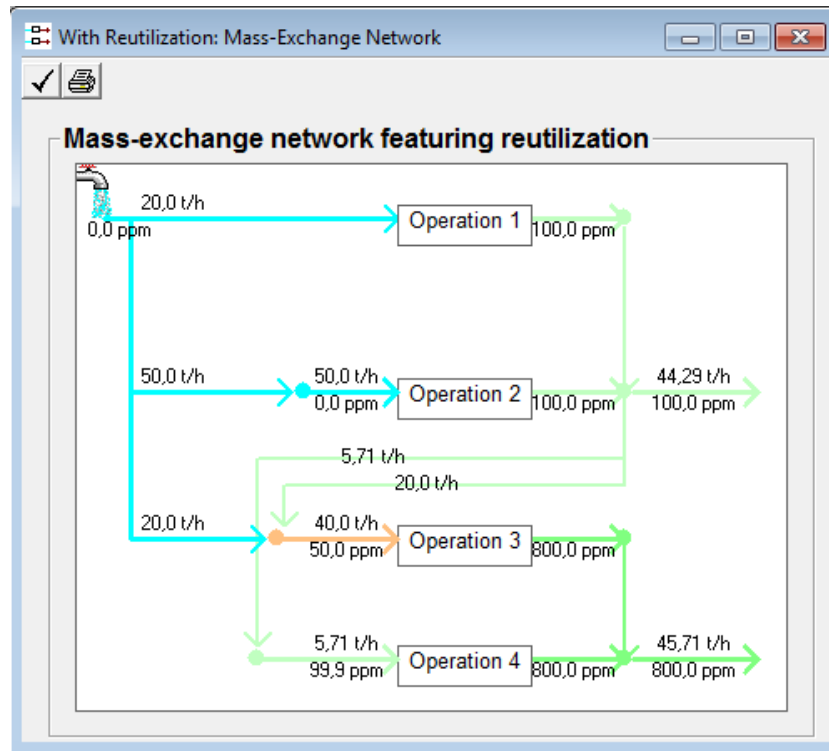

Figure 2.11. *Final MEN design*

In this MEN the necessary mass load of contaminant is removed using less external water flowrate than the corresponding flow obtained with the no integration strategy Figure 2.5.

Chapter 3

Heat Integration using *FI²EPI*

In this chapter the software FI²EPI is presented. This program performs the energy integration between hot streams and cold streams in a generic process, to obtain the minimum utilities consumption.

FI²EPI is an application developed by Instituto Superior Técnico (IST) in partnership with ADENE to support studies of Heat Integration Processes under internal or external audits. It combines both the pinch approach and the algebraic approach explained in §1.3 and can be used both as in the design phase as in process retrofit.

It is a tool that allows a comparative analysis of different scenarios of energy integration for decision support.

3.1 Input Data

The program will be described by a tutorial that can be found inside FI²EPI.

The example consist in six streams (three hot and three cold) and two utilities (saturated steam and cold water).

The data-input is the first step that the user is called to fulfill. The program starts with an introduction window followed by a screen that shows all the inputs and results.

The first data that the user have to input and that are mandatory for the study are the following:

1. The driving force of the heat exchange (ΔT_{min}).
2. The process streams data (Figure 3.1): for every stream it is required to input the inlet and outlet temperatures, the flowrate and the specific heat, C_P (or directly the heat capacity flowrate, i.e. the flowrate times the C_P);

no	Description	Ti (°C)	Tf (°C)	h (kW/m²·°C)	MCp (kW/°C)	Q (kW)	Stream type
1	1	210	70.0	2.00	49.0	6860	Hot
2	2	130	105	2.00	90.0	2250	Hot
3	3	60.0	160	2.00	50.0	5000	Cold
4	4	110	210	1.00	30.0	3000	Cold
5	5	120	175	1.00	30.0	1650	Cold
6	6	160	90.0	2.00	25.0	1750	Hot

Figure 3.1. *Process stream input table*

3. Utilities data (Figure 3.2): it is required to select the number of utilities available for the study and the class of the utilities used; such as saturated stream, thermal fluid, condensate, refrigerated water and refrigerated fluid. This data is actually not mandatory to obtain the composite curve and the heat cascade, but it is necessary to calculate the heat exchange network (HEN) without integration and the minimum energy requirements (MER) network. It is required to input.:

- For the liquids utilities: the source and discharge temperature of the utility, the price, the specific heat, *Cp*, and, optionally, the available mass of the utility or the maximum value of heat that can be exchanged by the utility;

- For the vapors utilities: the temperature (or the pressure) at which the utility is available, the price and, optionally, the available mass of the utility or the maximum value of heat that can be exchanged by the utility.

no	Description	Existing	Ti (°C)	Tf (°C)	h (kW/m²·°C)	Q (kW)	Price	Use in MER Network
1	Saturated Steam	YES	220	220	2.00	5200	180.00 €/kWyear	✓
2	Cold Water	YES	25.0	35.0	2.00	6410	7.50 €/kWyear	✓

Figure 3.2. *Utilities input table*

Note that in the second column of Figure 3.2, it is possible to identify if the utilities already exist, so as to be used in the analysis of the existing heat exchangers network, while in the last column it is possible to select which stream can be used for the construction of the MER network.

3.2 Main features

As said, FI^{2}EPI utilize both the pinch and the algebraic approaches. The features used in this work are discussed in the following.

3.2.1 Determination of the minimum consumption of utilities (Heat cascade, Composite Curves)

The determination of the minimum consumption of utilities is actually the very purpose of FI^{2}EPI, and it is the feature that express the real energy saving that a process can achieve using the energy integration method. As said in chapter 1, the program utilizes two different types of approach:

- Pinch point approach (§1.3.1). It is the point where the two composite streams touch; corresponds to the optimal solution so as the minimum heating and cooling utility requirements (Figure 3.3).
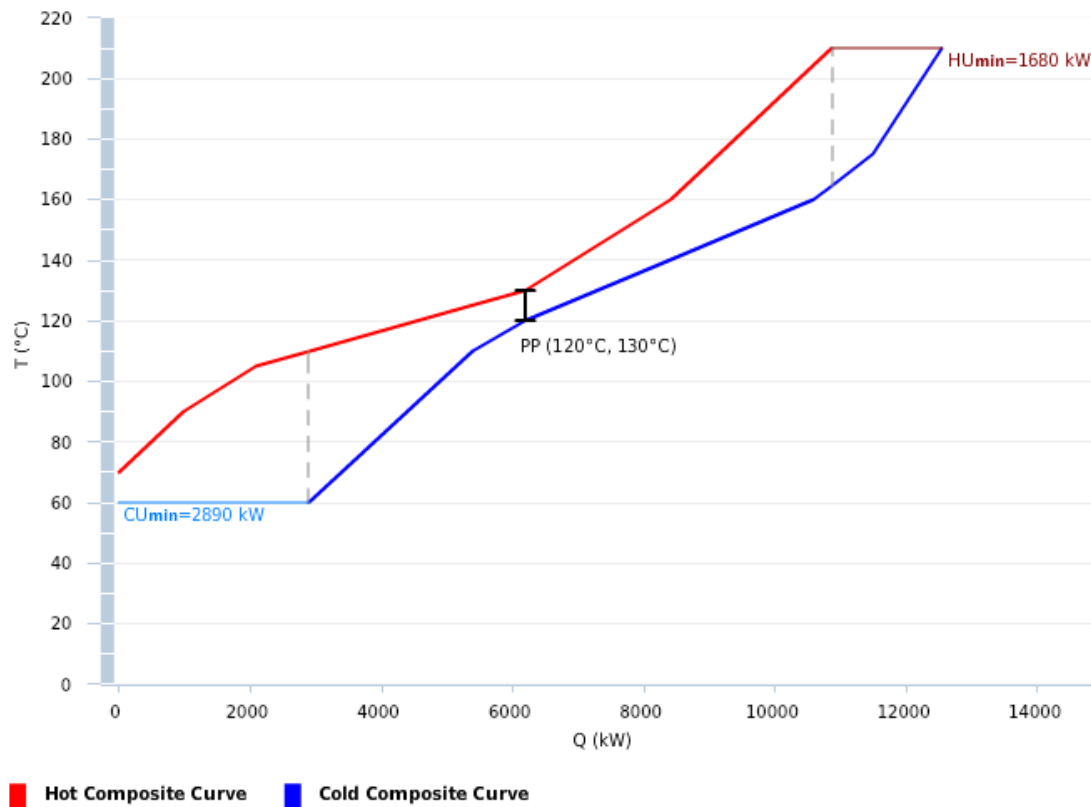
Figure 3.3. *Composite Curve*

- Problem table (§1.3.2). It concerns with the solving of a heat balance around several temperature intervals. The scale correspondence is determined using (1.5). It allows obtaining a heat cascade made of the whole temperature intervals that show the minimum heating and cooling utility requirements (Figure 3.4).

The heat cascade allow also plotting the global composite curve (Figure 3.6). The Global composite curve shows the variation of heat supply and demand within the process, helping the designer to maximize the use of cheaper utility levels and minimize the use of expensive utility levels.

The data required for the construction of the global composite curve comes directly from the problem table algorithm. Considering the Figure 3.5, the shaded pockets represent the process-to-process heat exchange and purple and green lines represent respectively the hot and cold utilities available for the process example. The global composite curve shows that, to fulfill the total hot utility required by the process, it is not necessary to supply all the hot utility at the top temperature level (purple line); but it is possible to supply the hot utility over two temperature levels: Th1 and Th2 (cheaper than Th1).

Similarly, to fulfill the cold utility requirements, it is not necessary to supply the cold utility at the temperature of the green line in Figure 3.5; but it is possible to supply the cold utility over two temperature levels: Tc1 and Tc2 (cheaper than Tc1). The points Tc2 and Th2 are called "Utility Pinches"

| T' (°C)	Process Streams	ΔT'i (°C)	ΔMCpi (kW/°C)	ΔQi (kW)	Heat Cascade (kW)
215					QHU = 0 QHU = 1680
205	[1]	10	30.0	300	-300 Q1=300 1380
180		25	-19.0	-475	175 Q2=-475 1855
165		15	11.0	165	10.0 Q3=165 1690
155	[6]	10	61.0	610	-600 Q4=610 1080
125	[2] [5]	30	36.0	1080	-1680 Q5=1080 0
115	[4]	10	-84.0	-840	-840 Q6=-840 840
100		15	-114	-1710	870 Q7=-1710 2550
85.0		15	-24.0	-360	1230 Q8=-360 2910
65.0	[3]	20	1.00	20.0	1210 Q9=20.0 2890
MCp (kW/°C)	49.0 90.0 25.0 50.0 30.0 30.0				QCU = 2890

Figure 3.4. *Heat Cascade*
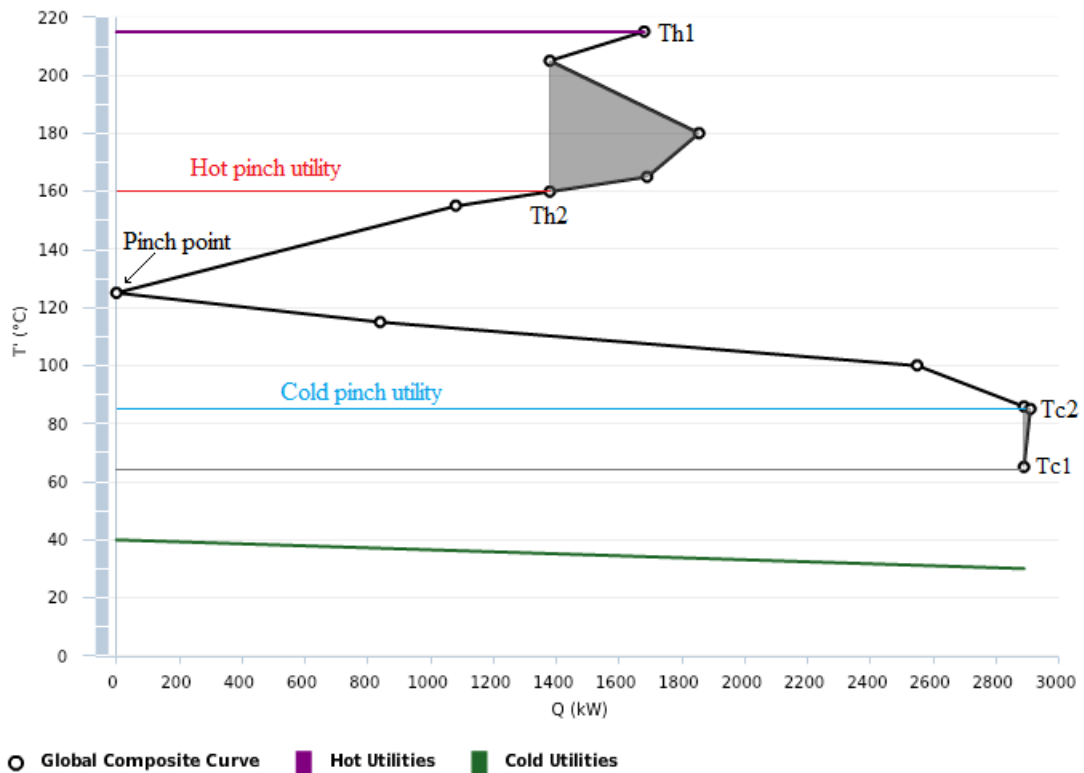
Figure 3.5. *Global Composite Curve*

3.2.2 MER Network Construction

As one of the most important feature of the program, FI²EPI gives the possibility to construct the MER network of the process.

After the input data step the program automatically provide the user with the heat exchangers network without integration Figure 3.6

After the program find the minimal energy requirement (MER) for the process in study, the construction of the MER network has to be done manually by the user. As can be seen in Figure 3.7, the interface of the construction is user friendly, and gives a help to spot which are the streams that can exchange each other (painted in yellow in Figure 3.7) and which are not.

As can be seen, the program allows also splitting the streams to meet the following thermodynamical constraints (for every couple of hot and cold streams):

- Above the pinch point: $M_h C_{Ph} \leq M_c C_{Pc}$ and n° hot streams ≤ n° cold streams;
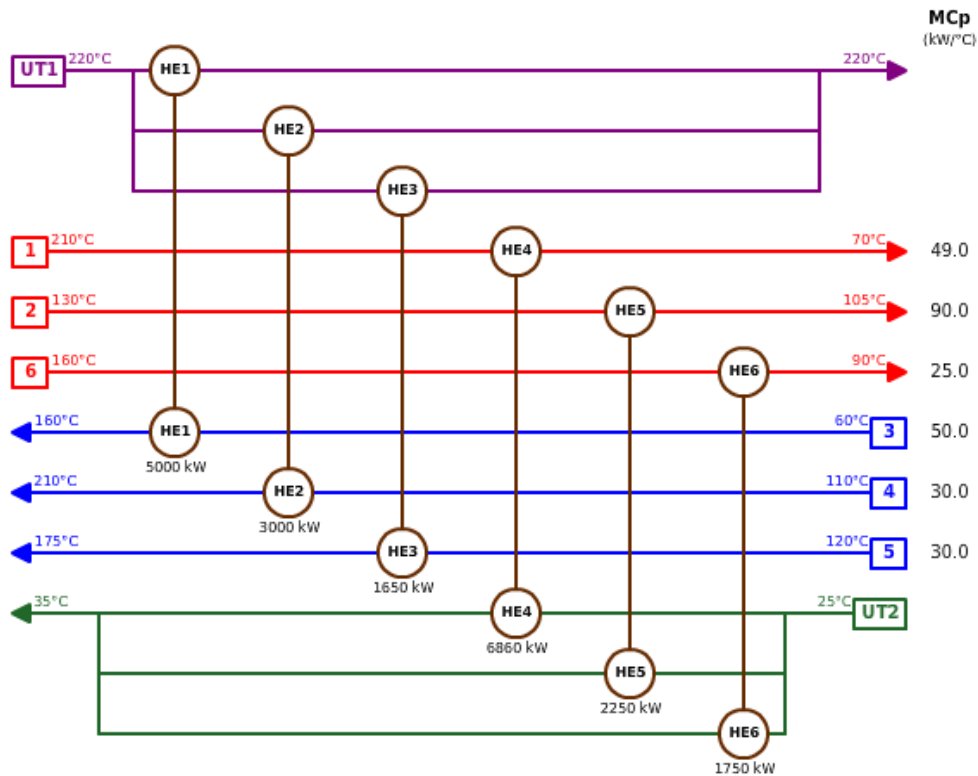- Below the pinch point: $M_h C_{Ph} \geq M_c C_{Pc}$ and n° hot streams ≥ n° cold streams

Figure 3.6. *HEN network without integration*

Figure 3.7. *MER construction Interface*

Once selected the right solution (zero heat remaining for every streams) the program return the actual MER network, as it can be seen in Figure 3.8.
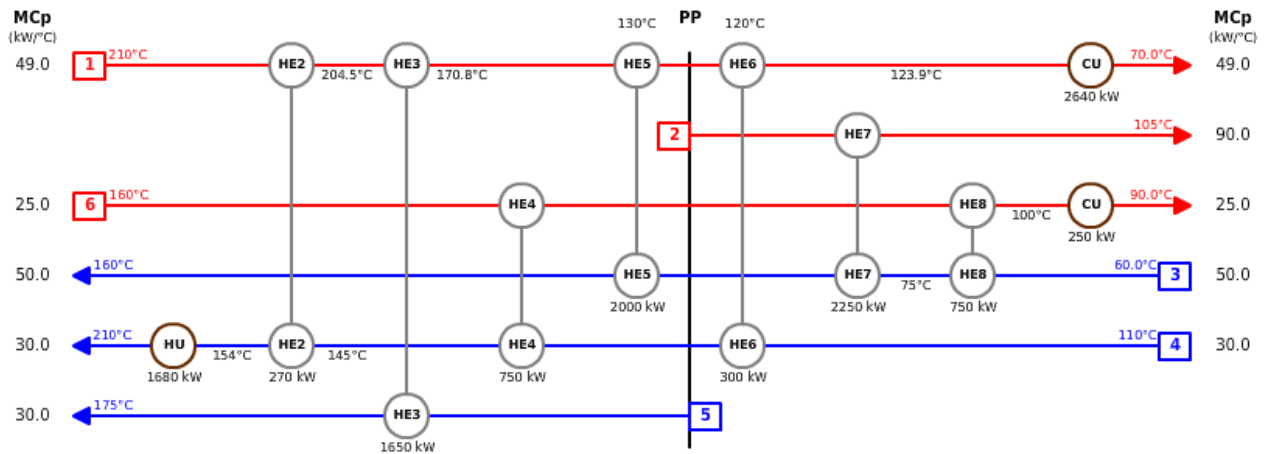

Figure 3.8. *MER network*

3.3 Other features

In the following the other features provided by FI²EPI software that have not be used for this study are described.

3.3.1 Analysis of the Existing Heat Exchangers Network

One important feature of FI²EPI, that is not used for this work, is the possibility to implement an already existent network of heat exchangers to work as a comparative tool for the MER networks obtained with the energy integration approach. It is required for the user to input the values of temperatures of the process streams and utilities data of the existing network (Figure 3.9). The program automatically generate the resultant HEN as in (Figure 3.10).

Streams/ Utilities	HE1 Q=2700 kW		HE2 Q=1750 kW		HE3 Q=4160 kW		HE4 Q=2250 kW		HE5 Q=300 kW		HE6 Q=3250 kW		HE7 Q=1650 kW	
	Ti (°C)	Tf (°C)	Ti (°C)	Tf (°C)	Ti (°C)	Tf (°C)	Ti (°C)	Tf (°C)	Ti (°C)	Tf (°C)	Ti (°C)	Tf (°C)	Ti (°C)	Tf (°C)
PS1	210	155			155	70.0								
PS2							130	105						
PS3			60.0	95.0							95.0	160		
PS4	110	200							200	210				
PS5													120	175
PS6			160	90.0										
UT1									220	220	220	220	220	220
UT2					25.0	35.0	25.0	35.0						

Figure 3.9. *Temperature Input table to construct the network of existing heat exchangers*
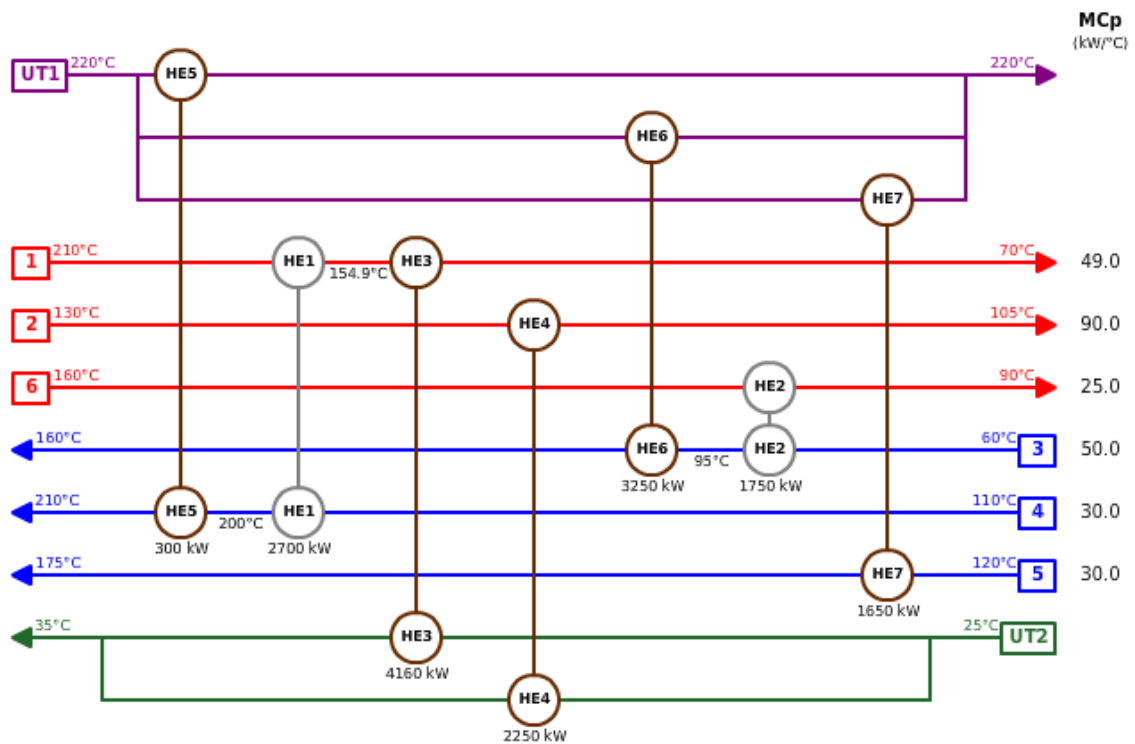

Figure 3.10. *Existing Heat Exchangers Network*

3.3.2   Determination of the optimum ΔTmin

It is a feature that allows the user to analyze and plot how the ΔT_{min} affect the cost of utilities, the area of the heat exchangers and the operating/equipment/total cost Figure 3.11 and give as a result the best option of ΔT_{min}.

To do that, the user must provide to the program the cost of utilities and the parameters to calculate the area of the heat exchangers and the equipment cost.

The program calculate the costs of the heat exchangers (equipment/capital cost) through the equation

$$HE\ cost\ (\text{€}) = a + bA^c \tag{3.1}$$

a,b,c = Parameters that the user have to insert. The program provide a set of plausible parameters as a default;

A = Total area of the heat exchanges [m^2].

The program provide also as a default a set of economical parameters (that can be modified by the user) for the calculation of the annualized equipment cost:

- Interest rate (i) sets at 4%;
- Payback time (n) sets at 5 years;
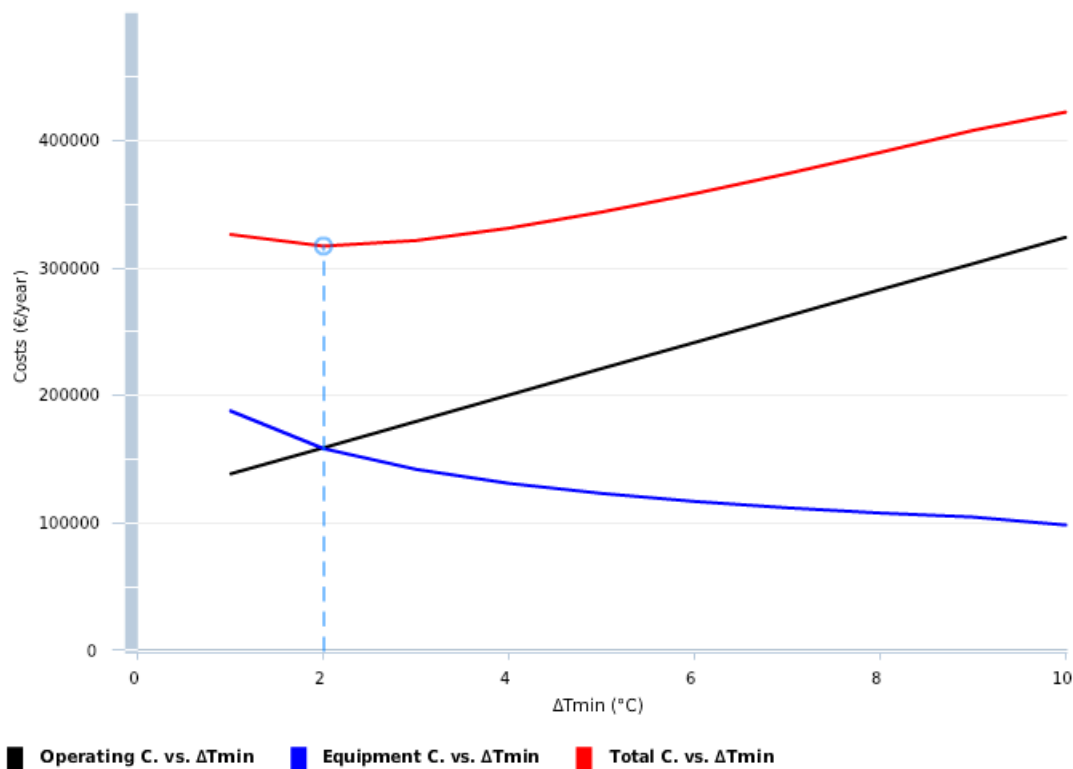- Capital recovery factor (CRF) sets at 0,225.

Figure 3.11. *Sensitive Analysis of various costs vs. ΔTmin*

The annualized equipment cost is calculated with the following equation found in Smith, 2005:

$$\text{Annualized capital cost} = \text{capital cost} \times CRF \tag{3.2}$$

where

$$CRF = \frac{i(1 + i)^n}{(1 + i)^n - 1} \tag{3.3}$$

FI²EPI sets also as a default the operation time sets at 8500 hours/year (that can be modified by the user) to calculate the operating cost, i.e. the cost of the utilities on annual basis.

The total cost is obtained by summing the operating cost and the annualized equipment cost.

3.2.5 MER Network Evolution Scenarios

The MER network evolution scenarios is an advanced tool that allows the user to further improve the economics of the process by trying to remove manually the internal loops in the network.

In Figure 3.12, it is possible to see the loops that are possible to remove (note that removing a loop will change the ΔT_{min}).

Figure 3.13 and Figure 3.14 show how the network become after removing for instance the first loop shown in Figure 3.12. Note that removing the loop in Figure 3.15 implies a changing on the ΔT_{min} to 6.5°C from 10°C.

Once all the possibilities of removing loops are took in account by the user, the program return the table of comparison of the scenario shown in Figure 3.15.

As for the other tools of FI²EPI, it is required for the user to input the cost of the utilities and the parameters to calculate the equipment costs through (3.1), (3.2).
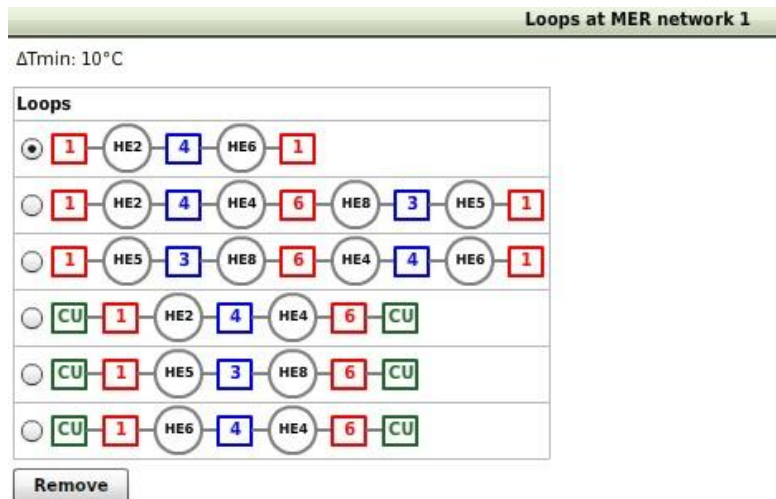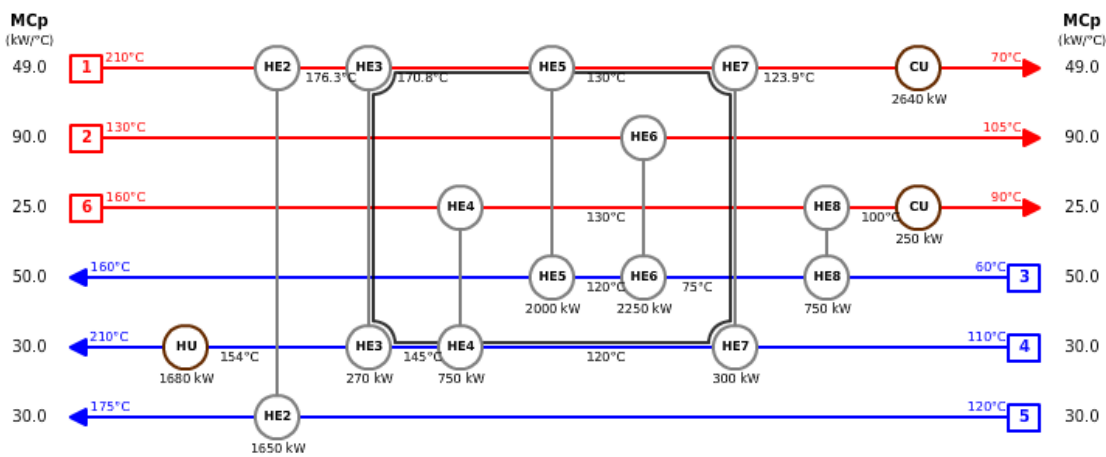
Figure 3.12. *Removing Loops interface*

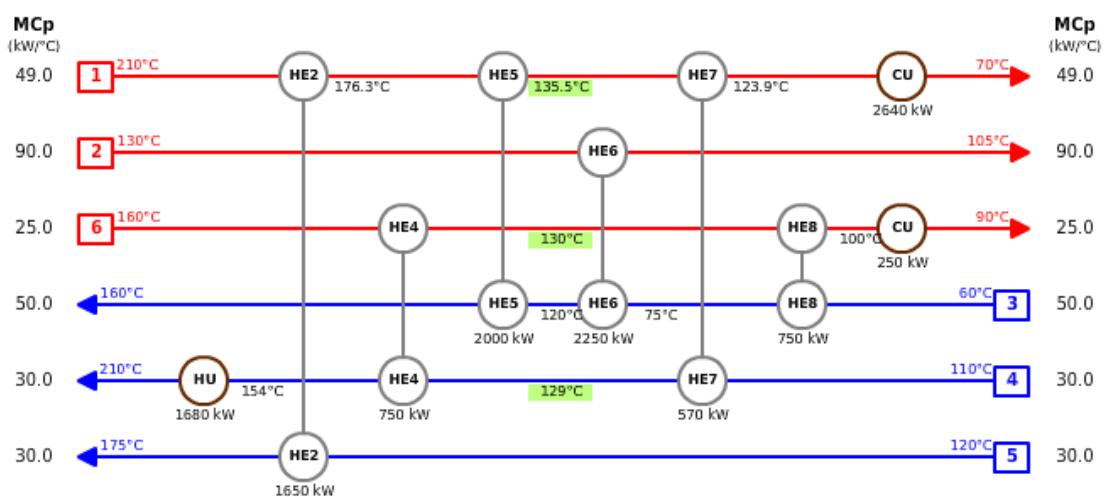**Figure 3.13.** *Example of loop in the network*

Figure 3.14. *How the network become after removing the loop in Figure 3.16*

Scenario	ΔTmin (°C)	HE's no.	Total Area (m²)	HU (kW)	CU (kW)	Operating Cost (€/year)	Capital Cost	Total Annual Cost (€/year)
HEN without Integration	10	6	309	9650	10860	1818450.00	68865.73	1887315.73
Existing HEN	10	7	397	5200	6410	984075.00	86006.38	1070081.38
MER Network 1	10	10	661	1680	2890	324075.00	137615.39	461690.39
Scenario 1 MER Network 1	1	9	941	1680	2890	324075.00	178303.12	502378.12
Scenario 2 MER Network 1	4.5	9	677	1785	2995	343705.10	136703.41	480408.51
Scenario 3 MER Network 1	10	9	576	1950	3160	374700.00	120846.18	495546.18
Scenario 4 MER Network 1	8	8	581	1950	3160	374700.00	118355.72	493055.72
Scenario 5 MER Network 1	10	8	558	2000	3210	384075.00	114711.68	498786.68
Scenario 6 MER Network 1	10	7	578	2000	3210	384075.00	114441.80	498516.80
Scenario 7 MER Network 1	10	8	556	2000	3210	384075.00	114385.16	498460.16
Scenario 8 MER Network 1	10	7	578	2000	3210	384075.00	114441.80	498516.80

Figure 3.15. *Table of scenarios*

Chapter 4

The AFI software

AFI was developed in this study with the purpose of combining AquoMin (Chapter 2) and FI^{2}EPI (Chapter 3). As said, the first is a program that performs the minimization of the fresh water consumption and wastewater production in a generic process using water as a contaminant remover; while the latter is a tool to perform energy integration between hot streams and cold streams in a generic process to obtain minimum utilities consumption.

The two aspects of water and utilities minimization are very much related, because the water used in the process as an extractive agent, is not merely used at the source conditions. In fact, it is usually heated to match the requirements of the operation, and before being discharge, the wastewater is generally cooled to observe the environmental constraint.

For that reason, having a tool that can minimize both energy and mass requirements for a generic process is indeed useful and quite innovative as at the moment, to our knowledge, there are no other programs that can perform that.

4.1 Work Flow

The approach used to combine Aquomin and FI^{2}EPI was to design of an interface between the two. More specifically, it was impossible to incorporate the AquoMin and FI^{2}EPI in a single bigger program, due to their different code languages; so the general method used is as follow (illustrated in Figure 4.1):

1. Input in AquoMin the following process data (with $i = 1,2..n$, operations):
   a. Concentration of contaminant in water source, C_{WS}, in ppm;
   b. Limit flowrate, M_{max}, in t/h;
   c. Maximum concentration of contaminant inlet, acceptable for each operation, $C_{i,IN}$, in ppm;
   d. Concentration of contaminant outlet for each operation, $C_{i,OUT}$, in ppm;
2. AquoMin performs the wastewater minimization (§1.2.3) and gives as a output the Mass Exchange Network (MEN) with the following data:
   a. Water consumptions with water-reutilization approach, W_W, in t/h;
   b. Water consumptions without water-reutilization approach, W_{WO}, in t/h;

(Note that AquoMin only works with values of flowrates in t/h and values of concentrations in ppm)

3. Input in the AFI software the following process data (with $i = 1,2..n°$ tot of operations):

    a. Concentration of contaminant in water source, C_{WS}, in ppm;

    b. Limit flowrate, M_{max}, in kg/s;

    c. Maximum concentration of contaminant inlet, acceptable for each operation, $C_{i,IN}$, in ppm;

    d. Concentration of contaminant outlet for each operation, $C_{i,OUT}$, in ppm;

    e. Temperature of water source, T_{WS}, in °C;

    f. Temperature of water discharge, T_{WD}, in °C;

    g. Temperature required for each inlet stream, $T_{i,IN}$, in °C;

    h. Temperature of each outlet stream, $T_{i,OUT}$, in °C;

    i. Water consumption with water-reutilization approach, W_W, in kg/s;

    j. Water consumption without water-reutilization approach, W_{WO}, in kg/s;

4. With the additional information on the temperatures, the AFI software is able to transform and optimize the output data from AquoMin, in input data for FI^{2}EPI.

5. FI^{2}EPI performs the energy integration (§1.3) and gives as a output the Heat Exchange Network (HEN) and the following data:

    a. Hot Utility consumptions with energy integration approach, HHC, in kW;

    b. Cold Utility consumptions with energy integration approach, HCC, in kW.

6. Input the utilities consumptions in the AFI software, to calculate the actual mass and energy saving performed by the analysis.

Note that the only way to proceed is to use first AquoMin and then FI^{2}EPI because water minimization actually modifies the streams, while energy integration uses the existing streams to find the MER. For that reason, performing the energy integration before the water minimization would end up in an illogical solution.
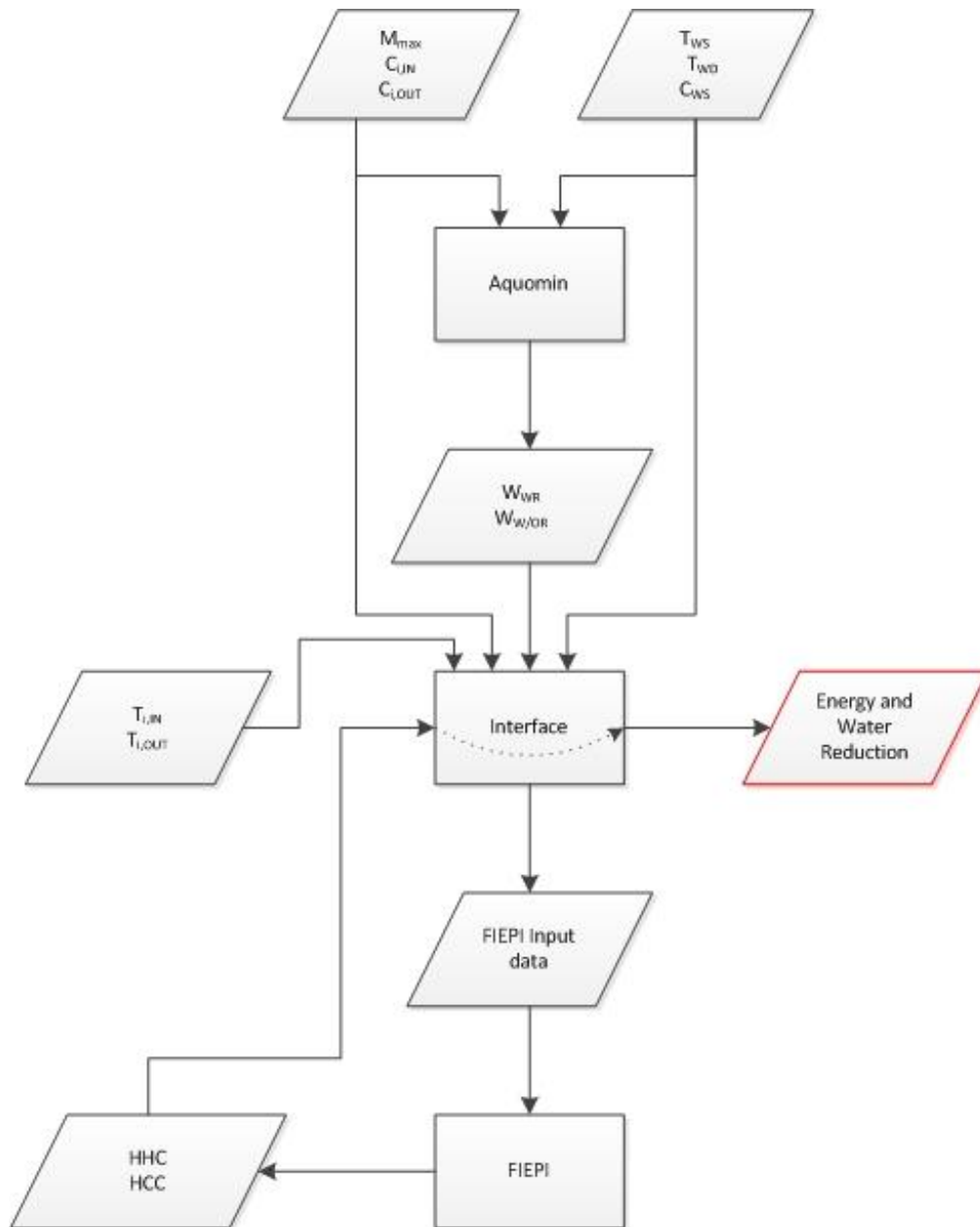
Figure 4.1. *Block diagram of the program information flux*

4.2 Program development

It is now possible to see in detail the calculations made by the AFI software to transform the output data of AquoMin, in input data of FI^{2}EPI, and all the aspect that were took in account for its construction.

For a better understanding, we used a numerical example that can be found in Savulescu, Kim et al., 2005 (Figure 4.2 and Table 4.1).

Based on Savulescu, Kim et al., 2005 and Leewongtanawit and Kim, 2009; using a value of ΔT_{min} of 10 °C, the best achievable integration for this example, with the minimum consumptions of both utilities and water, is summarized in Table 4.2

The expectations are to obtain the same results shown in Table 4.2, through the combination of AquoMin and FI^{2}EPI by the AFI software.
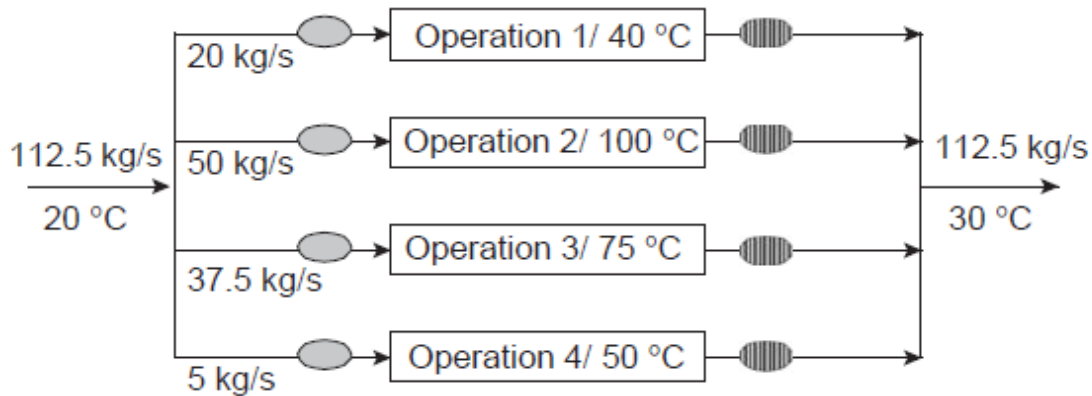

Figure 4.2. *Scheme of the example problem from Savulescu, Kim et al., 2005 .*

Table 4.1. *Data of the example problem from Savulescu, Kim et al., 2005*

Operation	$C_{P,IN}$ (ppm)	$C_{P,OUT}$ (ppm)	$T_{P,IN}$ (°C)	$T_{P,OUT}$ (°C)	Limiting water flowrate (kg/s)	Contaminant mass load (g/s)
Operation 1	0	100	40	40	20	2
Operation 2	50	100	100	100	100	5
Operation 3	50	800	75	75	40	30
Operation 4	400	800	50	50	10	4
Temperature of fresh water source, $T_{W,IN}$ = 20 (°C)						
Temperature of discharge wastewater, $T_{W,OUT}$ = 30 (°C)						

Table 4.2. *Best achievable consumptions of water and utilities*

Minimum water consumption (kg/s)	Minimum hot utility consumption (kW)	Minimum cold utility consumption (kW)
90	3780	0

4.2.1 Water and utilities consumption without mass and energy integration

In the first step, AFI collects in a table all the input data insert by the user, such as number of operations (max. four), data of the water source and, for every stream, the limit flow rate, temperature and concentration of contaminant. Note that the value of specific heat,

C_P, for the program is fixed and is equal at 4187 (J/kg°C), that is the one of the water. Changing that number is an operation that has to be done manually by the user.

Once the output data from AquoMin, W_W and W_{WO}, become available, AFI calculates the utilities and water consumption for the process without water minimization (Table 4.3.)

Table 4.3. *Input table of the flowrates without performing mass integration*

Operation	Water Flowrate (kg/s)	Hentalpy cold streams (kW)	Hentalpy hot streams (kW)
1	20	1674,800	837,400
2	50	16748,000	14654,500
3	37,5	8635,668	7065,563
4	5	628,050	418,700
Total fresh water Utilized (kg/s)	112,5		
Hot Utility (kW)	27686,538		
Cold Utility (kW)	22976,163		

4.2.2 Integration: attempt I

As a first attempt, we can try to combine AquoMin and FI²EPI directly, i.e. without any relevant interface between the two of them.

At first, it is necessary to input the data from Table 4.1 in AquoMin, so it is able to return the MEN with the values of water consumptions with water-reutilization approach (Figure 4.3). In Figure 4.3, it is also shown the position in which all the streams are heated/cooled.

With the values of water consumptions with water-reutilization approach, it is now possible to calculate the temperature of the four inlet streams and the two outlet streams, so as to obtain the input data for FI²EPI (Table 4.4). As said, AquoMin works only with the unit measure of the flowrate in t/h, so it is necessary to convert them in the units measure used in this example, i.e. kg/s.

With the data in Table 4.4, FI²EPI is able to plot the composite curve with the final amount of utilities consumption (Figure 4.4), with which it is possible to calculate the energy and water saving (Table 4.5),

As can be seen from Table 4.5, the minimum water consumption is already achieved but the utilities consumption, although it shows good reduction values, are still far from the target.

Figure 4.3. *Mass-exchange network of the first attempt*

Table 4.4. *FI²EPI input data for the first integration attempt*

Inlet streams			Outlet streams		
Flowrate (kg/s)	**Stream temperature (°C)**	**Target temperature (°C)**	**Flowrate (kg/s)**	**Stream temperature (°C)**	**Target temperature (°C)**
20,0	20,0	40,0	44,29	82,9	30,0
50,0	20,0	100,0			
40,00	51,4	75,0	45,71	71,9	30,0
5,71	82,9	50,0			
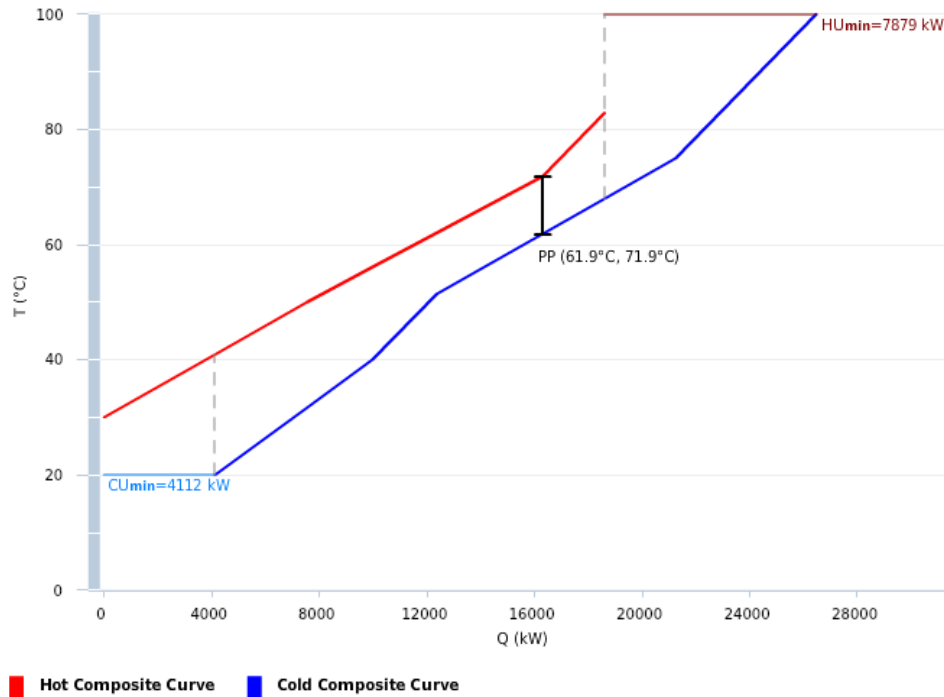
Figure 4.4. *Composite curve for the first integration attempt*

Table 4.5. *Mass and Utilities reduction with the first attempt of integration*

Total fresh water Utilized (kg/s)	90	Water reduction	-20,00%
Hot Utility (kW)	7879	Hot utility reduction	-71,5%
Cold Utility (kW)	4112	Cold utility reduction	-82,1%

4.2.3 Integration: attempt II

It is also possible to perform a variation of the first attempt, changing the position in which the outlet streams are heated (Figure 4.5). As can be seen comparing Figure 4.3 and Figure 4.5, in this case we have four (instead of two) outlet streams that can be used for the energy integration. On the other hand, in this case we have a waste of utilities because some of the four outlet streams are cooled to 30°C only to be partially reutilized to be hated again.

As done before, with the values of water consumptions with water-reutilization approach (Figure 4.5), we are able to calculate the temperature of the inlet and outlet streams, so as to obtain the input data for FI^{2}EPI (Table 4.6)

With the data in Table 4.6, FI^{2}EPI is able to plot the composite curve with the final amount of utilities consumption (Figure 4.6) with which it is possible to calculate the energy and water saving (Table 4.7).
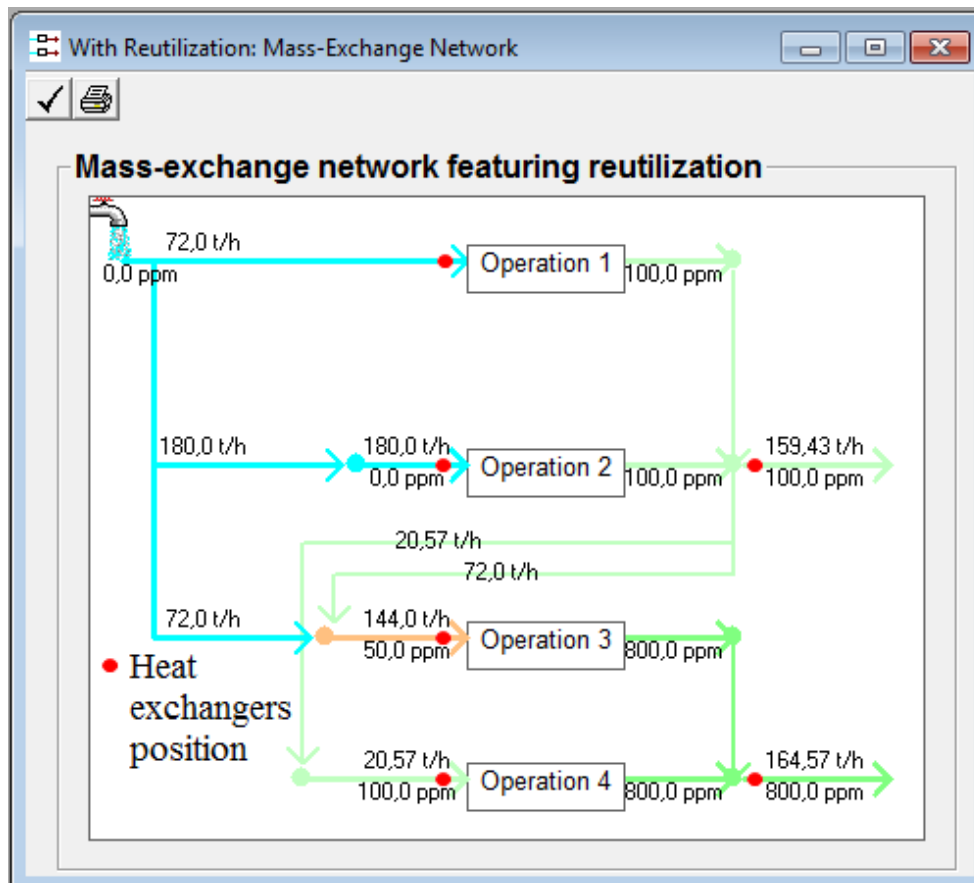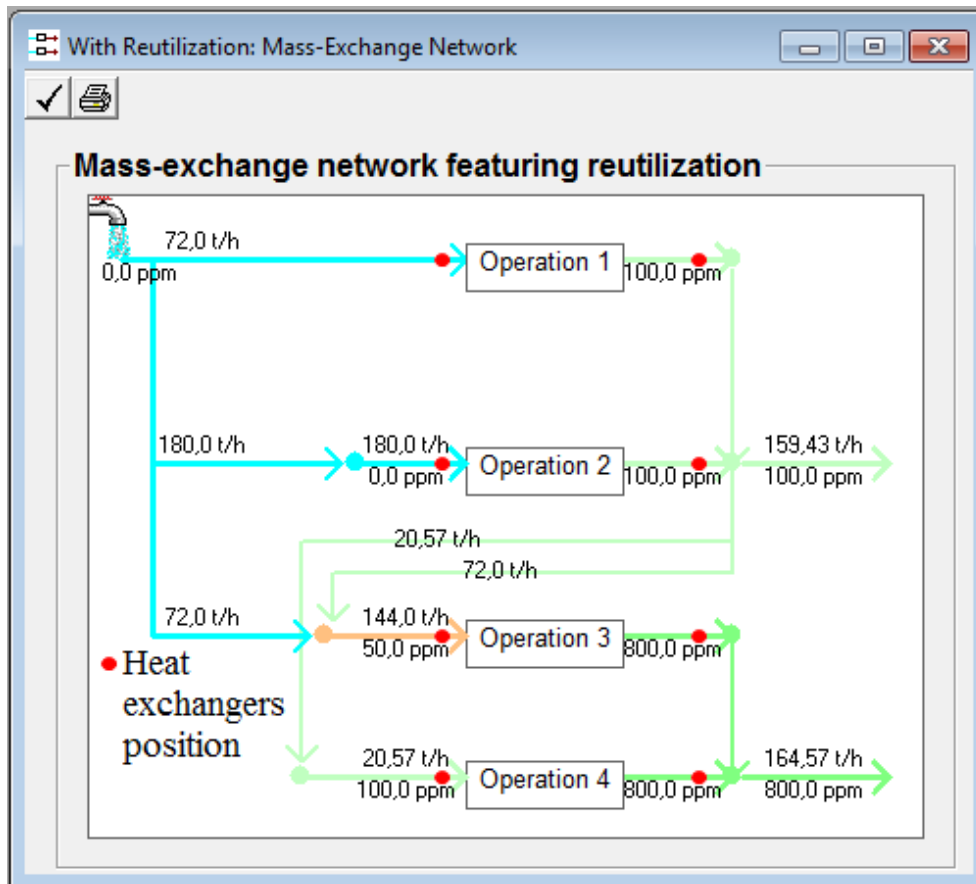
Figure 4.5. *Mass-exchange network of the second attempt*

Table 4.6. *FI²EPI input data for the second integration attempt*

Inlet streams			Outlet streams		
Flowrate (kg/s)	Stream temperature (°C)	Target temperature (°C)	Flowrate (kg/s)	Stream temperature (°C)	Target temperature (°C)
20,00	20,0	40,0	20,0	40,0	30,0
50,00	20,0	100,0	50,0	100,0	30,0
40,00	25,0	75,0	40,00	75,0	30,0
5,71	30,0	50,0	5,71	50,0	30,0

As can be seen from the results of these two attempts (Table 4.5 and Table 4.7), while in the second case (show in Figure 4.5) there is an obvious loss of heat because some streams are cooled and then heated again, the utilities consumption reduction is even greater than in the first case.

Thanks to those results, it was possible to discover the key points to work on to improve the energy integration:

    i.   Maximize the number of streams that are heated/cooled to exploit a wider range of temperatures during the energy integration;

ii. Prevent the heat losses, that occur when we cool a stream that has to be reused to be heated again;

iii. Take in account the quality of the heat in the streams, i.e. to do not mix a stream at high temperature with a stream at low temperature, because that narrows the range of temperatures that can be exploited during the energy integration.
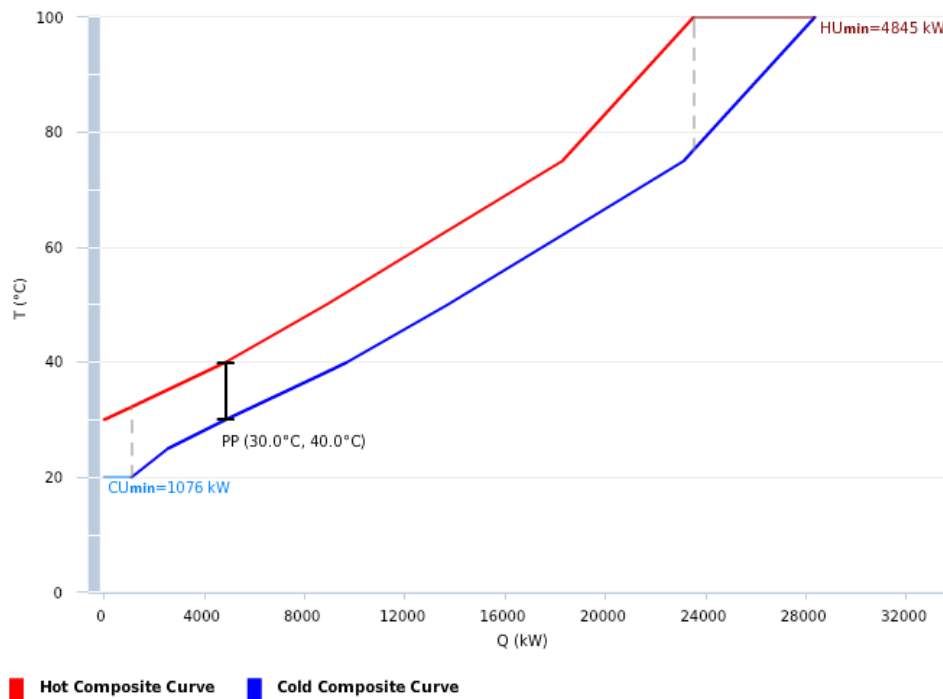

Figure 4.6. *Composite curve for the second integration attempt.*

Table 4.7. *Mass and Utilities reduction for the second integration attempt.*

Total fresh water Utilized (kg/s)	90	Water reduction	-20,00%
Hot Utility (kW)	4845	Hot utility reduction	-82,5%
Cold Utility (kW)	1075	Cold utility reduction	-95,3%

4.2.4 Improvement I: Mass Exchange Network (MEN)

It is now possible to develop an interface (the AFI software) to improve the values of utilities consumption. Taking into account the conclusion of §4.2.3, it is possible to suppose that the biggest hindrance to achieve said improvement is a particular behavior of AquoMin.

Namely, when AquoMin constructs the MEN, it combines all the outlet streams with the same concentration of contaminant (as it is possible to see in Figure 4.5). Combining the outlet streams, while it may have a sense to mass integration only, it becomes a problem for the energy integration because it does not take in account the quality of the heat in the streams; and this narrows the range of temperatures that could be exploited during the

heat integration. For instance, as shown in Figure 4.3 and Table 4.4, the 100°C stream coming from operation 2 could be used for the heating of a cold stream, up to 90°C (as we are always considering a ΔT_{min} of 10°C). Combining the 100°C stream coming from operation 2 with the 40°C stream coming from operation 1 produces a bigger stream at 82,9°C that could be used to heat a cold stream up to 72,9°C only.

For this reason, our goal now is to modify the MEN given by AquoMin, and force it to keep the outlet streams separated.

It was not actually possible to modify AquoMin itself, but we tried to develop an interface that takes the values of water flowrates given by AquoMin and, through a number of calculations, develops a new network with the outlet streams separated.

To fulfill that goal, taking into account a generic case of four inlet four outlet streams, it is necessary to consider all the different networks that Aquomin is able to return for a case of four inlet/outlet streams.

Considering c_i as the concentration of the outlet stream of the ith operation, with $i = 1, 2, 3, 4$; it is possible to find seven different network scenarios:

1) $c_1 \neq c_2 \neq c_3 \neq c_4$;
2) $c_1 = c_2 = c_3 \neq c_4$;
3) $c_1 = c_2 \neq c_3 \neq c_4$;
4) $c_1 = c_2 \neq c_3 = c_4$;
5) $c_1 \neq c_2 = c_3 = c_4$;
6) $c_1 \neq c_2 = c_3 \neq c_4$;
7) $c_1 \neq c_2 \neq c_3 = c_4$;

In Figure 4.7 and Figure 4.8 it is shown an example of the fourth and fifth scenarios.

The improvement achieved by separating the streams, implies also the generation of a new variable in the process. Namely, the amount of flowrate that has to be reutilized, for every of the streams that once were mixed together. In this work, this new variable was called split ratio.

For instance, as can be seen in Figure 4.5, 72 t/h are reutilized from the streams 1 and 2 combined, to operate in stream 3. Forcing the streams 1 and 2 to divide makes necessary to determine how much of those 72 t/h comes from the stream 1, and how much comes from the stream 2. Due to the different coding language of the software and considering the fact that those software are actually separated entities, it was not possible to code a function to determine the values of split ratios that give the best energy saving, so it has to be made by trial and error.
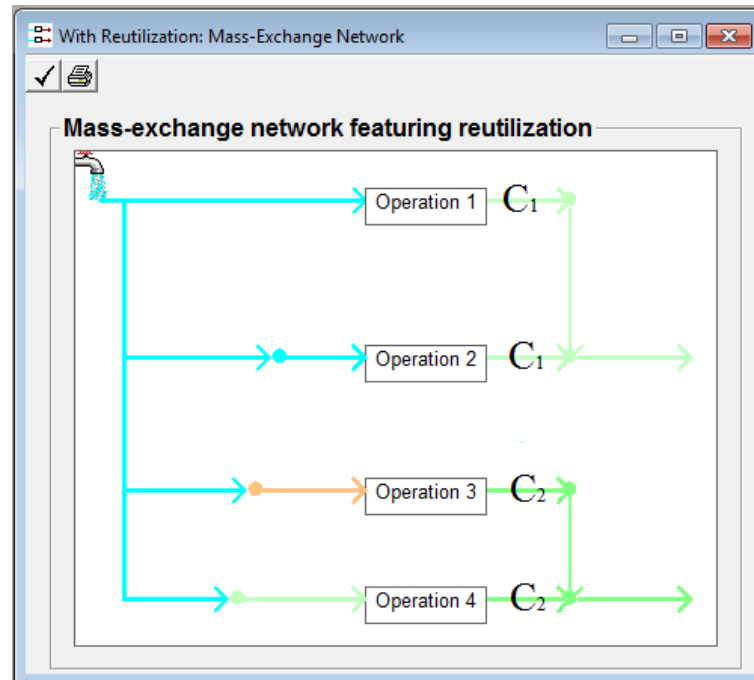
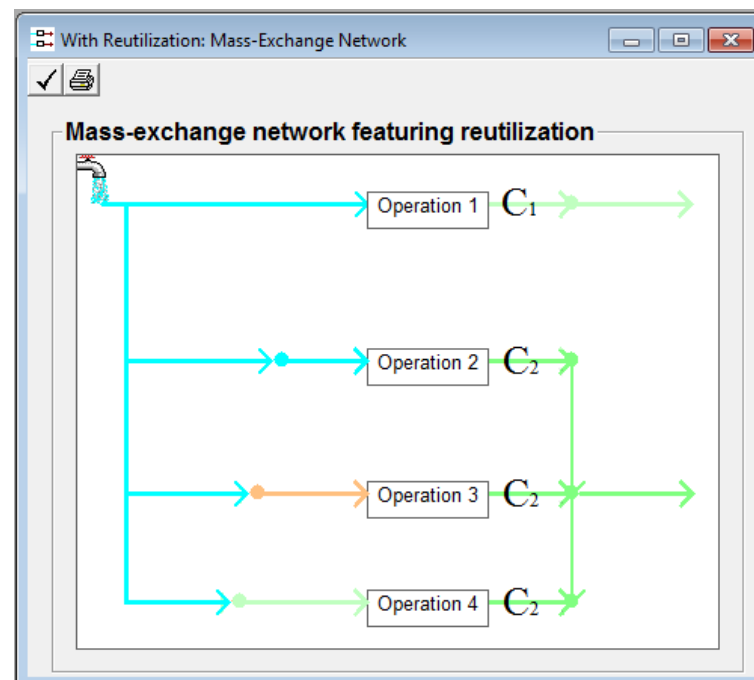**Figure 4.7.** *Mass-exchange network of fourth scenario.*

Figure 4.8. *Mass-exchange network of fifth scenario.*

For the example in Table 4.1, the best values of split ratios are shown in Table 4.8 and coincide with the data found in Savulescu, Kim et al., 2005.

Table 4.8. *Split ratios for the example in Table 4.1*

72 t/h reutilized from Operations 1 an 2 to Operation 3	
18 t/h reutilized from Operation 1	54 t/h reutilized from Operation 2
20,57 t/h reutilized from Operations 1 an 2 to Operation 4	
17,14 t/h reutilized from Operation 1	3.43 t/h reutilized from Operation 2

For each of the seven scenarios, a box of calculation has been developed. The software AFI has been coded to read the values of concentration outlet in the input data. It then automatically choose the correct network case, asks the user the values of the split ratios and finally generates a table with the input data for FI^{2}EPI. Note that the limit of four operation in the AFI software has been set up because adding more operations, would end up in a much higher number of scenarios to take in account.

For the example in exam, Figure 4.9 shows the new MEN with the separated outlet streams and Table 4.9 shows the input data for FI^{2}EPI.

With the data in Table 4.9, FI^{2}EPI is able to plot the composite curve with the final amount of utilities consumption (Figure 4.10) with which it is possible to calculate the energy and water saving (Table 4.10).

As can be seen by the results in Table 4.10, the energy saving in this case is better than the results obtained with the attempt I (Table 4.5), but it is worse than the results obtained with the attempt II (Table 4.7). We were not able to find an exact reason for this behavior, as it probably depends on the interactions between the streams during the energy integration. However, the effectiveness of this improvement will be displayed later in §4.2.5.
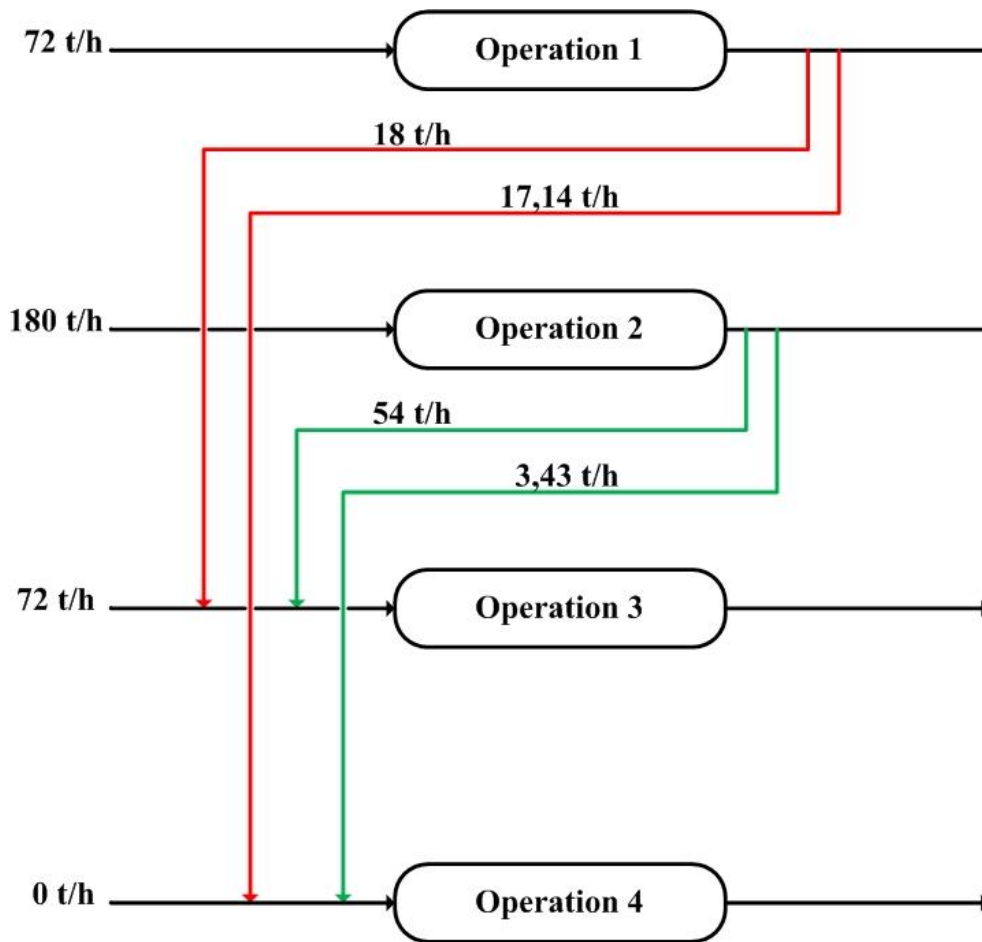
Figure 4.9. *New Mass-exchange network with the outlet streams separated*

Table 4.9. *FI²EPI input data of the first improvement attempt*

Inlet streams			Outlet streams		
Flowrate (kg/s)	Stream temperature (°C)	Target temperature (°C)	Flowrate (kg/s)	Stream temperature (°C)	Target temperature (°C)
20,00	20,00	40,0	10,24	40,0	30,0
50,00	20,00	100,0	34,05	100,0	30,0
40,00	52,50	75,0	40,00	75,0	30,0
5,71	50,00	50,0	5,71	50,0	30,0

Figure 4.10. *Composite curve for the first improvement attempt.*

Table 4.10. *Mass and Utilities reduction of the first improvement attempt.*

Total fresh water Utilized (kg/s)	90	Water reduction	-20,00%
Hot Utility (kW)	6273	Hot utility reduction	-77,3%
Cold Utility (kW)	2525	Cold utility reduction	-89,0%

4.2.5 Improvement II: Heat integration

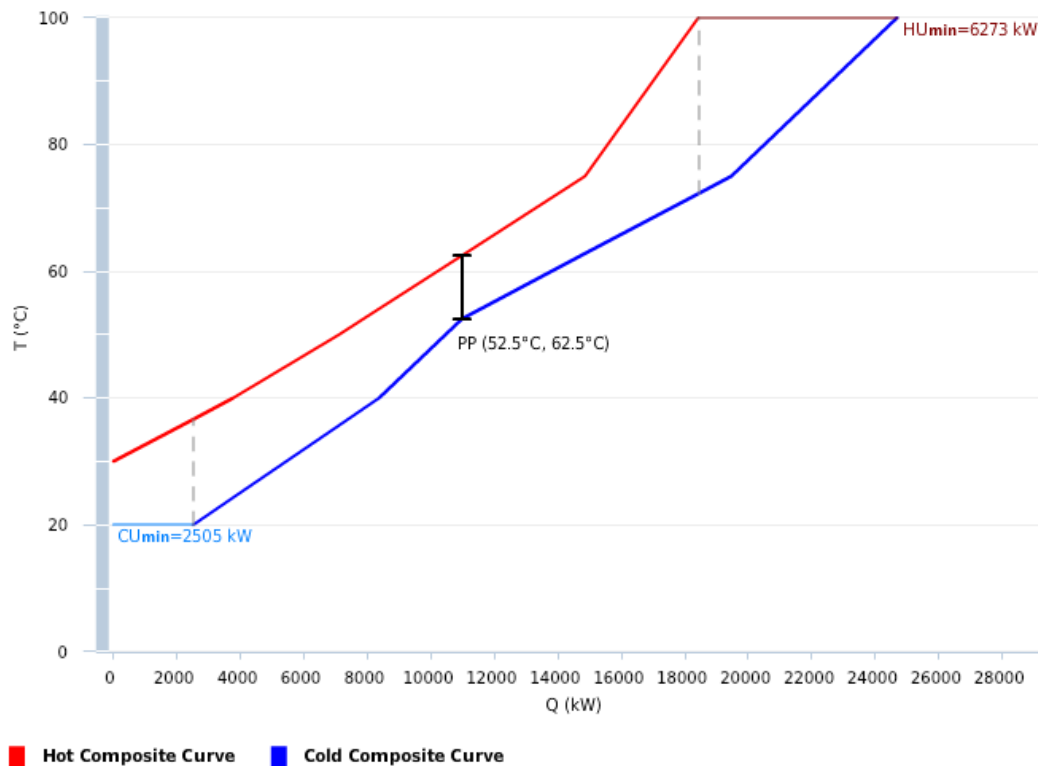One important improvement that could be made at this point regards, as said in §4.2.3, the quality of the heat in the streams. Until now, we have always focused on the outlet streams, but one important aspect that could be taken in account to reduce the utilities consumption is to analyze where a heat exchanger should be placed.

As can be seen in Figure 4.11, the possibilities for a generic inlet stream are two:

- Heat exchanger placed before the mixing point (Position 1 in Figure 4.11), to heat the stream so as to obtain the exact temperature required for the operation, with the mixing;
- Heat exchanger placed after the mixing point (Position 2 in Figure 4.11), to heat the stream at the exact temperature required for the operation.

For this example, the only stream involved is the inlet stream of operation 3. Even if the amount of heat to give to the stream is the same regardless the position of the heat exchanger, when talking about heat integration, the two situations are very different.

Considering a ΔT_{min} of 10 °C, it is possible to see that in position 1 the stream that has to be heated is made by fresh water (at 20 °C) that be heated with hot streams at 30 °C or more. In position 2, instead, the stream that has to be heated is at higher temperature (in Figure 4.4 and Figure 4.9 the stream temperature is over 50°C) and can be heated only with hot streams at high temperature (narrowing the temperature range available for the energy integration).
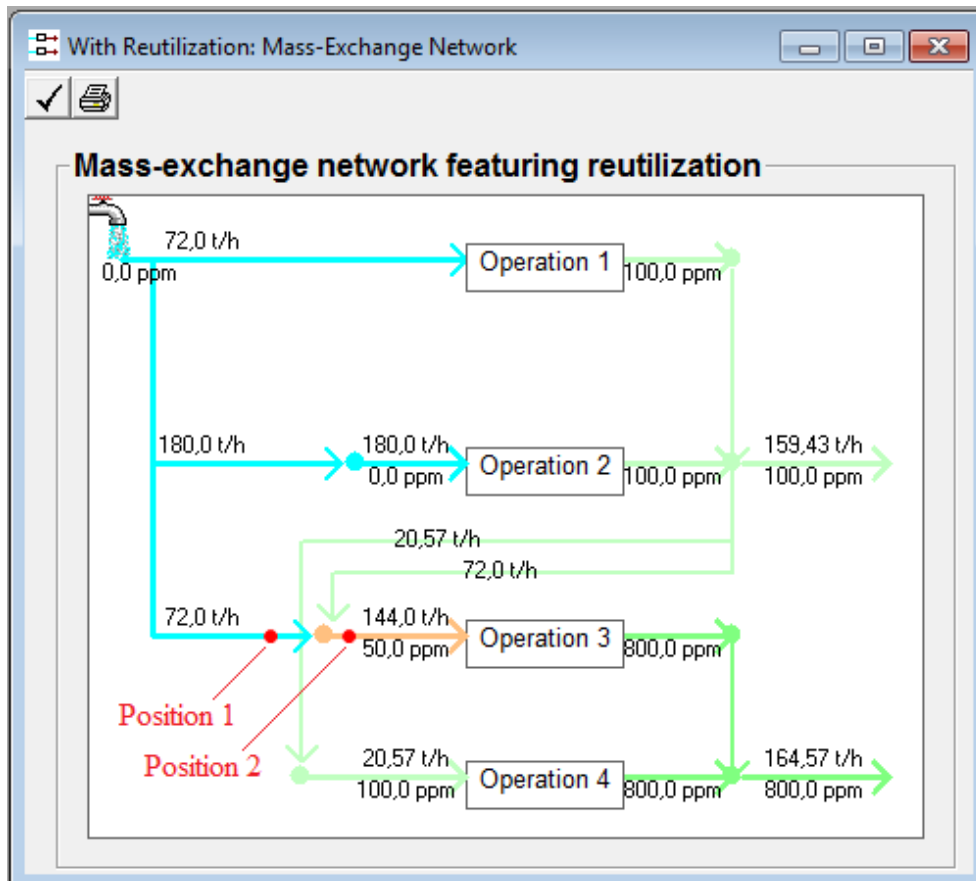
Figure 4.11. *MEN with the inlet streams possible heat positions*

However, even if the solution in position 1 seems to be better, that is not always the case, due to some boundaries that have to be placed. Namely, the solution in position 2 become the better choice when:

- the stream have to be cooled; putting the heat exchanger before the mixing point means the cooling of low temperature water, that is very expensive in terms of utilities;
- achieving the temperature required for the operation with the heat exchanger in position 1, means to heat the water at a temperature higher than 100°C; because to maintain the liquid form the pressure must be increased.

Given these hypotheses and taking in account the boundaries, the AFI software has been coded to automatically select which of the two options are better for a generic four operations process.

It is now possible to apply this second improvement to all the integration attempts and improvements exposed previously in this chapter (§4.2.2, §4.2.3, §4.2.4):

1) Integration: attempt I (§4.2.2): Here it is explained the heat integration improvement (II) applied to the integration attempt I. Table 4.11 shows how the streams data of the integration attempt I (Table 4.4) become after the application of the heat integration improvement.

Comparing the data in the two tables, it is possible to notice how the inlet stream of operation 3, which flowrate is 40 kg/s, to be heated from 51,4°C to 75°C, changes to be a stream of 20 kg/s flowrate, to be heated from 20°C to 67,14°C. It is clear that in the first case only the outlet streams from operation 1, 2, 3 could be used for the heat integration, while in the second case all the four outlet stream are available for the heat integration. In Figure 4.12 it is shown the new composite curve with the data from Table 4.11.

Table 4.12 shows the energy saving compared to the first integration attempt (*f.i.a.*), and the total one.

Table 4.11. *FI²EPI new input data for the first integration attempt*

Inlet streams			Outlet streams		
Flowrate (kg/s)	**Stream temperature (°C)**	**Target temperature (°C)**	**Flowrate (kg/s)**	**Stream temperature (°C)**	**Target temperature (°C)**
20,00	20,0	40,00	44,29	82,9	30,0
50,00	20,0	100,0			
20,00	20,00	67,14	45,71	71,9	30,0
5,71	82,90	50,00			

Figure 4.12. *New composite curve of the first integration attempt*

Table 4.12. *Mass and Utilities reduction with the new first attempt of integration*

Total fresh water Utilized (kg/s)	90	Water reduction from the *f.i.a*.	-0,00%	Water reduction	-20,00%
Hot Utility (kW)	6122	**Hot utility reduction from the *f.i.a*.**	-22,3%	**Hot utility reduction**	-78,9 %
Cold Utility (kW)	2355	**Cold utility reduction from the *f.i.a*.**	-42,7%	**Cold utility reduction**	-89,8%

2) Integration: attempt II (§4.2.3): Here it is explained the heat integration improvement (II) applied to the integration attempt II. The integration remains unchanged because the values of temperature of the fresh water exceed the boundaries requiring to be heated to 120°C.

3) Improvement I: MEN (§4.2.4): Here it is explained the heat integration improvement (II) discussed in this chapter, combined with the improvement I. Table 4.13 shows how the streams data of the first integration approach (Table 4.9) become after the application of the heat integration improvement.

Table 4.13. *FI²EPI input data with the MER and heat integration improvements*

Inlet streams			Outlet streams		
Flowrate (kg/s)	**Stream temperature (°C)**	**Target temperature (°C)**	**Flowrate (kg/s)**	**Stream temperature (°C)**	**Target temperature (°C)**
20,00	20,00	40,0	10,24	40,0	30,0
50,00	20,00	100,0	34,05	100,0	30,0
20,00	20,00	65,00	40,00	75,0	30,0
5,71	50,00	50,0	5,71	50,0	30,0

Also in this case it is possible to see how the inlet stream of operation 3, which flowrate is 40 kg/s, to be heated from 52,5°C to 75°C, changes to be a stream of 20 kg/s to be heated from 20°C to 65°C. In Figure 4.13 it is shown the new composite curve with the data from Table 4.13. Table 4.14 shows the energy saving achieved with the improvements.
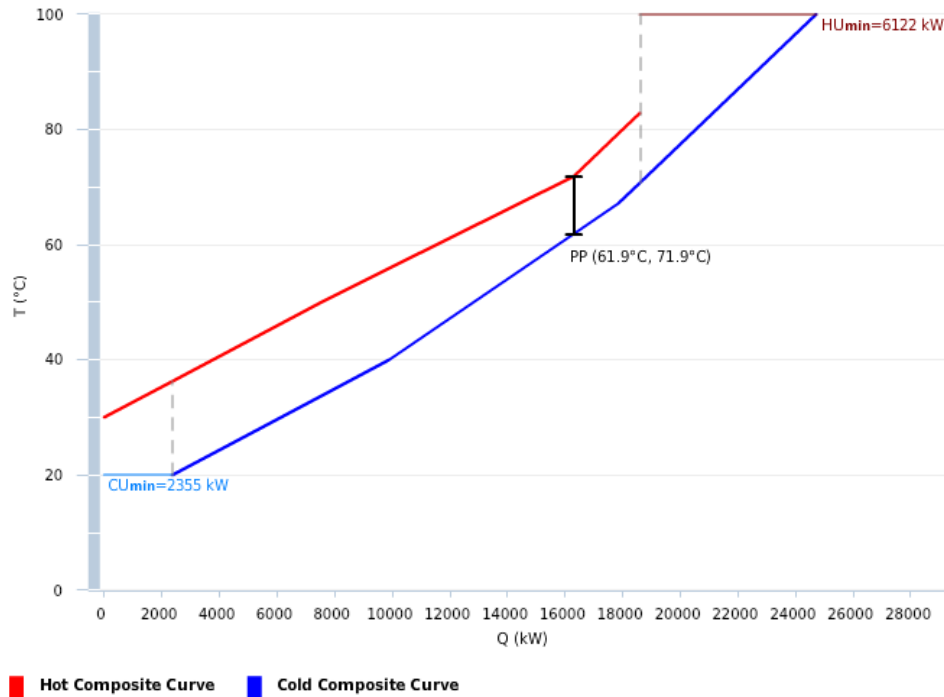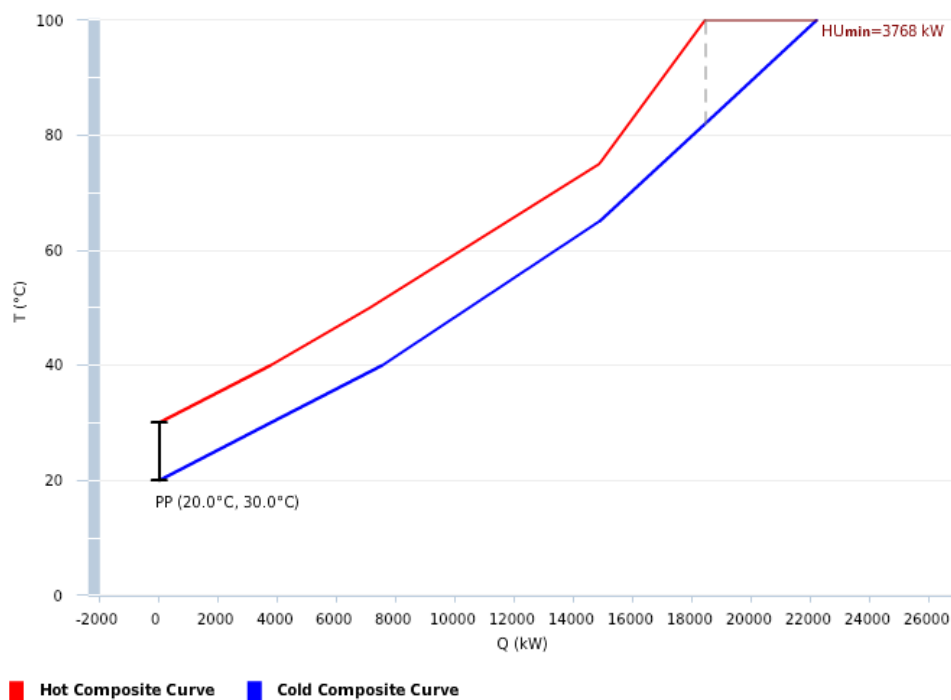

Figure 4.13. *New composite curve of the first integration attempt*

Table 4.14. *Mass and Utilities reduction with the first attempt of integration*

Total fresh water Utilized (kg/s)	90	Water reduction	-20,00%
Hot Utility (kW)	3768	Hot utility reduction	-86,4%
Cold Utility (kW)	0	Cold utility reduction	-100,0%

As can be seen from those results, we were able to achieve the same consumption savings reached by Savulescu, Kim et al., 2005 and Leewongtanawit and Kim, 2009. Comparing Table 4.14 with Table 4.3, it is possible to notice that the values of utilities consumption are not identical, but it is reasonable to assume that this small difference may be caused by a difference on the value of specific heat, *Cp*, used for the calculations.

4.3 Network design

It is now possible to design and compare the networks of the initial process without any form of integration (Table 4.1), and the final process (third case in §4.2.5;Table 4.14).

4.3.1 Initial process design

In regards of the initial process data (Table 4.1) without mass and/or energy integration being performed, Figure 4.14 and Figure 4.15 show the Mass Exchange Network (MEN) and the Heat Exchange Network (HEN). The two combined together form the complete process network (Figure 4.16).
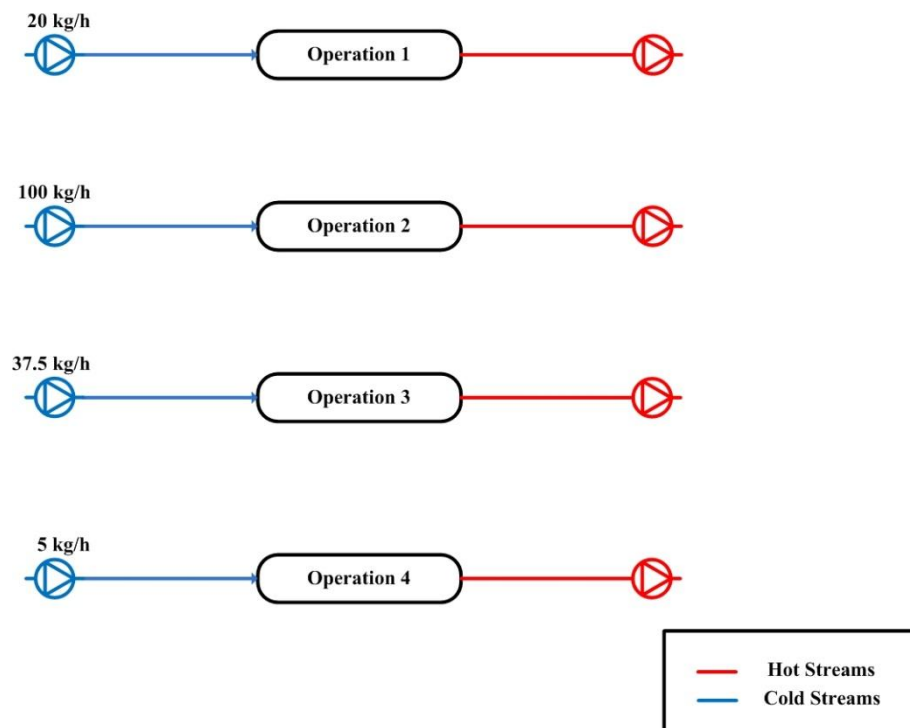
Figure 4.14. *MEN of the initial process without mass and/or energy integration*
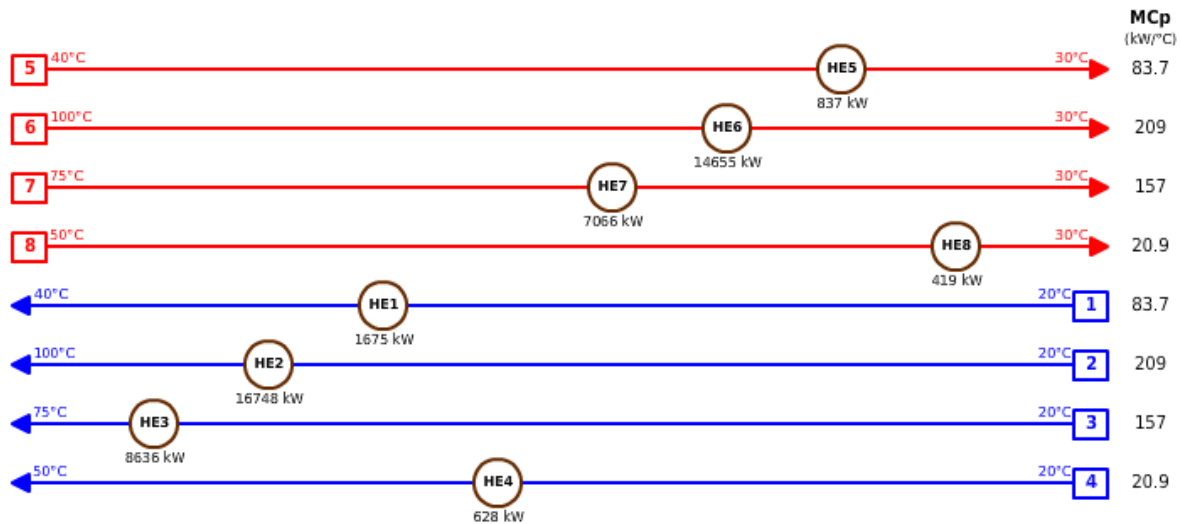
Figure 4.15. *HEN of the initial process without mass and/or energy integration*
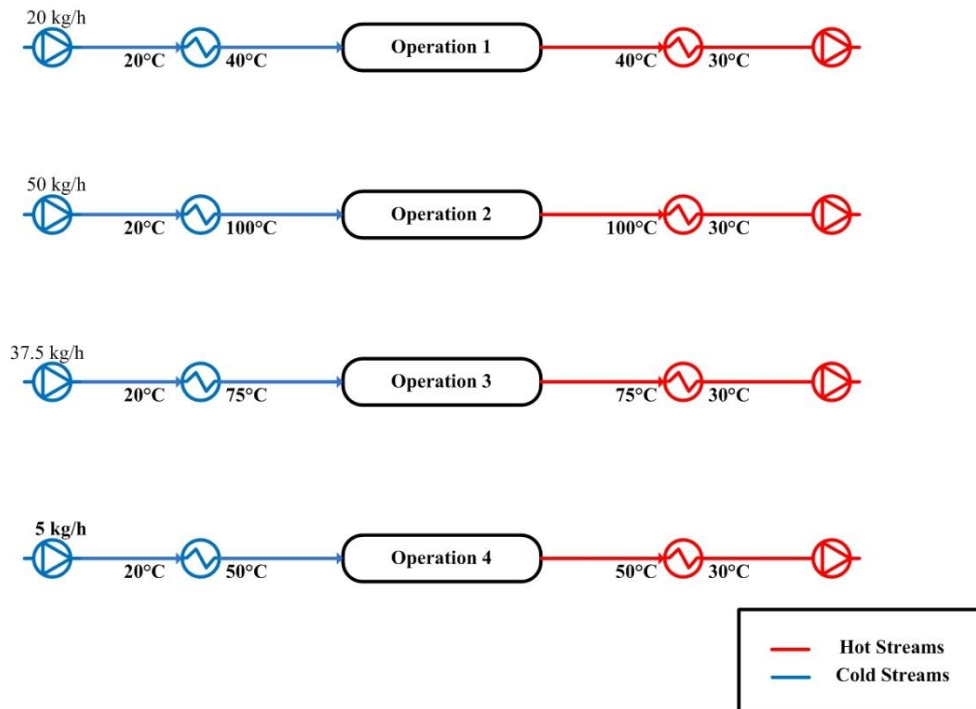
Figure 4.16. *Complete network of the initial process without mass and/or energy integration*

As can be seen in Figure 4.16, the network design is very simple. With a total of eight streams and eight heat exchangers, the process need a high amount of utilities and fresh water (Table 4.2) but it does not require much equipment.

4.3.2 Final process design

Here we describe the design networks of the final process (third case in §4.2.5, Table 4.13), i.e. the one that was able to reach the best in terms of fresh water and utilities consumptions. Figure 4.17, Figure 4.18 and Figure 4.19 show the Mass Exchange

Network (MEN), the Heat Exchange Network (HEN) and the combined complete process network, respectively.
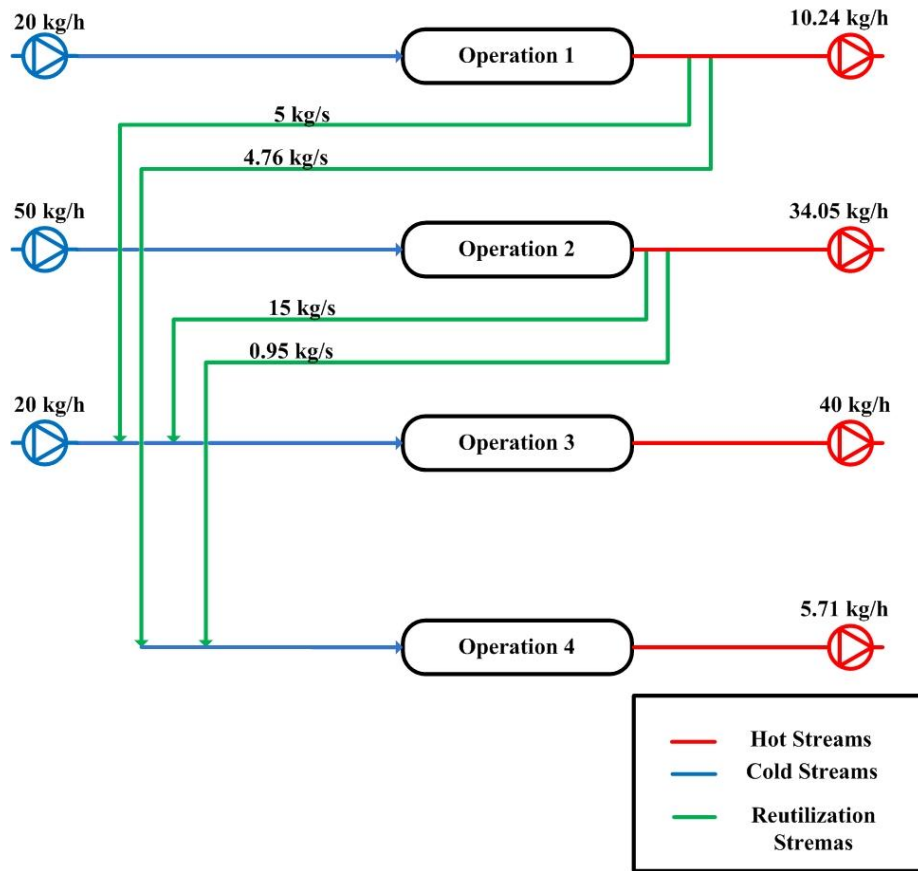
Figure 4.17. *MEN of the final process*
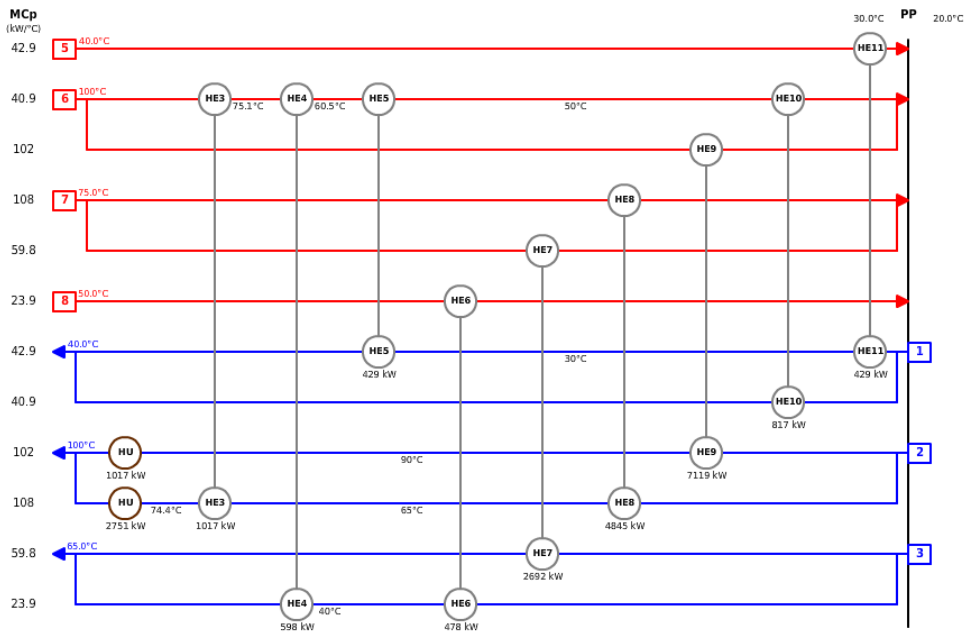
Figure 4.18. *HEN of the final process*

As is shown in Figure 4.19, the final design of the process is much more complex than the initial one in Figure 4.16. In order to achieve the consumptions reduction listed in Table 4.14, additional three heat exchangers and eight streams must be added to the process.

Figure 4.19. *Complete network of the final process*

4.4 Graphical Interface

The second goal of this work revolves around the implementation, in the AFI software, of a user-friendly interface coded in Visual Basic (Appendix A), for the resolution of a generic maximum-four operations process using AquoMin and FI^{2}EPI.

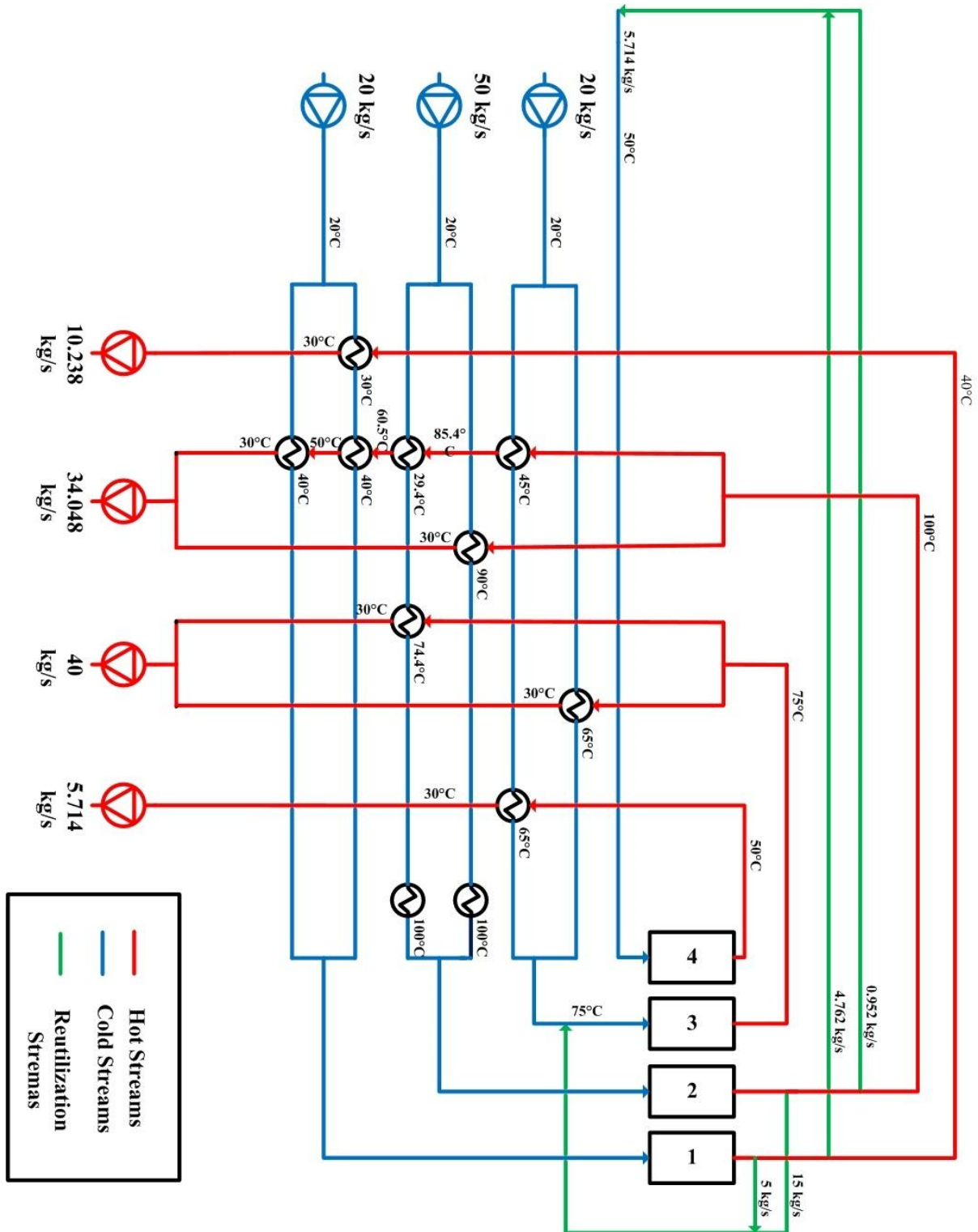This paragraph shows the graphical interface that has been implemented and describes the walkthroughs for the proper utilization of the AFI software. To achieve this goal, the same example reported in Figure 4.2 and Table 4.1 has been used (Savulescu, Kim et al., 2005).

The steps the user has to go through for the proper utilization of the AFI software are explained in the following:

1) First step: As can be seen in Figure 4.20, the AFI software starts with an introduction window that allows to start the program (button "Start Program"), or to open the excel box to see/modify the workbook in which are made the calculations (button "Edit Code").

Figure 4.20. *Initial interface box*

2) Second step: After pressing the button "Start Program" an input box (Figure 4.21) pops up to collect the data of the water source and water discharge (Table 4.1). Namely the input box asks to manually insert the temperature of the water source, T_{WS}, in °C; the temperature of the water discharge, T_{WD}, in °C; and the concentration of contaminant in the water source, C_{WS}, in ppm.

3) Third step: The AFI software pops up another input box (Figure 4.22) to collect the operations data (Table 4.1). As can be seen in Figure 4.22, the first column contains the values of the Limit flowrates of each operations, M_{max}, in kg/s. The second column contains the values of temperature required for each inlet stream, $T_{i,IN}$, in °C. The third column contains the values of temperature of each outlet stream, $T_{i,IN}$, in °C. While the fourth and fifth column contain the maximum concentration of contaminant inlet,

acceptable for each operation, $C_{i,IN}$, in ppm; and the concentration of contaminant outlet of each operation, $C_{i,OUT}$, in ppm;

Figure 4.21. *Input box for water source and discharge data*

The data insert for every operation will automatically be auto-sorted in the workbook from the lowest concentration outlet to the highest to match AquoMin method of operation.

The input box of Figure 4.22 is then followed by a message box that instructs the user to manually input the same data of Figure 4.21 and Figure 4.22, in the AquoMin software.

Figure 4.22. *Input box for operations data*

4) Fourth step: Manually input the data of Table 4.1 also in the AquoMin software. Note that AquoMin only works with the values of flowrates in t/h. AquoMin is now able to return the MEN without mass integration approach (Figure 4.14), and the MEN with water reutilization approach (Figure 4.17). This networks contain the values of water consumption with water-reutilization approach, W_W, in t/h, and water consumption without water-reutilization approach, W_{WO}, in t/h, that are needed to continue the energy integration.

5) Fifth Step: The AFI software continues by showing a chart (Figure 4.23) in which it is necessary to manually insert the data of water consumption, for each operation, as obtained according to the water-reutilization approach, W_W, in kg/s. The AFI software works also for a generic process with less than four operations. If for instance the process in exam is a three operations process, the first operation in the networks should be left blank; if the process is a two operations process, the first two operations in the networks need to be left blank; and so on.
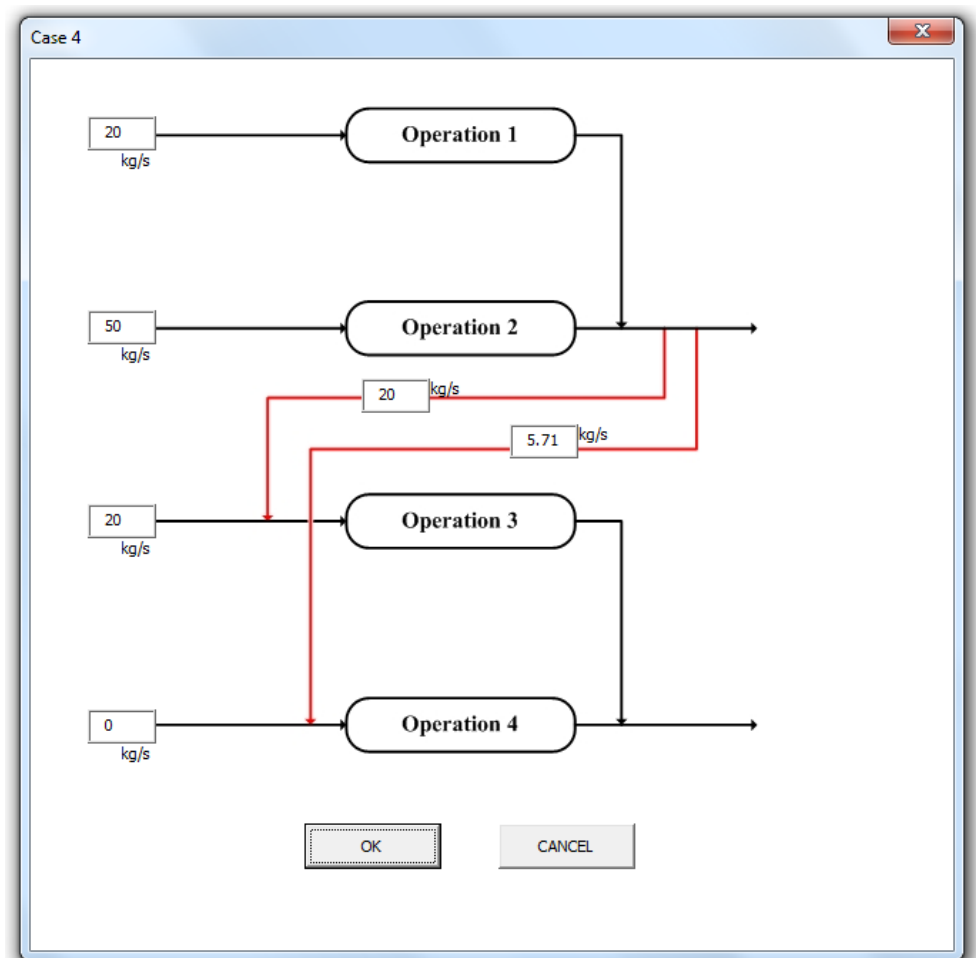
Figure 4.23. *Program's Mass-exchange network with reutilization*

The AFI software interface asks the user the values of the split ratio for the reutilization streams (Figure 4.24). For the example considered, we have a stream that combine the outlet streams from operation 1 and operation 2, that is been reutilized for an amount of 20 kg/s in the operation 3 and 5.71 kg/sin operation 4.

The software automatically checks the presence of mistake in the sums and warns the user.

6) Sixth Step: The AFI software continues by showing a chart (Figure 4.25) in which it is possible to manually insert the data of water consumption, for each operation, obtained without water-reutilization approach, W_{WO}, in kg/s. As said for the previous step, if a generic process with less than four operation is taken into account (for instance a three operations process) the first operation in the network needs to be left blank.

Figure 4.24. *Reutilization streams composition box*

7) Seventh Step: At this point, the AFI software returns a table with the data that have to be manually input by the user in the FI^{2}EPI software (Figure 4.26).
The AFI software interface allows also to export and save the data in Figure 4.27, by pressing the button "Generate Table".

8) Eight Step: Manually input the data of Figure 4.26 in the FI^{2}EPI software. FI^{2}EPI is now able to return the composite curve (Figure 4.13) and allows the user to construct the HEN (Figure 4.18). The composite curve contain the values of hot utility consumptions with energy integration approach, HHC, in kW; and cold utility consumptions with energy integration approach, HCC, in kW.

9) Ninth Step: The AFI software pops up an input box (Figure 4.27) to collect the values of hot utility consumptions with energy integration approach, HHC, in kW; and cold utility consumptions with energy integration approach, HCC, in kW obtained by FI^{2}EPI,

10) Tenth step: The AFI software is now ready to return the results with the final energy and water consumption, and the percentage of reduction from the initial case without mass

and energy integration (Figure 4.28). The AFI software interface allows also to export and save the data in Figure 4.28, by pressing the button "Generate Table.
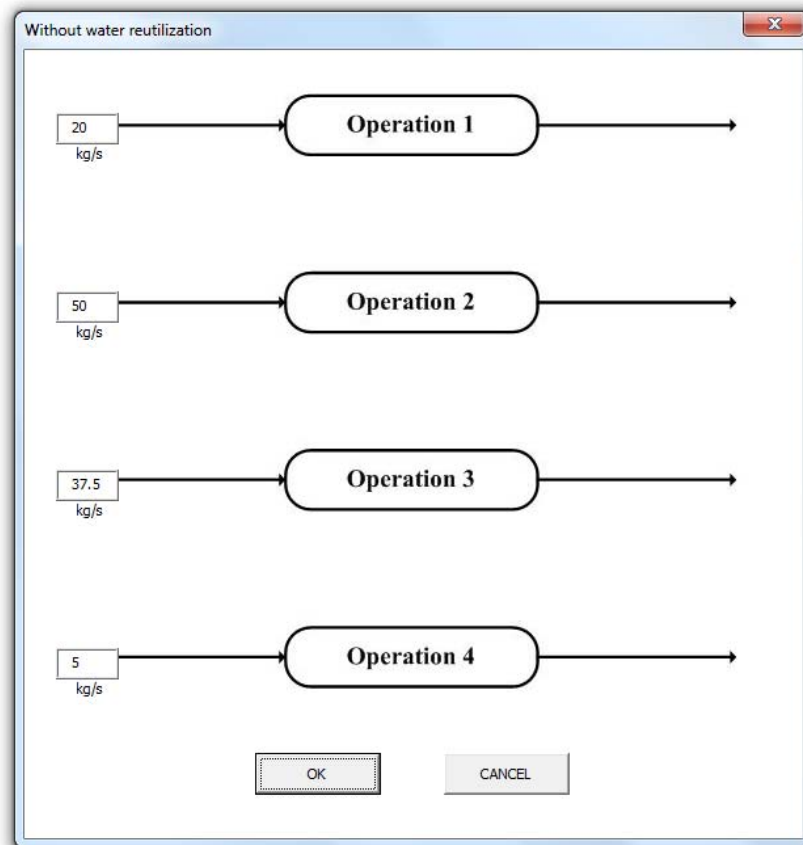

Figure 4.25. *Program's Mass-exchange network without reutilization*

Figure 4.26. *Table of the input data of F²IEPI*

Figure 4.27. *Utility Consumption box*

Figure 4.28. *Results box*

Conclusions

The goal of this thesis was the simultaneous minimization of wastewater and energy consumption, through a combination of two existing programs, FI^{2}EPI and AquoMin. AquoMin is a program coded in Visual Basic (VBA) that performs the minimization of the fresh water consumption and wastewater production in a generic process that uses water as a contaminant remover. FI^{2}EPI is a software coded in Java that performs energy integration between hot streams and cold streams in a generic process so as to obtain the minimum utilities consumption.

The study was divided in two parts: the first part concerned with the actual achievement of the simultaneous minimization of wastewater and energy consumption; the second part was the design of a third software (AFI) coded in Visual Basic, which aims at building an user-friendly interface between AquoMin and FI^{2}EPI. To achieve the process integration, a numerical example of a four operations process taken from the literature was reproduced.

At first, some integration attempts were tried combining AquoMin and FI^{2}EPI directly, i.e. without any relevant interface between the two of them. The best results achievable with this approach showed that the minimum value of wastewater consumption was already obtained, but the minimum energy consumptions, although showing a relevant decrease, did not reach the expectations.

Thanks to these first attempts, it was noticed that the key points to work on to improve the energy consumptions were:

  i.   To maximize the number of the heated/cooled streams, so as to exploit a wider range of temperatures during the energy integration;
  ii.   To prevent the heat losses that occur when a hot stream is cooled, drown and then reutilized and heated again;
  iii. To take in account the quality of the heat in the streams, i.e. not to mix a stream at high temperature with a stream at low temperature, because that narrows the range of temperatures that can be exploited during energy integration.

With the implementation of improvements on these key points, the application of the process integration to the case study showed a reduction of water utilization by 20%, and an 86.4% and 100% decrease with respect to heating and cooling utility requirements.

The main limit of this work is that the simultaneous minimization of wastewater and energy consumption is not made with a single program, but it is necessary to use all the three software (AquoMin, AFI and FI^{2}EPI). An additional improvement can be obtained by implementing an optimization function to determine the correct values for the split ratio (i.e. the values that give the best energy consumption). At the moment, the optimum

values of split ratio is determined by trial and error. Another relevant limit is that at the moment only four operations can be dealt with by the software.

Appendix A

In the Appendix A it is shown the code used to develop the graphical interface of the AFI software. Namely, the software has been coded in Visual Basic (VBA). Every Userform described in the following represents a popup box; for instance the Userform 2 represents the case 1 MEN scenario,vdescribed in § 4.2.4 (Figure A.1)
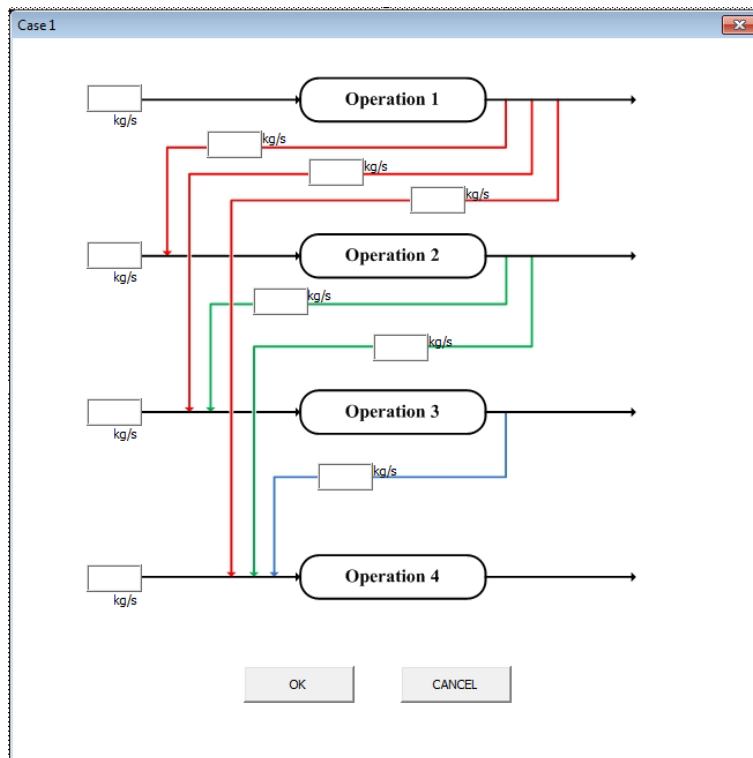
Figure A.1. *Case1 Mass Exchange Network*

Userform 1

This userform represents the streams input data box. Based on the data input by the user, this userform select the corresponding Mass Exchange Network scenario, as described in § 4.2.4

```
Private Sub cmdcancel2_Click()
UserForm1.Hide
UserForm9.Show
End Sub
Private Sub cmdok2_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("C3").Value = Me.L1.Value
sh2.Range("C4").Value = Me.L2.Value
sh2.Range("C5").Value = Me.L3.Value
sh2.Range("C6").Value = Me.L4.Value
```

```
sh2.Range("F3").Value = Me.Ti1.Value
sh2.Range("F4").Value = Me.Ti2.Value
sh2.Range("F5").Value = Me.Ti3.Value
sh2.Range("F6").Value = Me.Ti4.Value
sh2.Range("G3").Value = Me.To1.Value
sh2.Range("G4").Value = Me.To2.Value
sh2.Range("G5").Value = Me.To3.Value
sh2.Range("G6").Value = Me.To4.Value
sh2.Range("D3").Value = Me.Ci1.Value
sh2.Range("D4").Value = Me.Ci2.Value
sh2.Range("D5").Value = Me.Ci3.Value
sh2.Range("D6").Value = Me.Ci4.Value
sh2.Range("E3").Value = Me.Co1.Value
sh2.Range("E4").Value = Me.Co2.Value
sh2.Range("E5").Value = Me.Co3.Value
sh2.Range("E6").Value = Me.Co4.Value
Dim oneRange As Range
Dim aCell As Range
Set oneRange = sh2.Range("C2:I6")
Set aCell = sh2.Range("E3")
oneRange.Sort Key1:=aCell, Order1:=xlAscending, Header:=xlYes
If sh2.Range("E3").Value = sh2.Range("E4").Value Then
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Error, the concentrations output cannot be all equals!"
Else
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm3.Show
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm5.Show
Else
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm4.Show
End If
End If
Else
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm6.Show
Else
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm7.Show
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
```

```
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm8.Show
Else
MsgBox " Input the data also in Aquomin!"
UserForm1.Hide
MsgBox " Input in the following box the results given by Aquomin!"
UserForm2.Show
End If
End If
End If
End Sub
Private Sub cmdok1_Click()
End Sub
Private Sub L1_Change()
End Sub
Private Sub UserForm_Click()
End Sub
```

Userform 2

As said previously, the Userform 2 represents the case 1 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm2.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b37").Value = Me.w1.Value
sh2.Range("b42").Value = Me.w2.Value
sh2.Range("b47").Value = Me.w3.Value
sh2.Range("b52").Value = Me.w4.Value
sh2.Range("h36").Value = Me.r12.Value
sh2.Range("h37").Value = Me.r13.Value
sh2.Range("h38").Value = Me.r14.Value
sh2.Range("h42").Value = Me.r23.Value
sh2.Range("h43").Value = Me.r24.Value
sh2.Range("h47").Value = Me.r34.Value
UserForm2.Hide
UserForm11.Show
End Sub
Private Sub Image1_Click()
End Sub
Private Sub UserForm_Click()
End Sub
```

Userform 3

Userform 3 represents the case 2 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm3.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b91").Value = Me.w1.Value
sh2.Range("b94").Value = Me.w2.Value
sh2.Range("b97").Value = Me.w3.Value
sh2.Range("b101").Value = Me.w4.Value
sh2.Range("b100").Value = Me.r14.Value
UserForm3.Hide
UserForm14.Show
End Sub
Private Sub Image1_Click()
End Sub
Private Sub UserForm_Click()
End Sub
```

Userform 4

Userform 4 represents the case 3 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm4.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b142").Value = Me.w1.Value
sh2.Range("b146").Value = Me.w2.Value
sh2.Range("b150").Value = Me.w3.Value
sh2.Range("b154").Value = Me.w4.Value
sh2.Range("b149").Value = Me.r13.Value
sh2.Range("b152").Value = Me.r14.Value
sh2.Range("b153").Value = Me.r34.Value
UserForm4.Hide
UserForm15.Show
End Sub
Private Sub Image1_Click()
End Sub
```

```
Private Sub UserForm_Click()
End Sub
```

Userform 5

Userform 5 represents the case 4 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm5.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b194").Value = Me.w1.Value
sh2.Range("b198").Value = Me.w2.Value
sh2.Range("b203").Value = Me.w3.Value
sh2.Range("b206").Value = Me.w4.Value
sh2.Range("b202").Value = Me.r13.Value
sh2.Range("b205").Value = Me.r14.Value
UserForm5.Hide
UserForm16.Show
End Sub
Private Sub Image1_Click()
End Sub
```

Userform 6

Userform 6 represents the case 5 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm6.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b248").Value = Me.w1.Value
sh2.Range("b253").Value = Me.w2.Value
sh2.Range("b256").Value = Me.w3.Value
sh2.Range("b259").Value = Me.w4.Value
sh2.Range("i247").Value = Me.r12.Value
sh2.Range("i248").Value = Me.r13.Value
sh2.Range("i249").Value = Me.r14.Value
UserForm6.Hide
```

```
UserForm11.Show
End Sub
Private Sub Image1_Click()
End Sub
```

Userform 7

Userform 7 represents the case 6 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm7.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b299").Value = Me.w1.Value
sh2.Range("b304").Value = Me.w2.Value
sh2.Range("b307").Value = Me.w3.Value
sh2.Range("b311").Value = Me.w4.Value
sh2.Range("i298").Value = Me.r12.Value
sh2.Range("i299").Value = Me.r13.Value
sh2.Range("i300").Value = Me.r14.Value
sh2.Range("b310").Value = Me.r24.Value
UserForm7.Hide
UserForm17.Show
End Sub
Private Sub Image1_Click()
End Sub
Private Sub UserForm_Click()
End Sub
```

Userform 8

Userform 8 represents the case 7 of the Mass Exchange Network Scenarios in which the user have to input the data of water consumption, for each operation, as obtained according to the water-reutilization approach.

```
Private Sub cmdcancel1_Click()
UserForm8.Hide
UserForm1.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("b353").Value = Me.w1.Value
sh2.Range("b357").Value = Me.w2.Value
sh2.Range("b362").Value = Me.w3.Value
```

```
sh2.Range("b366").Value = Me.w4.Value
sh2.Range("i351").Value = Me.r12.Value
sh2.Range("i352").Value = Me.r13.Value
sh2.Range("i353").Value = Me.r14.Value
sh2.Range("i356").Value = Me.r23.Value
sh2.Range("i357").Value = Me.r24.Value
UserForm8.Hide
UserForm11.Show
End Sub
Private Sub Image1_Click()
End Sub
```

Userform 9

This userform represents the water source/discharge input data box.

```
Private Sub cmdcancel1_Click()
UserForm9.Hide
ThisWorkbook.Close savechanges:=True
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("D7").Value = Me.tws.Value
sh2.Range("D8").Value = Me.twd.Value
sh2.Range("D9").Value = Me.ccw.Value
UserForm9.Hide
UserForm1.Show
End Sub
Private Sub Label3_Click()
End Sub
Private Sub UserForm_Click()
End Sub
```

Userform 10

The userform 10 represents the streams property table generated by the AFI software with the streams data that the user have to input in the FI^2EPI software. This userform allow also to export the data of the table in a excel file.

```
Private Sub cmdcancel1_Click()
UserForm10.Hide
UserForm9.Show
End Sub
Private Sub cmdok1_Click()
UserForm10.Hide
UserForm12.Show
End Sub
Private Sub CommandButton1_Click()
Dim sfName As String
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
```

```vba
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Activate
If sh2.Range("E3").Value = sh2.Range("E4").Value Then
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Error, the concentrations output cannot be all equals!"
Else
Range("i118:n126").Value = Range("b118:g126").Value
Range("I118:n126").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Range("i224:n232").Value = Range("b224:g232").Value
Range("I224:n232").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
Else
Range("i171:n179").Value = Range("b171:g179").Value
Range("I171:n179").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
```

```
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
End If
Else
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Range("i275:n283").Value = Range("b275:g283").Value
Range("I275:n283").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
Else
Range("i328:n336").Value = Range("b328:g336").Value
Range("I328:n336").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Range("i381:n389").Value = Range("b381:g389").Value
Range("I381:n389").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
```

```vba
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
Else
Range("i68:n76").Value = Range("b68:g76").Value
Range("I68:n76").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:F").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Table", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
End If
End If
End Sub
Private Sub fr1_Click()
End Sub
Private Sub UserForm_Initialize()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
If sh2.Range("E3").Value = sh2.Range("E4").Value Then
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Error, the concentrations output cannot be all equals!"
Else
Me.fr1 = sh2.Range("c119").Text
Me.fr2 = sh2.Range("c120").Text
Me.fr3 = sh2.Range("c121").Text
Me.fr4 = sh2.Range("c122").Text
Me.fr5 = sh2.Range("c123").Text
Me.fr6 = sh2.Range("c124").Text
Me.fr7 = sh2.Range("c125").Text
Me.fr8 = sh2.Range("c126").Text
Me.Ti1 = sh2.Range("d119").Text
Me.Ti2 = sh2.Range("d120").Text
Me.Ti3 = sh2.Range("d121").Text
Me.Ti4 = sh2.Range("d122").Text
Me.ti5 = sh2.Range("d123").Text
Me.ti6 = sh2.Range("d124").Text
```

```vba
Me.ti7 = sh2.Range("d125").Text
Me.ti8 = sh2.Range("d126").Text
Me.To1 = sh2.Range("e119").Text
Me.To2 = sh2.Range("e120").Text
Me.To3 = sh2.Range("e121").Text
Me.To4 = sh2.Range("e122").Text
Me.to5 = sh2.Range("e123").Text
Me.to6 = sh2.Range("e124").Text
Me.to7 = sh2.Range("e125").Text
Me.to8 = sh2.Range("e126").Text
Me.cp1 = sh2.Range("f119").Text
Me.cp2 = sh2.Range("f120").Text
Me.cp3 = sh2.Range("f121").Text
Me.cp4 = sh2.Range("f122").Text
Me.cp5 = sh2.Range("f123").Text
Me.cp6 = sh2.Range("f124").Text
Me.cp7 = sh2.Range("f125").Text
Me.cp8 = sh2.Range("f126").Text
MsgBox " Input the following data in FIEPI!"
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Me.fr1 = sh2.Range("c225").Text
Me.fr2 = sh2.Range("c226").Text
Me.fr3 = sh2.Range("c227").Text
Me.fr4 = sh2.Range("c228").Text
Me.fr5 = sh2.Range("c229").Text
Me.fr6 = sh2.Range("c230").Text
Me.fr7 = sh2.Range("c231").Text
Me.fr8 = sh2.Range("c232").Text
Me.Ti1 = sh2.Range("d225").Text
Me.Ti2 = sh2.Range("d226").Text
Me.Ti3 = sh2.Range("d227").Text
Me.Ti4 = sh2.Range("d228").Text
Me.ti5 = sh2.Range("d229").Text
Me.ti6 = sh2.Range("d230").Text
Me.ti7 = sh2.Range("d231").Text
Me.ti8 = sh2.Range("d232").Text
Me.To1 = sh2.Range("e225").Text
Me.To2 = sh2.Range("e226").Text
Me.To3 = sh2.Range("e227").Text
Me.To4 = sh2.Range("e228").Text
Me.to5 = sh2.Range("e229").Text
Me.to6 = sh2.Range("e230").Text
Me.to7 = sh2.Range("e231").Text
Me.to8 = sh2.Range("e232").Text
Me.cp1 = sh2.Range("f225").Text
Me.cp2 = sh2.Range("f226").Text
Me.cp3 = sh2.Range("f227").Text
Me.cp4 = sh2.Range("f228").Text
Me.cp5 = sh2.Range("f229").Text
Me.cp6 = sh2.Range("f230").Text
Me.cp7 = sh2.Range("f231").Text
Me.cp8 = sh2.Range("f232").Text
MsgBox " Input the following data in FIEPI!"
Else
Me.fr1 = sh2.Range("c172").Text
Me.fr2 = sh2.Range("c173").Text
Me.fr3 = sh2.Range("c174").Text
```

```
Me.fr4 = sh2.Range("c175").Text
Me.fr5 = sh2.Range("c176").Text
Me.fr6 = sh2.Range("c177").Text
Me.fr7 = sh2.Range("c178").Text
Me.fr8 = sh2.Range("c179").Text
Me.Ti1 = sh2.Range("d172").Text
Me.Ti2 = sh2.Range("d173").Text
Me.Ti3 = sh2.Range("d174").Text
Me.Ti4 = sh2.Range("d175").Text
Me.ti5 = sh2.Range("d176").Text
Me.ti6 = sh2.Range("d177").Text
Me.ti7 = sh2.Range("d178").Text
Me.ti8 = sh2.Range("d179").Text
Me.To1 = sh2.Range("e172").Text
Me.To2 = sh2.Range("e173").Text
Me.To3 = sh2.Range("e174").Text
Me.To4 = sh2.Range("e175").Text
Me.to5 = sh2.Range("e176").Text
Me.to6 = sh2.Range("e177").Text
Me.to7 = sh2.Range("e178").Text
Me.to8 = sh2.Range("e179").Text
Me.cp1 = sh2.Range("f172").Text
Me.cp2 = sh2.Range("f173").Text
Me.cp3 = sh2.Range("f174").Text
Me.cp4 = sh2.Range("f175").Text
Me.cp5 = sh2.Range("f176").Text
Me.cp6 = sh2.Range("f177").Text
Me.cp7 = sh2.Range("f178").Text
Me.cp8 = sh2.Range("f179").Text
MsgBox " Input the following data in FIEPI!"
End If
End If
Else
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Me.fr1 = sh2.Range("c276").Text
Me.fr2 = sh2.Range("c277").Text
Me.fr3 = sh2.Range("c278").Text
Me.fr4 = sh2.Range("c279").Text
Me.fr5 = sh2.Range("c280").Text
Me.fr6 = sh2.Range("c281").Text
Me.fr7 = sh2.Range("c282").Text
Me.fr8 = sh2.Range("c283").Text
Me.Ti1 = sh2.Range("d276").Text
Me.Ti2 = sh2.Range("d277").Text
Me.Ti3 = sh2.Range("d278").Text
Me.Ti4 = sh2.Range("d279").Text
Me.ti5 = sh2.Range("d280").Text
Me.ti6 = sh2.Range("d281").Text
Me.ti7 = sh2.Range("d282").Text
Me.ti8 = sh2.Range("d283").Text
Me.To1 = sh2.Range("e276").Text
Me.To2 = sh2.Range("e277").Text
Me.To3 = sh2.Range("e278").Text
Me.To4 = sh2.Range("e279").Text
Me.to5 = sh2.Range("e280").Text
Me.to6 = sh2.Range("e281").Text
Me.to7 = sh2.Range("e282").Text
Me.to8 = sh2.Range("e283").Text
```

```vba
Me.cp1 = sh2.Range("f276").Text
Me.cp2 = sh2.Range("f277").Text
Me.cp3 = sh2.Range("f278").Text
Me.cp4 = sh2.Range("f279").Text
Me.cp5 = sh2.Range("f280").Text
Me.cp6 = sh2.Range("f281").Text
Me.cp7 = sh2.Range("f282").Text
Me.cp8 = sh2.Range("f283").Text
MsgBox " Input the following data in FIEPI!"
Else
MsgBox " Input the data also in Aquomin!"
Me.fr1 = sh2.Range("c329").Text
Me.fr2 = sh2.Range("c330").Text
Me.fr3 = sh2.Range("c331").Text
Me.fr4 = sh2.Range("c332").Text
Me.fr5 = sh2.Range("c333").Text
Me.fr6 = sh2.Range("c334").Text
Me.fr7 = sh2.Range("c335").Text
Me.fr8 = sh2.Range("c336").Text
Me.Ti1 = sh2.Range("d329").Text
Me.Ti2 = sh2.Range("d330").Text
Me.Ti3 = sh2.Range("d331").Text
Me.Ti4 = sh2.Range("d332").Text
Me.ti5 = sh2.Range("d333").Text
Me.ti6 = sh2.Range("d334").Text
Me.ti7 = sh2.Range("d335").Text
Me.ti8 = sh2.Range("d336").Text
Me.To1 = sh2.Range("e329").Text
Me.To2 = sh2.Range("e330").Text
Me.To3 = sh2.Range("e331").Text
Me.To4 = sh2.Range("e332").Text
Me.to5 = sh2.Range("e333").Text
Me.to6 = sh2.Range("e334").Text
Me.to7 = sh2.Range("e335").Text
Me.to8 = sh2.Range("e335").Text
Me.cp1 = sh2.Range("f329").Text
Me.cp2 = sh2.Range("f330").Text
Me.cp3 = sh2.Range("f331").Text
Me.cp4 = sh2.Range("f332").Text
Me.cp5 = sh2.Range("f333").Text
Me.cp6 = sh2.Range("f334").Text
Me.cp7 = sh2.Range("f335").Text
Me.cp8 = sh2.Range("f336").Text
MsgBox " Input the following data in FIEPI!"
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Input the data also in Aquomin!"
Me.fr1 = sh2.Range("c382").Text
Me.fr2 = sh2.Range("c383").Text
Me.fr3 = sh2.Range("c384").Text
Me.fr4 = sh2.Range("c385").Text
Me.fr5 = sh2.Range("c386").Text
Me.fr6 = sh2.Range("c387").Text
Me.fr7 = sh2.Range("c388").Text
Me.fr8 = sh2.Range("c389").Text
Me.Ti1 = sh2.Range("d382").Text
Me.Ti2 = sh2.Range("d383").Text
Me.Ti3 = sh2.Range("d384").Text
```

```vba
        Me.Ti4 = sh2.Range("d385").Text
        Me.ti5 = sh2.Range("d386").Text
        Me.ti6 = sh2.Range("d387").Text
        Me.ti7 = sh2.Range("d388").Text
        Me.ti8 = sh2.Range("d389").Text
        Me.To1 = sh2.Range("e382").Text
        Me.To2 = sh2.Range("e383").Text
        Me.To3 = sh2.Range("e384").Text
        Me.To4 = sh2.Range("e385").Text
        Me.to5 = sh2.Range("e386").Text
        Me.to6 = sh2.Range("e387").Text
        Me.to7 = sh2.Range("e388").Text
        Me.to8 = sh2.Range("e389").Text
        Me.cp1 = sh2.Range("f382").Text
        Me.cp2 = sh2.Range("f383").Text
        Me.cp3 = sh2.Range("f384").Text
        Me.cp4 = sh2.Range("f385").Text
        Me.cp5 = sh2.Range("f386").Text
        Me.cp6 = sh2.Range("f387").Text
        Me.cp7 = sh2.Range("f388").Text
        Me.cp8 = sh2.Range("f389").Text
        MsgBox " Input the following data in FIEPI!"
        Else
        Me.fr1 = sh2.Range("c69").Text
        Me.fr2 = sh2.Range("c70").Text
        Me.fr3 = sh2.Range("c71").Text
        Me.fr4 = sh2.Range("c72").Text
        Me.fr5 = sh2.Range("c73").Text
        Me.fr6 = sh2.Range("c74").Text
        Me.fr7 = sh2.Range("c75").Text
        Me.fr8 = sh2.Range("c76").Text
        Me.Ti1 = sh2.Range("d69").Text
        Me.Ti2 = sh2.Range("d70").Text
        Me.Ti3 = sh2.Range("d71").Text
        Me.Ti4 = sh2.Range("d72").Text
        Me.ti5 = sh2.Range("d73").Text
        Me.ti6 = sh2.Range("d74").Text
        Me.ti7 = sh2.Range("d75").Text
        Me.ti8 = sh2.Range("d76").Text
        Me.To1 = sh2.Range("e69").Text
        Me.To2 = sh2.Range("e70").Text
        Me.To3 = sh2.Range("e71").Text
        Me.To4 = sh2.Range("e72").Text
        Me.to5 = sh2.Range("e73").Text
        Me.to6 = sh2.Range("e74").Text
        Me.to7 = sh2.Range("e75").Text
        Me.to8 = sh2.Range("e76").Text
        Me.cp1 = sh2.Range("f69").Text
        Me.cp2 = sh2.Range("f70").Text
        Me.cp3 = sh2.Range("f71").Text
        Me.cp4 = sh2.Range("f72").Text
        Me.cp5 = sh2.Range("f73").Text
        Me.cp6 = sh2.Range("f74").Text
        Me.cp7 = sh2.Range("f75").Text
        Me.cp8 = sh2.Range("f76").Text
        MsgBox " Input the following data in FIEPI!"
        End If
        End If
        End If
```

```
End Sub
```

Userform 11

This userform represent the mass exchange network in which the user is required to insert the water consumption data obtained without the mass integration approach.

```
Private Sub cmdcancel2_Click()
UserForm11.Hide
UserForm9.Show
End Sub
Private Sub cmdok2_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("c16").Value = Me.w1.Value
sh2.Range("c17").Value = Me.w2.Value
sh2.Range("c18").Value = Me.w3.Value
sh2.Range("c19").Value = Me.w4.Value
UserForm11.Hide
UserForm10.Show
End Sub
Private Sub Image1_Click()
End Sub
Private Sub UserForm_Click()
End Sub
```

Userform 12

Userform 12 represents the utilities consumption input box, in which the user have to input the values of hot utility consumptions with energy integration approach and cold utility consumptions with energy integration approach obtained by FI^{2}EPI.

```
Private Sub cmdcancel2_Click()
UserForm12.Hide
UserForm9.Show
End Sub
Private Sub cmdok2_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
If sh2.Range("E3").Value = sh2.Range("E4").Value Then
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Error, the concentrations output cannot be all equals!"
Else
sh2.Range("c129").Value = Me.hu1.Value
sh2.Range("c130").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
End If
Else
```

```
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
sh2.Range("c235").Value = Me.hu1.Value
sh2.Range("c236").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
Else
sh2.Range("c182").Value = Me.hu1.Value
sh2.Range("c183").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
End If
End If
Else
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
sh2.Range("c286").Value = Me.hu1.Value
sh2.Range("c287").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
Else
sh2.Range("c339").Value = Me.hu1.Value
sh2.Range("c340").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
sh2.Range("c392").Value = Me.hu1.Value
sh2.Range("c393").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
Else
sh2.Range("c79").Value = Me.hu1.Value
sh2.Range("c80").Value = Me.cu1.Value
UserForm12.Hide
MsgBox "Final Results!"
UserForm13.Show
End If
End If
End If
End Sub
Private Sub UserForm_Initialize()
MsgBox "Input in the following box the values of hot and cold utilities after the
energy integration performed by FIEPI!"
End Sub
```

Userform 13

Userform 13 represents the final results box with the values of water and utilities consumption and the percentile of reduction of the consumptions, obtained thanks to the mass and energy integration.

```
Private Sub cmdcancel1_Click()
```

```vba
UserForm13.Hide
ThisWorkbook.Close savechanges:=True
End Sub
Private Sub cmdok1_Click()
ThisWorkbook.Close savechanges:=True
End Sub
Private Sub CommandButton1_Click()
Dim sfName As String
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
If sh2.Range("E3").Value = sh2.Range("E4").Value Then
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Error, the concentrations output cannot be all equals!"
Else
sh2.Activate
Range("h128:h130").Value = Range("c20:c22").Value
Range("i128:l130").Value = Range("b128:e130").Value
Range("g128:l130").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
sh2.Activate
Range("h234:h236").Value = Range("c20:c22").Value
Range("i234:l236").Value = Range("b234:e236").Value
Range("g234:l236").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
```

```
Application.Visible = False
Else
sh2.Activate
Range("h181:h183").Value = Range("c20:c22").Value
Range("i181:l183").Value = Range("b181:e183").Value
Range("g181:l183").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
End If
Else
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
sh2.Activate
Range("h285:h287").Value = Range("c20:c22").Value
Range("i285:l287").Value = Range("b285:e287").Value
Range("g285:l287").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
Else
sh2.Activate
Range("h338:h340").Value = Range("c20:c22").Value
Range("i338:l340").Value = Range("b338:e340").Value
Range("g338:l340").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
```

```
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
sh2.Activate
Range("h391:h394").Value = Range("c20:c22").Value
Range("i391:l394").Value = Range("b391:e394").Value
Range("g391:l394").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
Else
sh2.Activate
Range("h78:h80").Value = Range("c20:c22").Value
Range("i78:l80").Value = Range("b78:e80").Value
Range("g78:l80").Select
Selection.Copy
Workbooks.Add
ActiveSheet.Paste
ActiveSheet.Columns("A:f").AutoFit
Application.DisplayAlerts = False
Application.DisplayAlerts = True
sfName = Application.GetSaveAsFilename("Results", "Excel files (*.xls), *.xls")
If sfName <> "False" Then
ActiveWorkbook.SaveAs sfName
ActiveWorkbook.Close savechanges:=False
Else
MsgBox "You pressed Cancel!"
Exit Sub
End If
sh1.Activate
Application.Visible = False
End If
End If
End If
End Sub
Private Sub UserForm_Initialize()
Dim sh1 As Worksheet
```

```
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
If sh2.Range("E3").Value = sh2.Range("E4").Value Then
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
MsgBox " Error, the concentrations output cannot be all equals!"
Else
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c128").Text
Me.rw = sh2.Range("e128").Text
Me.h = sh2.Range("c129").Text
Me.rh = sh2.Range("e129").Text
Me.c = sh2.Range("c130").Text
Me.rc = sh2.Range("e130").Text
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c234").Text
Me.rw = sh2.Range("e234").Text
Me.h = sh2.Range("c235").Text
Me.rh = sh2.Range("e235").Text
Me.c = sh2.Range("c236").Text
Me.rc = sh2.Range("e236").Text
Else
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c181").Text
Me.rw = sh2.Range("e181").Text
Me.h = sh2.Range("c182").Text
Me.rh = sh2.Range("e182").Text
Me.c = sh2.Range("c183").Text
Me.rc = sh2.Range("e183").Text
End If
End If
Else
If sh2.Range("E4").Value = sh2.Range("E5").Value Then
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c285").Text
Me.rw = sh2.Range("e285").Text
Me.h = sh2.Range("c286").Text
Me.rh = sh2.Range("e286").Text
Me.c = sh2.Range("c287").Text
Me.rc = sh2.Range("e287").Text
Else
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c338").Text
Me.rw = sh2.Range("e338").Text
```

```
Me.h = sh2.Range("c339").Text
Me.rh = sh2.Range("e339").Text
Me.c = sh2.Range("c340").Text
Me.rc = sh2.Range("e340").Text
End If
Else
If sh2.Range("E5").Value = sh2.Range("E6").Value Then
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c391").Text
Me.rw = sh2.Range("e391").Text
Me.h = sh2.Range("c392").Text
Me.rh = sh2.Range("e392").Text
Me.c = sh2.Range("c393").Text
Me.rc = sh2.Range("e393").Text
Else
Me.iw = sh2.Range("c20").Text
Me.ih = sh2.Range("c21").Text
Me.ic = sh2.Range("c22").Text
Me.w = sh2.Range("c78").Text
Me.rw = sh2.Range("e78").Text
Me.h = sh2.Range("c79").Text
Me.rh = sh2.Range("e79").Text
Me.c = sh2.Range("c80").Text
Me.rc = sh2.Range("e80").Text
End If
End If
End If
End Sub
```

Userform 14

Userform 14 represents the split ratio input box of the case 2 MEN scenario.

```
Private Sub cmdcancel1_Click()
UserForm14.Hide
UserForm9.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("i91").Value = Me.r14.Value
sh2.Range("i94").Value = Me.r24.Value
sh2.Range("i97").Value = Me.r34.Value
If sh2.Range("b103").Text < 0 Or sh2.Range("b103").Text > 0 Then
MsgBox ("Error,the sum is not correct!")
Else
If sh2.Range("i92").Text < 0 Or sh2.Range("i95").Text < 0 Or sh2.Range("i98").Text
< 0 Then
MsgBox ("Error, maximum available flowrate has been exceeded")
Else
UserForm14.Hide
UserForm11.Show
End If
End If
```

```
End Sub
Private Sub t24_Click()
End Sub
Private Sub UserForm_Initialize()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
Me.tot1 = sh2.Range("b100").Value
Me.t14 = sh2.Range("b91").Value
Me.t24 = sh2.Range("b94").Value
Me.t34 = sh2.Range("b97").Value
End Sub
```

Userform 15

Userform 15 represents the split ratio input box of the case 3 MEN scenario.

```
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("i142").Value = Me.r14.Value
sh2.Range("i146").Value = Me.r24.Value
sh2.Range("i141").Value = Me.r13.Value
sh2.Range("i145").Value = Me.r23.Value
If   sh2.Range("b156").Text   <   0   Or   sh2.Range("b156").Text   >   0   Or
sh2.Range("b157").Text < 0 Or sh2.Range("b157").Text > 0 Then
MsgBox ("Error,the sum is not correct!")
Else
If sh2.Range("i143").Text < 0 Or sh2.Range("i147").Text < 0 Then
MsgBox ("Error, maximum available flowrate has been exceeded")
Else
UserForm15.Hide
UserForm11.Show
End If
End If
End Sub
Private Sub CommandButton2_Click()
UserForm15.Hide
UserForm9.Show
End Sub
Private Sub UserForm_Initialize()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
Me.tot4 = sh2.Range("b152").Value
Me.tot3 = sh2.Range("b149").Value
Me.t14 = sh2.Range("c159").Value
Me.t24 = sh2.Range("c160").Value
Me.t13 = sh2.Range("c159").Value
Me.t23 = sh2.Range("c160").Value
End Sub
```

Userform 16

Userform 16 represents the split ratio input box of the case 4 MEN scenario.

```
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
sh2.Range("i195").Value = Me.r14.Value
sh2.Range("i199").Value = Me.r24.Value
sh2.Range("i194").Value = Me.r13.Value
sh2.Range("i198").Value = Me.r23.Value
If  sh2.Range("b208").Text  <  0  Or  sh2.Range("b208").Text  >  0  Or
sh2.Range("b209").Text < 0 Or sh2.Range("b209").Text > 0 Then
MsgBox ("Error,the sum is not correct!")
Else
If sh2.Range("i196").Text < 0 Or sh2.Range("i200").Text < 0 Then
MsgBox ("Error, maximum available flowrate has been exceeded")
Else
UserForm16.Hide
UserForm11.Show
End If
End If
End Sub
Private Sub CommandButton2_Click()
UserForm16.Hide
UserForm9.Show
End Sub
Private Sub Frame2_Click()
End Sub
Private Sub UserForm_Initialize()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
Me.tot4 = sh2.Range("b205").Value
Me.tot3 = sh2.Range("b202").Value
Me.t14 = sh2.Range("c212").Value
Me.t24 = sh2.Range("c213").Value
Me.t13 = sh2.Range("c212").Value
Me.t23 = sh2.Range("c213").Value
End Sub
```

Userform 17

Userform 17 represents the split ratio input box of the case 6 MEN scenario.

```
Private Sub cmdcancel1_Click()
UserForm17.Hide
UserForm9.Show
End Sub
Private Sub cmdok1_Click()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
```

```
sh2.Range("i303").Value = Me.r24.Value
sh2.Range("i306").Value = Me.r34.Value
If sh2.Range("b313").Text < 0 Or sh2.Range("b313").Text > 0 Then
MsgBox ("Error,the sum is not correct!")
Else
If sh2.Range("i304").Text < 0 Or sh2.Range("i307").Text < 0 Then
MsgBox ("Error, maximum available flowrate has been exceeded")
Else
UserForm17.Hide
UserForm11.Show
End If
End If
End Sub
Private Sub UserForm_Initialize()
Dim sh1 As Worksheet
Dim sh2 As Worksheet
Set sh1 = ActiveWorkbook.Sheets("Interface")
Set sh2 = ActiveWorkbook.Sheets("Example1")
Me.tot1 = sh2.Range("b310").Value
Me.t24 = sh2.Range("c317").Value
Me.t34 = sh2.Range("c318").Value
End Sub
```

Userform 18

Userform 18 represents the software initial window box, with which it is possible to start the program
or edit the software coding/calculations.

```
Private Sub CommandButton1_Click()
UserForm18.Hide
UserForm9.Show
End Sub
Private Sub CommandButton2_Click()
UserForm18.Hide
Application.Visible = True
End Sub
Private Sub Label1_Click()
End Sub
Private Sub UserForm_Click()
End Sub
```

Nomenclature

a	=	correlating parameter (-)
A	=	total area of the heat exchangers (m^2)
b	=	correlating parameter (-)
c	=	correlating parameter (-)
C	=	concentration (ppm)
ΔC	=	concentration difference (ppm)
$C_{i,IN}$	=	maximum concentration of contaminant inlet, acceptable for each operation (ppm)
$C_{i,OUT}$	=	concentration of contaminant outlet for each operation (ppm)
C_P	=	heat capacity (J/kg°C)
C_{WS}	=	external water source concentration (ppm)
F	=	flowrate, based on AquoMin nomenclature (t/h, kg/s)
F_{min}	=	external water source flowrate (t/h)
G	=	flowrate of waste (rich) stream (units depends on application)
HC	=	heat exchanged from cold streams (kW)
HCC	=	cold utility consumptions with energy integration approach (kW)
HH	=	heat exchanged from hot streams (kW)
HHC	=	hot utility consumptions with energy integration approach (kW)
i	=	interest rate (-)
L	=	flowrate of lean stream (units depends on application)
L_c	=	flowrate of lean stream available on the plant (units depends on application)
M	=	flowrate, based on FI^{2}EPI nomenclature (t/h, kg/s)
Δm_c	=	Mass of contaminant (g/h, g/s)
MR	=	mass of pollutant lost by the rich stream (units depends on application)
MS	=	mass of pollutant gained by the lean stream (units depends on application)
m_w	=	limiting water flowrate (t/h)
n	=	payback time (y)
N_{IN}	=	Intervals number
N_{OP}	=	number of operations (-)
N_R	=	total number of rich streams (-)
N_S	=	total number of lean streams (-)

N_{SE}	=	number of external lean streams (-)
N_{SP}	=	number of process lean streams (-)
r	=	residual (-)
t	=	generic cold temperature (°C, K)
T	=	temperature (°C, K)
ΔT_{min}	=	minimum temperature difference (°C, K)
$T_{i,IN}$	=	temperature required for each inlet stream (°C, K)
$T_{i,OUT}$	=	temperature of each outlet stream (°C, K)
T_{WD}	=	temperature of the water discharge (°C, K)
T_{WS}	=	temperature of the water source (°C, K)
W_W	=	water consumptions with water-reutilization approach (t/h, kg/s)
W_{WO}	=	water consumptions without water-reutilization approach (t/h, kg/s)
x	=	lean stream composition (-)
y	=	rich stream composition (-)

<u>Acronyms</u>

AFI	=	AquoMin FI^{2}EPI interface
CIT	=	composition interval table
CRF	=	capital recovery factor
CWRT	=	center for waste reduction technologies
EWS	=	external water source
FI^{2}EPI	=	ferramenta informática para a integração energética de processos industriais
HE	=	heat exchanger
HEN	=	heat exchangers network
HENS	=	heat exchangers network synthesis
IST	=	instituto superior técnico
LCC	=	limiting composite curve
MEN	=	mass exchange network
MENS	=	mass exchange network synthesis
MER	=	minimal energy requirement
MPT	=	mass problem table
MSAs	=	mass separating agents
FIA	=	first integration attempt
VBA	=	visual basic
WSD	=	water sources diagram

Subscripts

c	=	cold stream
h	=	hot stream
i	=	stream number, or
		operation number, or
		interval number
j	=	stream number, or
		operation number, or
		interval number
max	=	maximum
nec	=	necessary
usd	=	used
z	=	temperature interval

Superscripts

in	=	inlet
out	=	outlet
s	=	supply
t	=	target
tot	=	total

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