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DESIGN OF WATER AND ENERGY NETWORKS USING TEMPERATURE-CONCENTRATION DIAGRAMS

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Abstract.

The reduction of energy and water demand is a critical issue in various industrial sectors like the pulp and paper industry. This objective may be achieved through properly designed heat and mass transfer networks.

This work introduces a new methodology for the synthesis of these systems.

The procedure here presented is specifically conceived for networks with two distinct sections: the simultaneous heat and mass transfer sub-network, which main goal is the removal of pollutants from processes and the heat exchange sub-networks (direct and indirect), which main goal is the thermal management of the water flows and the heat recovery. To keep the two sections separate, water reuse in the simultaneous heat and mass transfer network is operated by allowing non-isothermal mixing between the streams. These irreversibilities produce a negative impact on the primary energy savings, which is discussed, but have some advantages in terms of operation, design simplicity and in retrofit applications.

Keywords: *Process integration; Combined Heat and Mass Transfer, Thermal Pinch, Water Pinch*

1. INTRODUCTION

The methodologies that have been developed to date for the combined minimization of water and energy are based on Pinch analysis techniques. Since its popularization in the 1980's [1], Pinch Technology has been applied to achieve primary energy savings in different types of energy intensive industries. In the work of Linnhoff et al. [1], examples are given of the implementation of the methodology to different industries where energy savings in the order of 12% were obtained. In a newer edition, Kemp [2] presents other examples of the implementation of the methodology to other cases, such as the oil industry [3], organic chemicals manufacturing site [4], and applications in hospitals [5]. The percentage of savings in each type of industry depends on several factors such as the type of process, the available technology and the amount of investment, etc. In these cases, the amount of savings reported is around 25% [6].

The application of Pinch Analysis concepts to the case of water minimization has given rise to the Water Pinch methods. In this approach, the minimum flow of fresh water that a process requires given the amount of mass to be withdrawn within the minimum and maximum required concentrations is found [7-9]. Wang and Smith [7] presented a technique to minimize the consumption of water in industrial processes. This technique is based on graphical methods where concentrations of single contaminants versus flow rate profiles are produced. Olesen and Polley [8] noted that the methodology developed by Wang and Smith [7] for the design of water networks could be simplified and proposed a simpler methodology for single contaminant cases. The main feature of this work is that it treats inlet and outlet concentration limits as flexible variables, retaining

only as a fixed variable the amount of mass (contaminant) to be removed. However, the problem that is not discussed is the impact that different concentrations would have on the equipment dimensions.

Various recent researches on the subject are focused on simultaneous energy and water minimization design using heuristic rules [10,11] and optimization using mathematical programming [12,13]. Such approach is useful for the reduction of natural resources in energy and water intensive industries, as the pulp and paper industry, metallurgical industry, food industry, chemical industry, etc.

A water and energy network exhibits features that makes them different from ordinary heat recovery networks, namely: a) water represents the main component of the streams, b) water streams can mix c) the total mass flow rate of the inlet streams equals the mass flow rate of the outlet streams, and d) in the case of isothermal processes, the variation in the enthalpy flow associated with the cold streams (to be heated up) is very close to or even equal to the enthalpy change associated to the hot streams (to be cooled down) leaving the processes. A simplified representation of the interaction between water and energy stream temperature is shown in Figure 1. The features indicated above make it possible to build a system with minimum fresh water requirement and minimum energy demand. The minimum fresh water requirement, m_F , is obtained from water pinch analysis. Once this quantity is obtained, the energy demand Q (heating demand and cooling demand) determined as:

$$Q = m_F \cdot c \cdot \Delta T_{\min} \quad (1)$$

where c is the specific heat and ΔT_{\min} is the allowed minimum temperature difference between hot and cold streams, i.e. the temperature difference at the pinch [14]. To reach this target, it is necessary to keep the minimum temperature difference in all the sections of the heat exchangers and to avoid non-isothermal mixing. This means that when two or more streams enter a process, they must reach the process temperature, which is possible by installing heat exchangers throughout the processes. In this paper, the analysis is focused on networks where the two goals, i.e. temperatures and concentrations, are controlled in two separate sections: temperatures are controlled in the heat transfer sub-network (direct and indirect) while concentrations are controlled in the simultaneous heat and mass transfer sub-network. The consequence of this choice is that non-isothermal mixing is allowed in the simultaneous heat and mass transfer sub-network, as there are not heat exchangers in this section. This brings the disadvantage of increased primary energy demand. As discussed in the following section, the main advantages consist in a larger flexibility in the operation and the

possibility to implement the proposed procedure into existing systems without major changes to the process layout.

2. SIMULTANEOUS HEAT AND MASS TRANSFER SYSTEM.

The system is composed by three sub networks, as observed by Bagajewicz et al. [15] and Sorin M. et al.[16]:

1) Simultaneous Heat and Mass Transfer Network. This is the sub-network where water streams are distributed to the various operations to remove contaminants. The water streams are properly mixed so that used water exiting some of the operations is reused in these operations that not necessarily require fresh water. The network design is performed in order to provide the required mass flow rate and concentration to the various processes. As the use of heat exchangers is intentionally avoided in this section, direct heat transfer due to non-isothermal mixing is necessary to reach the target temperatures for the streams entering the processes.

2) Direct Heat Exchange Network. This is a sub-network of water streams where the streams exiting the processes are properly mixed together to achieve the required temperatures and flow rates to enter the following sub-network.

3) Indirect Heat Exchange Network. This is a sub-network where the enthalpy flow of the streams exiting the processes is recovered to heat fresh water streams through heat exchangers and where the necessary external heating and cooling loads are supplied to the fresh water and effluent water respectively.

The way these sub-networks are linked is shown in Figure 2. In the diagram, j streams leave the indirect heat transfer network toward the simultaneous heat and mass transfer network; at the outlet of this section, k streams combine to produce the i number of streams required for indirect heat transfer in the HEN. In Figure 2, the number of streams entering and exiting the Indirect Heat Exchange Network (i and j) are equal.

One of the advantages of this scheme is that it can be easily applied to the retrofit of existing plants where no heat recovery is involved.

3. CONSTRUCTION OF THE TEMPERATURE VS CONCENTRATION DIAGRAM.

The objective in the design of energy and water networks is to find the structure that minimizes the total costs so that the elimination of a given contaminant is achieved within the specified process constraints. Such

process constraints are: maximum inlet concentration, mass of contaminant to be removed and operating temperature. If the operating temperature is uniform throughout the process, the solution to the problem gives the interconnection of fresh water streams and used water (which has been used to remove contaminants in other operations), so as to meet the maximum acceptable concentration of contaminant at the inlet of downstream operations. When the inlet target temperature is different for each operation, a new variable comes into play and the problem is described as the design of simultaneous heat and mass transfer system. In the proposed approach, the design of such systems starts with the Simultaneous Heat and Mass Transfer Network. The required process data include: specification of the various water consuming operations, inlet temperatures, mass load of contaminant to be removed, minimum and maximum concentrations permitted on the water streams, allowable discharge temperature and fresh water inlet temperature. With this information, the minimum fresh water consumption considering water reuse is determined [7].

The next step consists in the determination of the distribution of fresh water and the flow interconnections within the process for maximum water reuse, for minimum external energy consumption and minimum number of heat exchangers. The solution to this problem is highly combinatorial since each of the water using operations that make up the whole process will have its own operating temperature and maximum permitted concentration. The complexity of the problem can be reduced by means of a heuristic approach, such as the one introduced in this work, which is described below using a Temperature vs. Concentration diagram.

The Temperature vs Concentration diagram contains the following information: Number of water using operations, temperature of the operation, maximum permitted inlet water concentration, mass load of contaminant to be removed. This information is used to select the processes to feed with freshwater. Mass and energy balances are then used to complete the design.

In Figure 3a, the solid line represents the range over which the water concentration varies as the contaminant is removed from an inlet concentration ($C_{lim,in,i}$) to an outlet concentration ($C_{lim,out,i}$) at a constant temperature (T_i). In the diagram $C_{lim,in,i}$ represents the maximum inlet concentration permitted for the mass removal operation to take place. A significant feature is that water could be fed to such an operation even from a zero concentration as shown by the dotted line in Figure 3a. Operations are ordered according to the temperature they operate at and are numbered accordingly. The operations that require fresh water by specification are

positioned in the diagram at the corresponding temperature and start from the point at zero concentration as shown in Figure 3b.

There is a number of feasible solutions to achieve the temperature and concentration of downstream operations; each possible combination of water streams corresponds to a certain energy consumption. Figure 3c illustrates how the flow rate, temperature and concentration requirements of operation 2 are met by a combination of effluents from operations 1 and n .

For the establishment of the water flow rates and the interconnection between operations with minimum energy requirement the following guidelines are considered:

1. Supply fresh water to those operations that requires it, i.e. operations characterized by maximum inlet concentration equal to zero.
2. Meet the fresh water requirements of the two operations that need the highest and lowest temperatures.
3. Satisfy process requirements in terms of temperature, first, and then concentration. Used but less concentrated water from upstream processes should be used primarily and fresh water only when necessary.

3.1 Network structure for direct and indirect heat transfer

The difference between the fresh water entry temperature and the water discharge temperature represents the minimum temperature approach for the network design. So once its value is specified, the composite curve corresponding to the streams entering and exiting the simultaneous heat and mass transfer sub-network (cold and hot streams, respectively) can be constructed; this allows the calculation of the minimum heating and cooling load for the system. Once this target is obtained, the heat recovery network can be designed. This network is generally composed of direct and indirect heat transfer sub-networks. Direct heat transfer takes place during the mixing of water streams at different temperature, as already examined in the previous section. Non isothermal mixing has a detrimental effect upon the heat recovery network as it provokes additional irreversibilities that could be avoided by installing heat exchangers [14]. However, the positive side of non isothermal mixing is that it allows to reduce the number of heat exchanger without affecting the external load.

The way the number of heat exchangers is reduced to a minimum can be explained by analyzing the changes that direct heat transfer produces in the shape of the composite curves. For instance, if mixing is carried out on the hot side of the composite curve [16] the result is that temperature driving forces reduce; however, since

the profile of the new composite curve becomes practically parallel to the shape of the cold composite curve, the number of heat exchangers is equal to the number of sections on the composite curves as given by the number of slope changes plus one. In fact, on the cold side, the first heat exchanger must be sized to heat up the entire fresh water mass flow rate from the inlet temperature to the target temperature of the coldest process. After this point, the mass flow rate required by the first process is extracted. The remaining mass flow rate is heated up to the temperature of the next process and so on. The last heat exchanger is the one supplying the external heat requirement.

On the hot side, the streams exiting the simultaneous heat and mass transfer sub-network can be mixed so that each heat exchanger is fed with the same mass flow rate as the one flowing on the cold side and an inlet temperature equal to the outlet temperature of the cold fluid plus the minimum temperature difference. On the last heat exchanger all the streams that have not yet been used are mixed together with the main stream. The resulting temperature is generally higher than the minimum value (i.e. the temperature of the cold stream exiting the heat exchanger plus the minimum temperature difference) because of the irreversibilities in the simultaneous heat and mass transfer sub-network.

4. APPLICATION OF THE METHODOLOGY

In this section, the methodology is applied to a case study proposed by Wang and Smith [7]. The resulting system is then discussed and compared with a fully integrated system, i.e. a system where non-isothermal mixing is avoided.

The process operating data are presented in Table 1. The various mass removal operations are listed in relation to their temperature; other information includes: mass load of contaminant to be removed, maximum permitted inlet concentration and outlet concentration of the water streams, and the limiting water flow rate required to remove the specified amount of contaminant. Fresh water is available at 20 °C and it is assumed that the maximum permitted effluent discharge temperature is 30 °C. The Water Pinch technique is applied to the data of Table 1 in order to determine the minimum fresh water supply considering water reuse. The results are shown in Figure 4 where the minimum fresh water consumption is 90 kg/s.

Figure 5 shows a Temperature vs Concentration diagram where the four mass removal operations are depicted. This diagram also indicates the various opportunities for water stream combinations that can be used as feed of downstream operations. For instance, the combination of effluents from operations 1 and 4 can

meet the requirements of operations 2 and 3. The next step consists in the distribution of the fresh water. In this case, the operations requiring pure water will be favored; then any fresh water left will be distributed amongst the other operations. Figure 6 presents the Temperature vs Concentration diagram for case 1 and shows the various options for supplying operations 2 and 3. The first choice is to check whether a combination of stream fractions from operations 2 and 4 is able to meet the requirements of operation 3. For the case of operation 3, this would avoid destruction of temperature driving forces since they are available at a temperature immediately above and below the required by operation 3. Should the combination of streams from operation 2 and 4 not be enough to meet the demand of operation 3, a fraction from operation 1 must be considered. The solution to the problem is found by solving the mass and energy balance equations from where it can be seen that the effluent from operations 2 and 4 meet the demand of operation 3. Figure 7 shows the final mass flow rate distribution, the network structure and the effluent streams to be discharged.

The next step consists in the definition of the heat exchanger network for indirect heat transfer. To this end the composite curves are used (Figure 8). Table 2 contains the information regarding flow rates and temperatures for the construction of these curves. The cold composite curve is taken from the f_{FW} data and the hot composite curve uses the f_R flow rates. The various fresh water fractions must be heated from 20 °C to the temperature required at each operation, while the effluent discharges will have to be cooled to 30°C. The external heating and cooling load for a $\Delta T_{min} = 10$ °C are 4165 kW and 385 kW respectively. Thus, three exchangers and a heater are needed as shown in Figure 9.

As mentioned earlier, direct heat transfer takes place amongst the hot effluent streams; they are mixed in order to produce the number of streams for minimum number of exchangers in the heat transfer network shown in Figure 10 where the hot streams: $f_{R,1}$, $f_{R,2}$, $f_{R,3}$ y $f_{R,4}$ are combined to generate the streams: $f_{FR,1}$, $f_{FR,2}$ y $f_{FR,3}$ at the required temperatures. These combinations are generated by means of simple energy and mass balances.

With each of the different sub-network structures being designed, the final step consists in linking them into a single overall structure. This is shown in Figure 11; the total fresh water consumption is 90 kg/s, the external heating load is 4165 kW, the external cooling required is 385 kW and a total of 3 heat exchangers are needed. Table 3 shows a comparison between the designs obtained using other approach presented in the literature

(scenario A. [11]) and the design approach introduced in this work (scenario B) where it can be appreciated that the proposed approach (scenario B) requires less energy.

5. DISCUSSION

It has been already mentioned that it is possible to minimize the external heating load by avoiding non-isothermal mixing in the simultaneous heat and mass transfer sub-network. A possible system is presented in Figure 12.

The heat load of this system is 3777 kW, which is about 10% less than the system proposed in this paper. Such advantage reduces if the minimum temperature difference increases, as shown in Figure 13. In addition, in the case of the proposed system the heat load may be reduced by increasing the fresh water mass flow rate up to about 96.9 kg/s; beyond this value the heat load increases, as shown in Figure 14.

Another difference between the two systems is related with the effects of possible water losses. In the case of isothermal mixing, if a loss occurs in a process, the system is not able to fulfil the energy balances unless an additional heater is installed upstream the operation 4. In Figure 12, this heater is indicated as H3. Similar consideration may be drawn in the case of the other designs proposed in [14]. In the case of a system with non-isothermal mixing, it is possible to overcome losses in the process just by adjusting the mass flow rates to the various heat exchangers and by supplying a different heat load to the heater and to the cooler. Table 4 shows the various mass flow rates and temperatures in four scenarios corresponding with losses in each of the processes in the case of isothermal mixing, while Table 5 shows the data in the case of non-isothermal mixing. If a leak of 2 kg/s is considered in process 1, the heat load increases to 4365 kW for both isothermal and non-isothermal mixing. Similar result is obtained for a leak in process 2; in this case the heat load becomes 4161 kW. In the case of a leak in process 3 or 4, the heat load for non-isothermal mixing becomes lower than with isothermal mixing: 2695 kW instead of 3946 kW.

5. CONCLUSIONS

A tool for the design of water and energy networks is presented in this paper. This tool provides a simple means to design systems where the section for achieving the concentration targets in the processes is independent of the section devoted to heat recovery and heating/cooling supply. Such system is obtained by allowing non-isothermal mixing. Although non iso-thermal mixing reduces the available temperature driving

forces for heat transfer; it has the advantage of reducing the number of heat exchangers for heat recovery at the expense of increased surface area requirements. From the operational point of view, iso-thermal mixing might prove to show higher flexibility specially in cases of unexpected water losses. Work in this direction is undergoing.

6. NOMENCLATURE

C	Concentration	[ppm]
$C_{\text{lim, in}}$	Limiting inlet concentration,	[ppm]
$C_{\text{lim, out}}$	Limiting outlet concentration	[ppm]
CP	Heat capacity mass flowrate	[kW/°C]
C_p	Heat capacity	[kJ/kg°C]
ΔT_{min}	Minimum temperature approach	[°C]
f	Water flowrate	[kg/s]
$f_{WF, i}$	Fresh water flowrate to the ith operation	[kg/s]
$f_{FR, i}$	Wastewater flowrate from the ith operation	[kg/s]
$f_{R, i}$	Wastewater flowrate for heat recovery	[kg/s]
h	Enthalpy	[kW]
m	Mass load	[g/s]
Q_{cold}	Cold utility	[kW]
Q_{hot}	Hot utility	[kW]
T	Temperature	[°C]
T_{in}	Temperature of freshwater	[°C]
T_{out}	Discharge temperature of wastewater	[°C]

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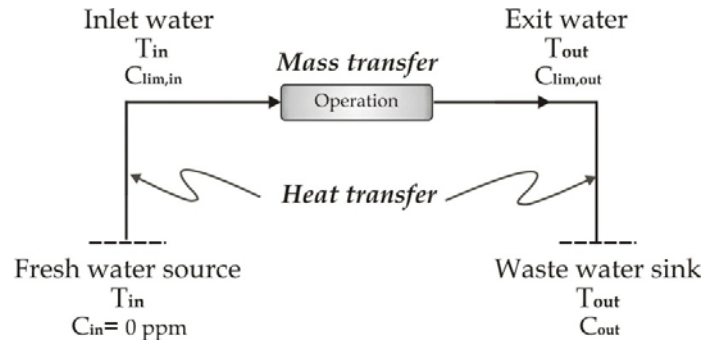


Figure 1. Mass transfer and heat transfer for operation.

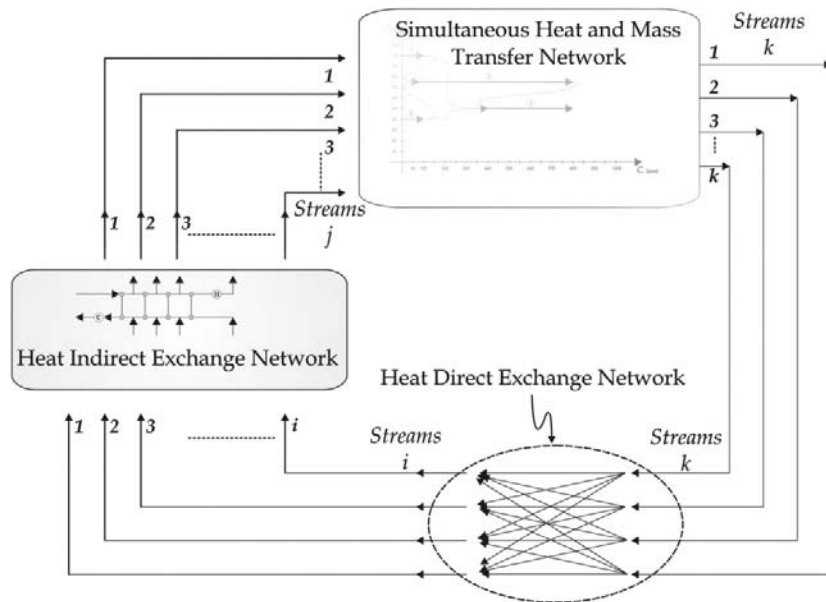


Figure 2. Simultaneous heat and mass transfer system.

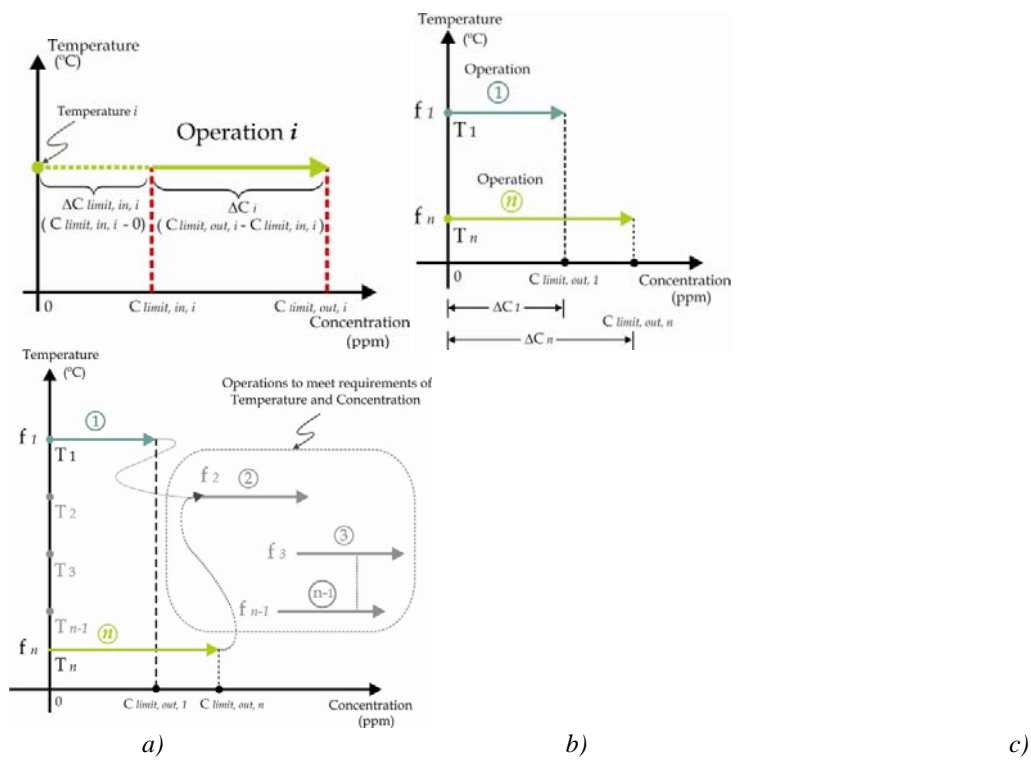


Figure 3. *a)* Temperature vs Concentration diagram for operation *i*. *b)* Representation of operations that require fresh water. *c)* Stream combinations to meet the temperature and concentration requirements of other operations.

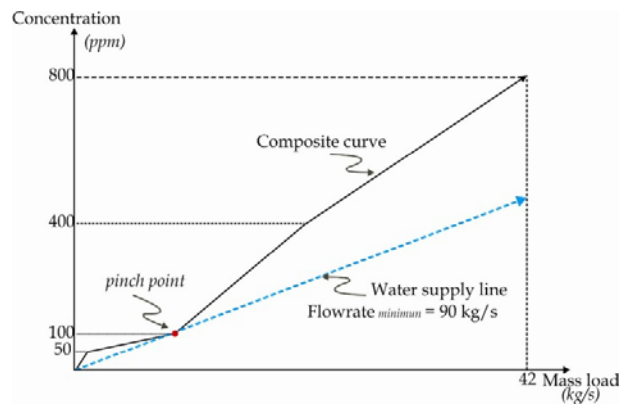


Figure 4. Limiting water composite curve and minimum fresh water supply for cases study.

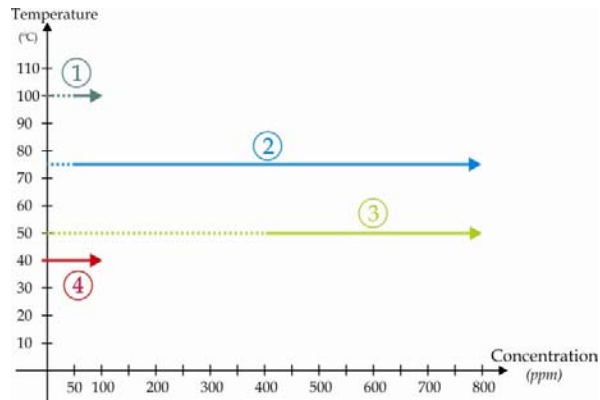


Figure 5. Temperature-Concentration diagram for case 1.

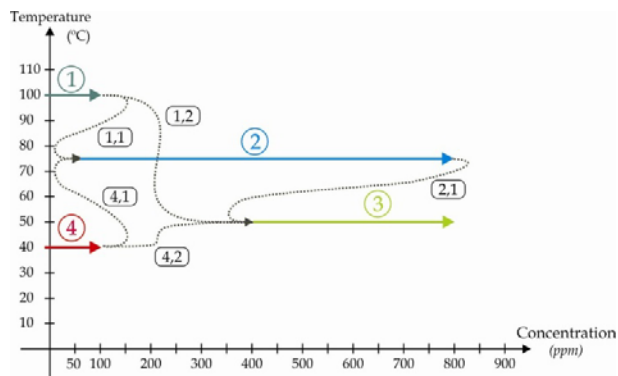


Figure 6. Possible combinations of streams to meet the requirements of operation 2 and 3.

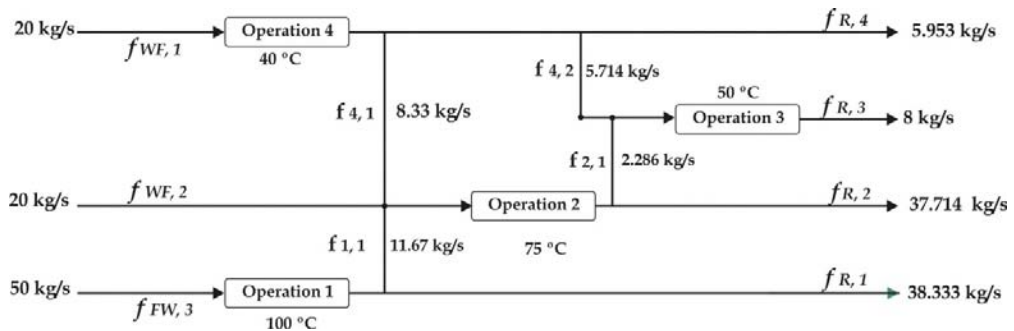


Figure 7. Simultaneous heat and mass exchange network structure.

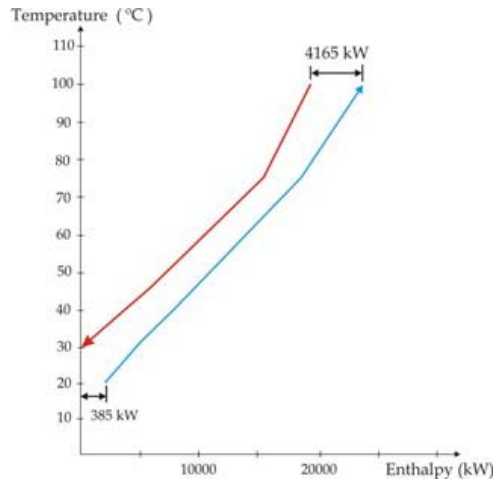


Figure 8. Composite curve.

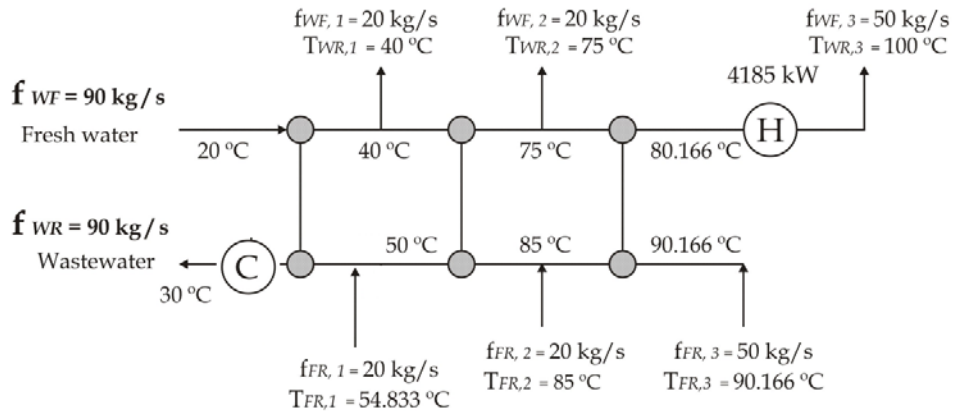


Figure 9. Network structure for indirect heat transfer.

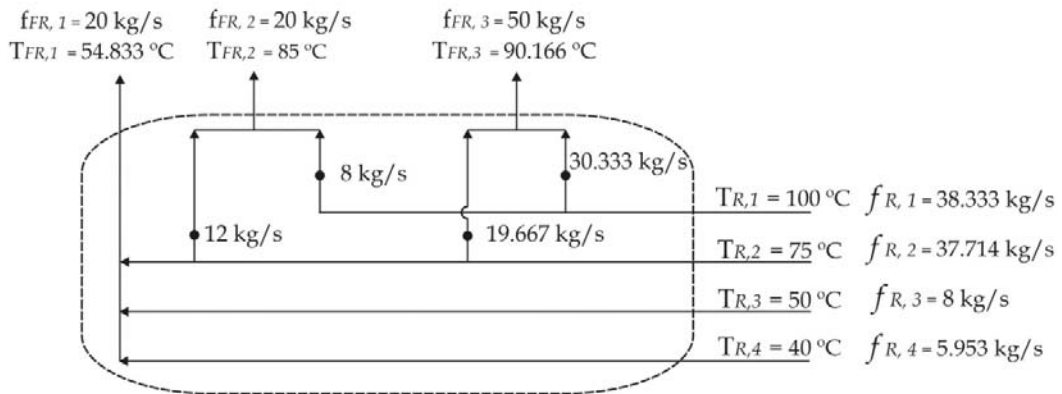


Figure 10. Heat direct exchange subnetwork.

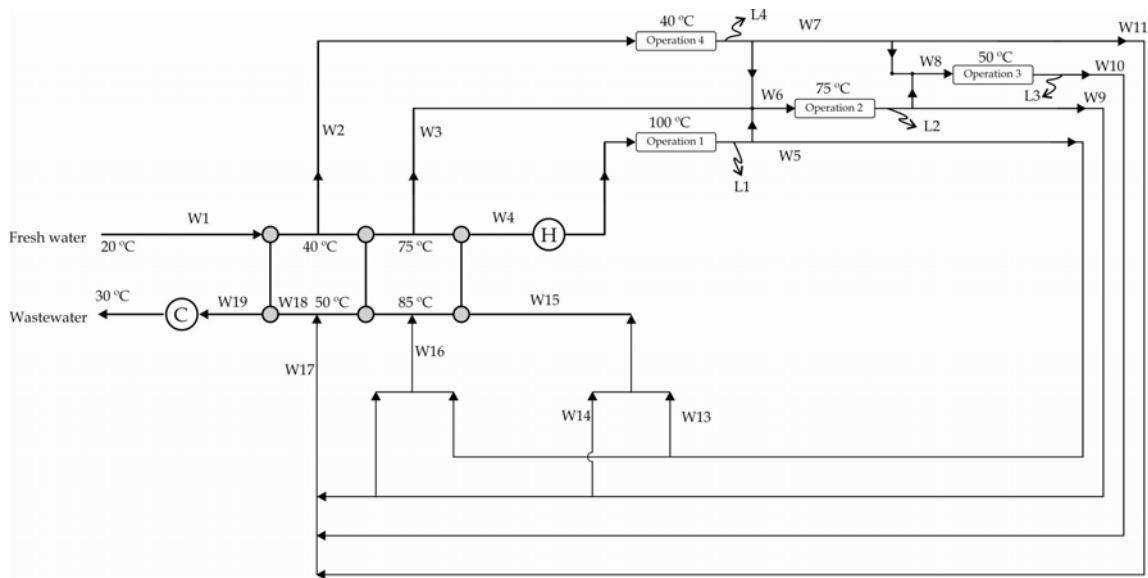


Figure 11. Overall network structure for the heat and mass transfer system.

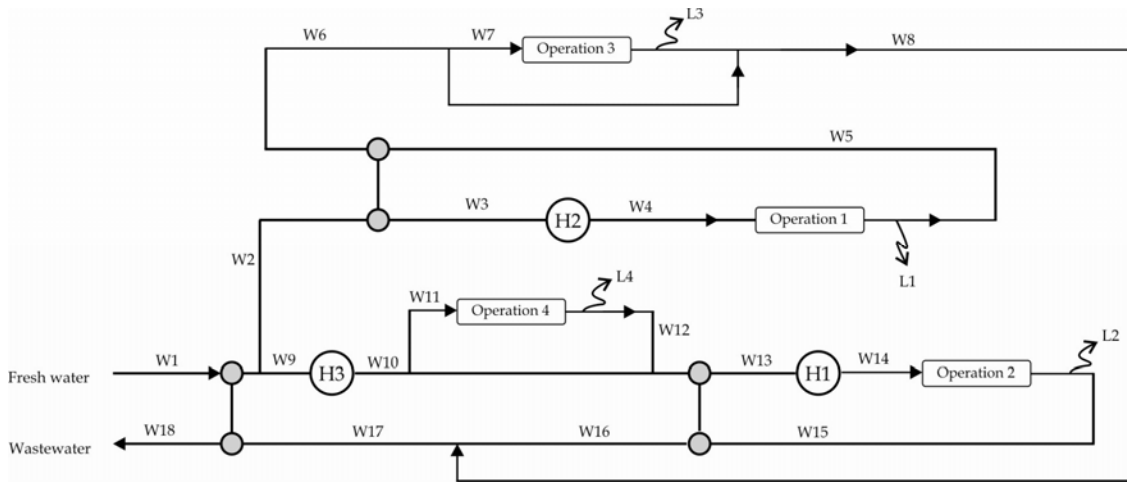


Figure 12. Network structure without non-isothermal mixing

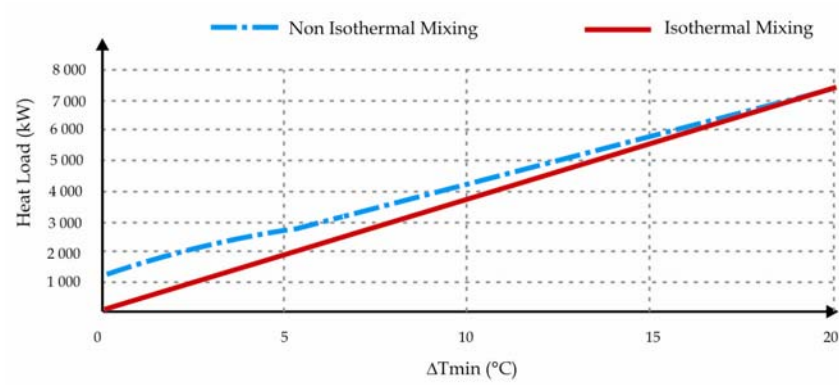


Figure 13. Heat load in the case of isothermal and non-isothermal mixing systems

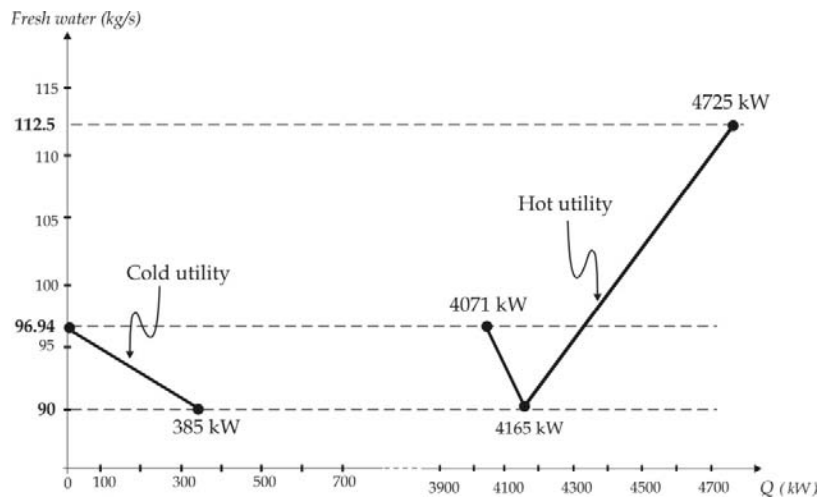


Figure 14. External heating and cooling as a function of fresh water flow rate for a minimum temperature difference of $\Delta T_{\min} = 10 \text{ }^{\circ}\text{C}$.

Table 1. Process data for case study.

Operation (No.)	Concentration _{in} (ppm)	Concentration _{out} (ppm)	Temperature _{in} (°C)	Temperature _{out} (°C)	Limiting water flowrate (kg/s)	Contaminant mass load (g/s)
1	50	100	100	100	100	5
2	50	800	75	75	40	30
3	400	800	50	50	10	4
4	0	100	40	40	20	2

Temperature of fresh water source: $T_{in} = 20 \text{ }^{\circ}\text{C}$

Temperature of discharge wastewater: $T_{out} = 30 \text{ }^{\circ}\text{C}$

Table 2. Information for the construction of the composite curves.

<i>Cold composite curve</i>					<i>Hot composite curve</i>				
f_{FW}	$T_{lim, in}$	T_{FW}	CP	$Enthalpy$	F_R	$T_{lim, in}$	T_{FW}	CP	$Enthalpy$
(kg/s)	(°C)	(°C)	(kW/°C)	(kW)	(kg/s)	(°C)	(°C)	(kW/°C)	(kW)
50	20	100	210	16800	38.33	100	30	161	11270
20	20	75	84	4620	37.71	75	30	158.4	7128
20	20	40	84	1680	8	50	30	33.6	672
					5.95	40	30	25	250

Table 3. Solution of case study and comparison with previous results reported in the open literature.

Scenario	Methodology	Hot utility consumption (kW)	Cold utility consumption (kW)	Water Consumption (kg/s)	ΔT_{\min} (°C)	Number of heat transfer units in HEN
A	1	4265	485	90	10	5
B	2	4165	385	90	10	5

Table 4. Temperatures and mass flow rates for the system with isothermal mixing (see Figure 12) without and with water losses in the processes

	no losses		L1=2 kg/s		L2=2 kg/s		L3=2 kg/s		L4=2 kg/s	
	f [kg/s]	T [°C]	f [kg/s]	T [°C]	f [kg/s]	T [°C]	f [kg/s]	T [°C]	f [kg/s]	T [°C]
W1	90	20	90	20	90	20	90	20	92	20
W2	50	40	50	39.56	50	39.56	50	39.56	50	39.57
W3	50	90	50	87.56	50	89.56	50	89.56	50	89.57
W4	50	100	50	100	50	100	50	100	50	100
W5	50	100	48	100	50	100	50	100	50	100
W6	50	50	48	50	50	50	50	50	50	50
W7	5.7	50	5.7	50	5.7	50	5.7	50	5.7	50
W8	50	50	48	50	50	50	48	50	50	50
W9	40	40	40	39.56	40	39.56	40	39.56	42	39.56
W10	40	40	40	40	40	40	40	40	42	40
W11	20	40	20	40	20	40	20	40	20	40
W12	40	40	40	40	40	40	40	40	40	40
W13	40	65	40	65	40	63.75	40	65	40	65
W14	40	75	40	75	40	75	40	75	40	75
W15	40	75	40	75	38	75	40	75	40	75
W16	40	50	40	50	38	50	40	50	40	50
W17	90	50	88	50	88	50	88	50	90	50
W18	90	30	88	30	88	30	88	30	90	30

Table 5. Temperatures and mass flow rates for the system with non-isothermal mixing (see Figure 11) without
and with water losses in the processes

	no losses		L1=2 kg/s		L2=2 kg/s		L3=2 kg/s		L4=2 kg/s	
	f [kg/s]	T [°C]	f [kg/s]	T [°C]	f [kg/s]	T [°C]	f [kg/s]	T [°C]	f [kg/s]	T [°C]
W1	90	20	90	20	90	20	90	20	90	20
W2	20	40	20	40	20	40	20	40	20	40
W3	20	75	20	75	20	75	20	75	20	75
W4	50	80.17	50	79.2	50	80.17	50	87.16	50	87.16
W5	38.33	100	36.33	100	38.33	100	38.33	100	38.33	100
W6	40	75	40	75	40	75	40	75	40	75
W7	11.66	40	11.66	40	11.66	40	11.66	40	9.66	40
W8	8	50	8	50	8	50	8	50	8	50
W9	37.71	75	37.71	75	35.71	75	37.71	75	37.71	75
W10	8	50	8	50	8	50	6	50	8	50
W11	5.95	40	5.95	40	5.95	40	5.95	40	3.95	40
W12	6.04	75	4.05	75	4.05	75	6.04	75	6.04	75
W13	30.33	100	28.33	100	30.33	100	30.33	100	30.33	100
W14	19.67	75	21.67	75	19.67	75	19.67	75	19.67	75
W15	50	90.17	50	89.2	50	90.17	50	90.17	50	90.17
W16	20	85	20	85	20	85	20	85	20	85
W17	20	54.58	18	52.32	18	52.32	18	55.09	18	56.20
W18	90	51.02	88	50.47	88	50.47	88	51.04	88	51.27
W19	90	31.02	88	30.02	88	30.02	88	30.59	88	30.81