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Simultaneous optimization of water and heat exchange networks

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Abstract−This paper focuses on the simultaneous optimization of the heat-integrated water allocation networks. A mathematic model is established to illustrate the modified state-space representation of this problem. An easy logical method is employed to help identify the streams of hot or cold ones. In this model, the water exchange networks (WEN), heat exchange networks (HEN), and the interactions between the WEN and HEN combine together as one unity. Thus, the whole network can be solved at one time, which enhances the possibility to get a global optimal result. Examples from the literature and a PVC plant are analyzed to illustrate the accuracy and applicability of this method.

Keywords: Optimization, Chemical Processes, Mathematical Modeling, Heat-integrated Water Allocation Networks, State-space Representation

INTRODUCTION

Heat and mass are both important utilities used in a plant. After the 1980s, heat exchange networks as well as mass exchange networks made great improvements. However, in practice, when the workers are dealing with the problem of mass exchange network in the process, we inevitably find that heat is also an important factor in the mass integration process. That is, heat and mass are two significant elements that should be considered simultaneously. Therefore, research on simultaneously minimizing heat and mass, water allocation heat exchange network (WAHEN), inevitably is brought up. However, WAHEN is not a process that just combines the process of MEN and the process of HEN together [1]. The simultaneous heat and water minimization was proposed at the first time, and they attempted to solve the problem mathematically [2]. Then, the importance of simultaneous minimization of energy and water was first illustrated by Savelski and Bagejewicz [3]. According to these methods used to solve heat and water minimization, the methods adopted to solve the WAHEN can also be divided into two: conceptional method and mathematical approach.

The conceptional method is useful and widely employed in practical operation in industry. At first, Huang and Edgar [4] solved the problem of the simultaneous minimization in a petroleum refinery by a knowledge-based design approach. The concept of a combined-exchange network (CEN), which contains a mass exchange network (MEN) and a heat exchange network (HEN), was proposed. Savulescu and Smith [5] discussed creating a separate system and introduced new insights into the HEN design approach for water streams. Also, a new graphical approach, the superimposed mass and energy transfer-based system (SMEC), was provided on mass and energy reduction [6].

The mathematical approach, overcoming the drawbacks of the conceptional method which is restricted to single contaminant networks and does not give optimal results, is suitable for solving complex networks and multi-objective situations. Bagajewicz et al. [7] presented a state space approach to the synthesis process. The state space, which is divided into two parts, the distribution network and other participating networks, contains the concept of heat exchange network and water exchange network in a whole graph. Bagajewicz et al. [8] introduced a new mathematic approach for the design of water utilization networks and a specific state space representation of the network. The whole process exchange network is obtained after the minimum freshwater usage and energy consumption are identified. The optimization process is a sequential one with two steps. What's more, the pinch method is introduced to solve heat network. This may lead to a non-optimal result. Then, to circumvent the difficulty of dealing with wastewater-treatment system, a systematic design methodology and a modified state-space representation [9] were developed for simultaneously synthesizing multi-contaminant WAHENs. But the mathematical model is complex and not easy to understand. In the same year, in order to reduce the number of heat exchangers and the process complexity, Bagajewicz et al. [10] proposed a new MINLP with a new superstructure of the HEN. Liao et al. [11] proposed a new mathematic model to simultaneously solve the heat-integrated water allocation networks, and they suggested a new method of identifying hot and cold streams in the model. The hot and cold stream labeling strategy not only effectively decreases the relative number of hot and cold streams while maintaining the diversity of potential heat exchange matches, but also captures some unique network structures that might be ignored by heuristics. All these published papers which refer to WAHEN analyzed this problem by discussing HEN and WEN in the same model, and they also combined these two networks by analyzing the connections between them. At these points, a mathematical method which is solved in single step with a new hot and stream labeling strategy is brought up in the following.

Others focused their attention on the HEN to optimize the WAHEN; they added non-isothermal mixing in the HEN. The direct heat transfer focus on non-isothermal mixing was firstly proposed by Savulescu [5]. Graphical thermodynamic rules [12] were formalized by Sorin

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and Savulescu in 2004 to design WAN and corresponding HEN. This new graphical thermodynamic rule avoided the deterioration of energy targets while minimizing the number of heat transfer units as well as the mixing and splitting network complexity. Smith and Savulescu [13,14] proposed a method on simultaneous energy and water minimization, discussing non-isothermal mixing which can lead to separate systems. However, this method is only applied when there is only one kind contaminant in the water. However, in 2012, Chandra Sahu and Bandyopadhyay [15] developed linear programming formulations to target the minimum energy requirements, and also discussed the heat integration through isothermal and non-isothermal mixing involving single as well as multiple contaminants in mathematic theory. In these WAHEN papers concerning non-isothermal, we found that the whole framework or main structures of the mathematic model are not changed. After non-isothermal mixing is added in the HEN model, the complexity and energy consumption are reduced. They improved the result by discussing more details of the system.

In this paper, to clearly illustrate the connections, a different mathematic model combining a model for water exchange networks proposed by Feng et al. [16] and another model for heat exchange networks proposed by Grossamnn et al. [17] is employed to solve simultaneously the water and heat minimization problem. The established model is mixed-integer non-linear problem (MINLP) and the main differences between this paper and those published papers are that the models adopted in this paper to analyze WAHEN are different, and the connections between HEN and WEN are discussed more deeply. What's more, we focus on the main framework of the method; other details such as non-isothermal are ignored. Compared with the model suggested by Dong et al. [9], the model in this paper is easier to understand, and when compared to the model suggested by Bagajewicz et al. [8], this model solves the problem in only one step. Because water and heat cannot be separated in the system, there are two approaches which we use to analyze the connections: one from the heat view and the other from the water view. Then, these two problems are both solved.

PROBLEM STATEMENT

The main process of this system consists of several water using processes with particular temperature and concentration demands. Each process' inlet and outlet must be satisfied with the maximum stream concentration and temperature constrains. The objective is to find the most optimal network of these processes and streams with minimum capital costs.

Assumptions:

1. The regeneration recycle is not considered in this system. However, the reuse and regeneration are taken into consideration.
2. If the concentration of the contaminant in the stream is low, the heat capacity of these streams can be fixed as 4.2 kJ/kg·°C.
3. All processes are isothermally operated and the no water losses occur.
4. The temperature of the freshwater is 20 °C, the temperature of the wastewater is 30 °C. In practice, the temperature of most operations is greater than 30 °C, so the freshwater streams belong to the cold streams and the wastewater streams are identified as the hot streams.

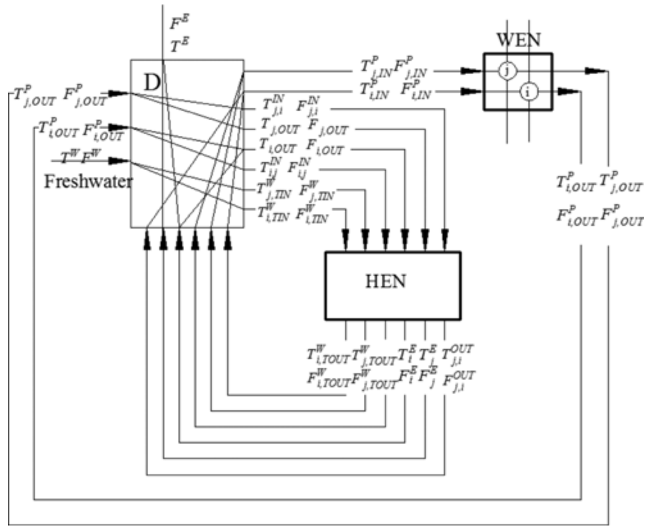

Fig. 1. Water-allocated heat exchange networks superstructure.

5. There is only one hot utility and one cold utility in this system.

SUPERSTRUCTURE

This superstructure of water-allocated heat exchange networks, as shown in Fig. 1 [8], is divided into two parts according to Dong et al. [9]: the distribution network and the operation network. The distribution network consists of the connections between the heat and water exchange networks, and the operation network consists of the water exchange network and the heat exchange network. In this superstructure, the water exchange network, which is shown in Fig. 2, is derived from the paper proposed by Feng et al. [16], the heat exchange network is similar to the one presented by Grossmann et al. [17]; the superstructure of heat is shown in Fig. 3, and the state-space superstructure proposed by Bagajewicz et al. [8] is adopted to account for the whole framework.

In the superstructure proposed in the following, before the fresh water from the source F^W is piped to the water using processes, the

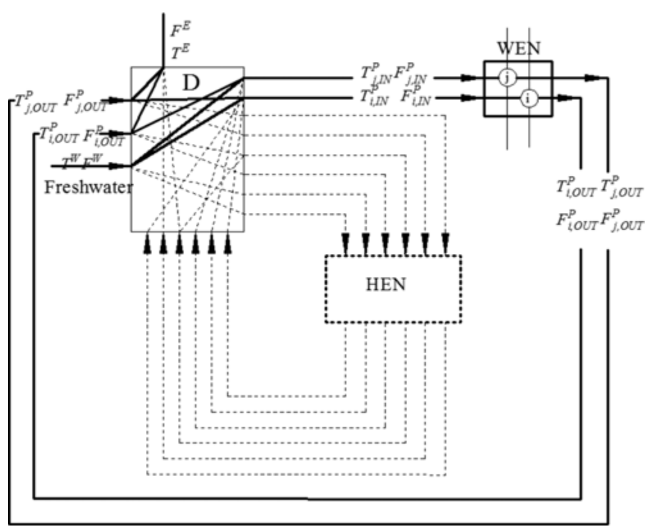

Fig. 2. Water exchange networks in the superstructure.

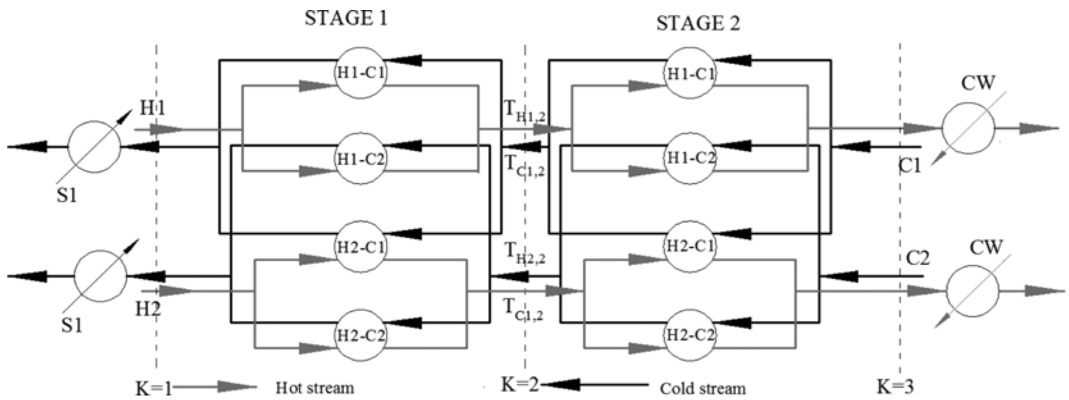

Fig. 3. Heat exchange networks Yee and Grossmann [17].

water should be directed to the heat exchange network to satisfy the temperature demand. The temperature of the stream from the source piped to process j at the inlet of heat exchange system is marked as $F^{W}_{j,TIN}$ and the temperature of this stream at the outlet of the heat exchange network is marked as $F^{W}_{j,TOUT}$. Then the freshwater stream with particular temperature $T^{P}_{j,IN}$ is used by these processes; the water discharged from these processes with contaminants and temperature $F^{P}_{j,OUT}$ is split into several streams, some of which are reused by other processes $F^{IN}_{j,i}$ and some of them marked as F^{E}_{j} are discharged to the environment. The streams reused always exchange heat in the HEN before they are piped to the destination processes because different processes have different temperature demands, and these streams can be either hot ones or cold ones. The waste water streams must be directed to the HEN to lower the temperature because of environmental regulations. From Fig. 1, more variables than needed can be found, and these variables are created for the convenience of integrating the heat and water system. The relationship of these variables will be explained in the following equations. All streams have two properties: the temperature, which is mainly discussed in the heat exchange network, and the flow rate, which is mainly discussed in the water exchange network.

The framework of water exchange network in this superstructure is different from the one proposed by the Feng et al. [16]. The superstructure of the WEN in this work is not just confined in the operation network and is extended into the distribution network as shown in Fig. 2. Because each stream from the WEN will be employed to exchange heat, the streams confined in the WEN cannot show the connections between WEN and HEN. In Fig. 2, the HEN is illustrated in dashed lines, which means it was ignored in order to show the trace of the WEN in this superstructure.

The detail of the HEN is shown in Fig. 3, which is the same as the one proposed by Yee and Grossmann [17]. There are only two stages in this model and the possibilities of the match between all heat and cold streams are totally discussed.

MATHEMATICAL MODEL

According to what has been discussed above, the mathematical model can be divided into three parts: water part, heat part, and connections between water and heat. The mathematical formulations of water and heat model are from Feng et al. [16] and Yee and Grossmann [17], respectively. These equations are based on energy balance, mass balance, and common sense. In the following mathematical model, the water using processes as well as the regeneration processes are both considered, and in the objective functions only freshwater and utility consumptions are considered. To understand more easily the integrated water allocation and heat exchanger networks, the developed connections and a new hot and cold stream labeling strategy are also introduced. Then, this model begins with these connections.

1. The Connections between the HEN and the WEN

1-1. The Connections between HEN and WEN Concerning the Water Using Process

The total freshwater demand:

$$F^{W}=\sum F^{W}_{j,TIN} \quad j\in P \tag{1}$$

The flowrate balance for the water using process:

$$F^{P}_{j,IN}=F^{P}_{j,OUT} \quad j\in P \tag{2}$$

The flowrate balance for the mixer before the water using process:

$$F^{P}_{j,IN}=\sum F^{OUT}_{i,j}+\sum F^{OUT}_{r,j}+F^{W}_{j,TIN} \quad i,j\in P;\ r\in R;\ i\neq j \tag{3}$$

The flowrate balance for the splitter after the water using process:

$$F^{P}_{j,OUT}=\sum F^{IN}_{j,i}+\sum F^{IN}_{j,r}+F^{E}_{j} \quad i,j\in P;\ r\in R;\ i\neq j \tag{4}$$

The flowrate balance for the final emission point:

$$F^{E}=\sum F^{E}_{j}+\sum F^{E}_{r} \quad j\in P;\ r\in R \tag{5}$$

The flowrate balance for the heat exchanger:

$$F^{IN}_{j,i}=F^{OUT}_{j,i};\ F^{IN}_{j,r}=F^{OUT}_{j,r} \quad i,j\in P;\ r\in R;\ i\neq j \tag{6}$$

1-2. The Connections between HEN and WEN Concerning the Water Regeneration Process

The flowrate balance for the water using process:

$$F^{R}_{r,OUT}=R^{R}_{r,IN} \quad r\in R \tag{7}$$

The flowrate balance for the mixer before the water using process:

$$F^{R}_{r,IN}=\sum F^{OUT}_{j,r}+\sum F^{OUT}_{r',r} \quad j\in P;\ r,r'\in R \tag{8}$$

The flowrate balance for the splitter after the water using process:

$$F^{R}_{r,OUT}=\sum F^{IN}_{r,r'}+\sum F^{IN}_{r,j}+F^{E}_{r} \quad r,r'\in R;\ j\in P;\ i\neq j \tag{9}$$

The flowrate balance for the heat exchanger:

$$F^{IN}_{r,r'}=F^{OUT}_{r,r'} \quad r, r'\in R; r\neq r' \tag{10}$$

$$F^{OUT}_{r,j}=F^{IN}_{r,j} \quad j\in P; r\in R \tag{11}$$

1-3. The Connections between HEN and WEN Concerning the Heat System

Assuming that the temperature of the freshwater is 20 °C,

$$T^{W}=20\ ^{\circ}C \tag{12}$$

The temperature of the wastewater is fixed:

$$T^{E}=T^{E}_{j}=T^{E}_{r}=30\ ^{\circ}C \quad r\in R; j\in P \tag{13}$$

The temperature of the inlet of the heat exchanger is equal to that of the freshwater:

$$T^{W}_{j,TIN}=T^{W} \quad j\in P \tag{14}$$

The temperature relationship for the process connected the outlet of heat exchanger and the inlet of mass exchanger.

At this point, the problem can be discussed in two aspects: isothermal mixing and non-isothermal mixing, and only the isothermal mixing is discussed.

Inlet of water using process:

$$T^{W}_{j,TOUT}=T^{P}_{j,IN}=T^{OUT}_{i,j}=T^{OUT}_{r,j} \quad i, j\in P; r\in R; i\neq j \tag{15}$$

Inlet of water regeneration process:

$$T^{OUT}_{r',r}=T^{OUT}_{j,r}=T^{R}_{r,IN} \quad j\in P; r, r'\in R; r\neq r' \tag{16}$$

The temperature relationship for the process connected the outlet of mass exchanger and the inlet of heat exchanger:

$$T^{P}_{j,OUT}=T^{IN}_{j,i}=T^{IN}_{j,r}=T_{j,OUT} \quad i, j\in P; r\in R; i\neq j \tag{17}$$

$$T^{R}_{r,OUT}=T^{IN}_{r,j}=T^{IN}_{r,r'}=T_{r,OUT} \quad j\in P; r, r'\in R; r\neq r' \tag{18}$$

2. Water Exchange Network Model

In this part, to illustrate the water exchange network more clearly, we turn to both the rectangle and the lines to analyze the WEN. When we discuss the WEN, the HEN in the superstructure is eliminated and the remainder which on behalf of the WEN is shown in bold-faced lines. In the box which represents the WEN, there are two kinds of process; one is the processes which produce the contaminants and the other is the regeneration process based on absorbing the pollutants. The pipes that connect different processes which represent the water reuse are not included in the box because they carry heat energy and can be used to exchange energy to achieve temperature constraints. To illustrate the water exchange network more clearly, the regeneration part is only discussed in this section and it is ignored in the simultaneous heat and water minimization part.

According to the basic method we adopted to analyze the system and the representation in Fig. 2, a mass balance is conducted in terms of flow-rate and contaminant.

2-1. The Analysis of the Water Using Process in WEN

The total inlet flow rate of the process is equal to the total outlet flow-rate of the process:

$$F^{W}_{j,TIN}+\sum F^{OUT}_{i,j}+\sum F^{OUT}_{r,j}=\sum F^{IN}_{j,i}+\sum F^{IN}_{j,r}+F^{E}_{j} \quad i, j\in P; i\neq j; r\in R \tag{19}$$

The mass balance for the inlet point before the process:

$$\sum(F^{IN}_{i,j}\bullet C^{IN}_{i,j})+\sum(F^{IN}_{r,j}\bullet C^{IN}_{r,j})=(F^{W}_{j,TIN}+\sum F^{IN}_{i,j}+\sum F^{IN}_{r,j})\bullet C^{PS}_{j,IN} \quad i, j\in P; i\neq j; r\in R \tag{20}$$

The mass balance for the water using process:

$$F^{P}_{j,IN}\bullet C^{PS}_{j,IN}+M_{j,s}=F^{P}_{j,OUT}C^{PS}_{j,OUT} \quad j\in P; s\in C \tag{21}$$

The mass balance for the splitter point after the process:

$$F^{P}_{j,OUT}\bullet C^{PS}_{j,OUT}=\sum(F^{IN}_{j,i}\bullet C^{IN}_{j,i})+\sum(F^{IN}_{j,r}\bullet C^{IN}_{j,r})+F^{E}_{j}\bullet C_{j,out} \quad i, j\in P; r\in R; i\neq j \tag{22}$$

$$C^{PS}_{j,OUT}=C^{IN}_{j,i}=C_{j,OUT}=C^{IN}_{j,r} \quad i, j\in P; i\neq j; r\in R \tag{23}$$

The above equation is obtained by common sense, because when the stream is split into several streams the concentration of the stream before and after splitter will not change. This is definitely different from the condition of the mixer point in the system. However, in practice, the concentration of the inlet streams and outlet streams of these processes should be lower than the maximum concentration, which is determined by the practical operation condition. These constraints are expressed in the following equations:

$$C^{PS}_{j,IN}\leq C^{PS}_{j,INMAX} \quad j\in P \tag{24}$$

$$C^{PS}_{j,OUT}\leq C^{PS}_{j,OUTMAX} \quad j\in P \tag{25}$$

2-2. The Analysis of the Regeneration Process in WEN

The total inlet flow-rate of the regeneration process is equal to the total outlet flow-rate of the regeneration process:

$$\sum F^{OUT}_{j,r}+\sum F^{OUT}_{r',r}=\sum F^{IN}_{r,j}+\sum F^{IN}_{r,r'}+F_{r,OUT} \quad j\in P; r, r'\in R; r\neq r' \tag{26}$$

The mass balance for the regeneration process:

$$\sum(F^{OUT}_{j,r}\bullet C^{OUT}_{j,r})+\sum(F^{OUT}_{r',r}\bullet C^{OUT}_{r',r})-M^{L}_{r}=\sum(F^{IN}_{r,j}\bullet C^{IN}_{r,j})+\sum(F^{IN}_{r,r'}\bullet C^{IN}_{r,r'})+F_{r,OUT}\bullet C_{r,OUT} \quad j\in P; r, r'\in R; r\neq r' \tag{27}$$

The mass balance for the inlet point before the regeneration process:

$$\sum(F^{OUT}_{j,r}\bullet C^{OUT}_{j,r})+\sum(F^{OUT}_{r',r}\bullet C^{OUT}_{r',r})=(\sum F^{IN}_{j,r})\bullet C^{RS}_{r,IN} \quad j\in P; r, r'\in R; r\neq r' \tag{28}$$

The mass balance for the splitter point after the regeneration process:

$$F^{R}_{r,OUT}\bullet C^{RS}_{r,OUT}=\sum(F^{IN}_{r,j}\bullet C^{IN}_{r,j})+\sum(F^{IN}_{r,r'}\bullet C^{IN}_{r,r'})+F_{r,OUT}\bullet C_{r,OUT} \quad j\in P; r, r'\in R; r\neq r' \tag{29}$$

$$C^{RS}_{r,OUT}=C^{IN}_{r,j}=C^{IN}_{r,r'}=C_{r,OUT} \quad j\in P; r, r'\in R; r\neq r' \tag{30}$$

Also, in practice the concentration of the inlet streams and outlet streams of these processes should be lower than the maximum concentration, which is determined by the practical operation condition. These constraints are expressed in the following equations:

$$C^{RS}_{r,IN}\leq C^{RS}_{r,INMAX} \quad r\in R \tag{31}$$

$$C^{RS}_{r,OUT}\leq C^{RS}_{r,OUTMAX} \quad r\in R \tag{32}$$

3. Heat Exchange Network Model

The thermal data of the heat exchange network is obtained from the streams that exist in the water exchange network. In this simultaneous heat and water minimization method, two problems set barriers to solve the system. The first one is how to collect the data from the different kinds of streams and establish the fundament of the heat exchange networks. The second one is how to recognize the hot and cold streams.

After analyzing the connection between the WEN and the HEN, we found that the streams can be divided into three kinds. The first kind is the 20 °C freshwater streams which are treated as cold streams. The second one is the wastewater streams, the outlet temperature of these streams is 30 °C, and they are treated as hot streams. The third kind is the streams connecting different processes (water using processes or regeneration process), and they can be either cold streams or hot streams. The third kind of streams will add difficulty when we calculate the utility consumption because it will confuse the supply and demand energy in the system. To identify these streams, in this paper a mathematic logical method is proposed. After this logical method is applied to the third kind of streams, one can easily classify these streams.

3-1. How to Identify the Hot and the Cold Streams

When the streams come from the WEN join the heat exchange system, the program cannot tell whether these streams are hot or cold. To balance the energy, and avoid the incorrect energy identification which will lead to a wrong result of hot and cold utility consumption, we proposed a logical mathematical method to help identify these streams, and this logical method is easier to understand and simpler to conduct when compared with these methods proposed by other workers.

First, we rearrange the water-using processes in the WEN according to their ascending operational temperature. This can be easily realized no matter how many processes exist in the system, and it will never affect the final results.

Then, the processes are represented by subscripts i or j. For instance, $F_{i,j}^{IN}$ is the temperature at the inlet of the stream from the process i to j. If the index i is less than j, it means that the temperature of process i is less than that of j and that the stream is a cold stream which is from a process of lower temperature to that of higher temperature and needs heating. What's more, this method can be easily read by the program:

$$\text{If } i<j, \text{ then } F_{i,j}\in Sj \tag{33}$$

$$\text{If } i>j, \text{ then } F_{i,j}\in Si \tag{34}$$

Besides, we all know that

$$F^{W}_{j,TIN}\in Sj;\ R_{j,OUT}\in Si \tag{35}$$

Along with the problem we discussed above, how to integrate these different streams into the HEN to trigger the optimization is also a difficulty worth our attention. This problem will be solved using mathematic analysis.

3-2. The Details of the Heat Exchange Networks

The mathematical model in this paper is oriented from the model established by Yee and Grossmann in 1990.

The overall heat balance for each stream:

$$(T_{Si}^{IN}-T_{Si}^{OUT})\bullet F_{Si}=\sum_{K\in ST}\sum_{Sj\in CP} q_{SiSjK}+q_{CUSi}\quad Si\in HP \tag{36}$$

$$(T_{Sj}^{OUT}-T_{Sj}^{IN})\bullet F_{Sj}=\sum_{K\in ST}\sum_{Si\in CP} q_{SiSjK}+q_{HUSj}\quad Sj\in CP \tag{37}$$

Stage heat balance:

$$(t_{Si,K}-t_{Si,K+1})\bullet F_{Si}=\sum_{Sj\in CP} q_{SiSjK}\quad Si\in HP;\ K\in ST \tag{38}$$

$$(t_{Sj,K}-t_{Sj,K+1})\bullet F_{Sj}=\sum_{Si\in HP} q_{SiSjK}\quad Sj\in HP;\ K\in ST \tag{39}$$

Utility consumption:

$$(t_{Si,NOK+1}-T_{Si}^{OUT})\bullet F_{Si}=q_{CUSi}\quad Si\in HP \tag{40}$$

$$(T_{Sj}^{OUT}-t_{Sj,1})\bullet F_{Sj}=q_{HUSj}\quad Sj\in CP \tag{41}$$

Temperature conditions:

$$T_{Si}^{IN}=t_{Si,1}\quad Si\in HP \tag{42}$$

$$T_{Sj}^{IN}=t_{Sj,NOK+1}\quad Sj\in CP \tag{43}$$

$$t_{Si,K}\geq t_{Si,K+1}\quad Si\in HP;\ k\in ST \tag{44}$$

$$t_{Sj,K}\geq t_{Sj,K+1}\quad Sj\in CP;\ k\in ST \tag{45}$$

$$T_{Si}^{OUT}\leq t_{Si,NOK+1}\quad Si\in HP \tag{46}$$

$$T_{Sj}^{OUT}\leq t_{Sj,1}\quad Sj\in CP \tag{47}$$

Logical constraints

To illustrate the total number of heat exchangers, the 0-1 binary variables which are represented by Z_{ijk}, Z_{cui}, and Z_{huj} are used to analysis the system.

$$q_{SiSjK}-\Omega_1 Z_{ijk}\leq 0\quad Si\in HP;\ Sj\in CP\ 6 \tag{48}$$

$$q_{CUSi}-\Omega_2 Z_{cui}\leq 0\quad Si\in HP \tag{49}$$

$$q_{HUSj}-\Omega_3 Z_{huj}\leq 0\quad Sj\in CP \tag{50}$$

$$\Omega_1=\min\{(T_{Si}^{IN}-T_{Si}^{OUT})\bullet F_{Si},(T_{Sj}^{OUT}-T_{Sj}^{IN})\bullet F_{Sj}\} \tag{51}$$

$$\Omega_2=(T_{Si}^{IN}-T_{Si}^{OUT})\bullet F_{Si} \tag{52}$$

$$\Omega_3=(T_{Sj}^{OUT}-T_{Sj}^{IN})\bullet F_{Sj} \tag{53}$$

Temperature difference between different streams:

$$\Delta T_{ijk}\leq T_{Si,K}-T_{Sj,K}+\Gamma(1-Z_{ijk})\quad Si\in HP;\ Sj\in CP;\ K\in ST \tag{54}$$

$$\Delta T_{ijk+1}\leq T_{Si,K+1}-T_{Sj,K+1}+\Gamma(1-Z_{ijk})\quad Si\in HP;\ Sj\in CP;\ K\in ST \tag{55}$$

$$\Delta T_{CUSi}\leq T_{Si,NOK+1}-TOUT_{CU}+\Gamma(1-Z_{CUSi})\quad Si\in HP \tag{56}$$

$$\Delta T_{HUSj}\leq TOUT_{HU}-T_{Sj,1}+\Gamma(1-Z_{HUSj})\quad Sj\in CP \tag{57}$$

Objective function

In sequential optimization, the total water exchange network costs and total heat exchange network costs are optimized sequentially. However, in simultaneous water and heat minimization, these two objectives should be considered at the same time. Therefore, the objective function combines these two aspects.

$$COST=CO_{WEN}+CO_{HEN} \tag{58}$$

The cost of water exchange network mainly consists of the freshwater cost.

$$CO_{WEN}=C_{FW}\bullet F^{W} \tag{59}$$

The costs of the heat exchange network including the cost of the utility consumption:

$$CO_{HEN}=C_{CU}\bullet\sum q_{CUSi}+C_{HU}\bullet\sum q_{HUSj}\quad Si\in HP;\ Sj\in CP \tag{60}$$

APPLICATION EXAMPLE

In this section, three examples are discussed to show the accuracy and applicability of the approach proposed before. Because of

Table 1. Cost factors and parameters of the process

Cost factors		Parameters	
Hot utility (C_{HU})	100$/kW year	TIN_{HU} (°C)	150
Cold utility (C_{CU})	25$/kW year	$TOUT_{HU}$ (°C)	150
Freshwater (C_{FW})	2.5$/t	TIN_{CU} (°C)	10
		$TOUT_{CU}$ (°C)	20
		Tmin (°C)	10

Table 2. Process data of example 1

Operation	C_{in} (ppm)	C_{out} (ppm)	$T_{op, in}$ (°C)	$T_{op, out}$ (°C)	Contaminant mass load (g/s)
Operation 1	0	100	40	40	2
Operation 2	50	100	100	100	5
Operation 3	50	800	75	75	30
Operation 4	400	800	50	50	4

the complexity of solving non-linear programming, only freshwater and utility consumptions are included in the objective function. The operation costs and parameters involved in the following three examples are illustrated in Table 1. In the solution procedure, the operational software LINGO is employed to solve the mathematical model, because the GAMS is based more heavily on the initial values. The first example is the one first presented by Savulescu and Smith [18] and later discussed by Bagajewicz et al. [8], Savulescu et al. [13,14] and Dong et al. [9]. The second example is taken from Bagajewicz et al. [8]. And the third example is related to the VCM manufacturing process which is oriented from a workshop in a PVC plant.

1. Example 1

The data of example 1 is presented in Table 1 [8,9,13,14,18]. There are four water using processes and only one kind of contaminant is considered in this process.

Before optimizing this whole network, we arranged these operations according to the temperature of these processes. The connections between different processes were fully explored, and these streams can be either hot streams or cold streams. We used the method of how to identify hot and cold streams we proposed before to distinguish these streams. All the freshwater streams are cold streams and all the wastewaters are hot streams.

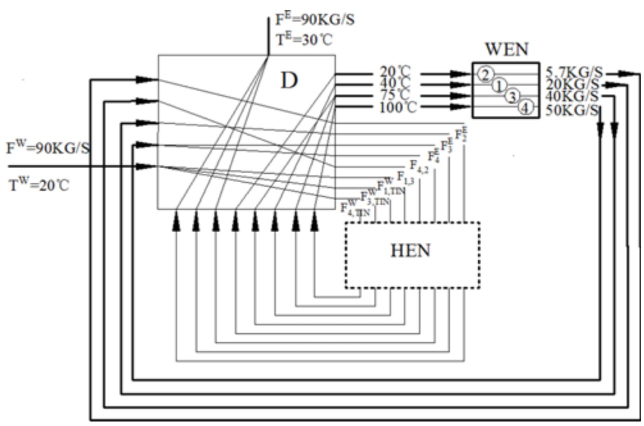

Fig. 4. Solution network of example 1.

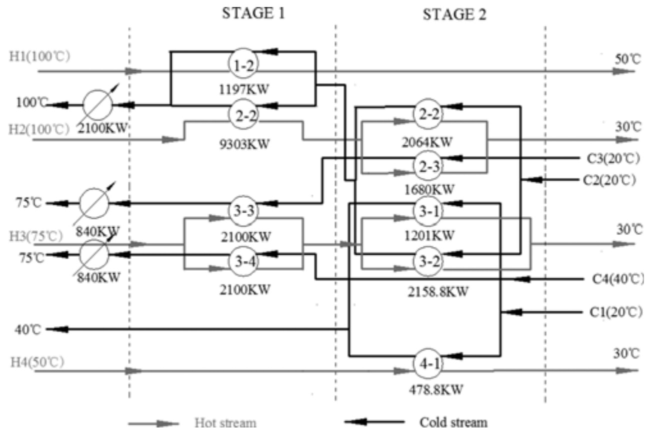

Fig. 5. Heat exchange network of example 1.

After simultaneous optimization, the whole network is illustrated in Fig. 4, and the details of the heat exchange network are shown in Fig. 5. The freshwater intake equals 90 kg/s; however, under this target many water exchange networks can be obtained if the water exchange network is only considered. The simultaneous water and heat minimization can help to choose a water exchange network, which leads to less utility consumption. Fig. 4 shows that there are only two streams existing between different streams. The connection details can be found in the Distribution part in the superstructure.

The hot utility and cold utility consumption are 3,780 kW and 0 kW, respectively. The whole superstructure is divided into two stages, and in order to satisfy the temperature demand of the system, three heaters and nine heat exchangers are needed in this network. The heat load and other parameters of the heat system can also be found in Fig. 5.

Compared to the results of others, which are listed in Table 3, the conclusions from our approach are almost the same if only the freshwater consumption and utility consumption are taken into consideration. This verifies that the approach is effective for simultaneous optimization of water and heat exchanger networks. As for the numbers of heaters and heat exchangers, they are not included in the objective. Consequently, the number we obtained in this work is not optimized. The final costs of the heat and water exchange system for the current example are 0.378 M$/year and 810$/h, respectively.

2. Example 2

The data listed in Table 4 is from Bagajewicz et al. [8]. By con-

Table 3. Comparisons of the results to others' work

Operation	Savulescu et al. [13,14]	Dong et al. [9]	This work
Freshwater (kg·s^{-1})	90	90	90
Cold utility (kW)	485	0	0
Hot utility (kW)	4265	3780	3780
Heater unit	1	1	3
Cooler unit	1	0	0
Heat exchanger unit	0	4	9

Table 4. Data for example 2 [8]

Operation	C_{in} (ppm)	C_{out} (ppm)	$T_{op, in}$ (°C)	$T_{op, out}$ (°C)	Contaminant mass load (g/s)
1	50	800	75	75	30
2	50	100	100	100	5
3	800	1100	100	100	50

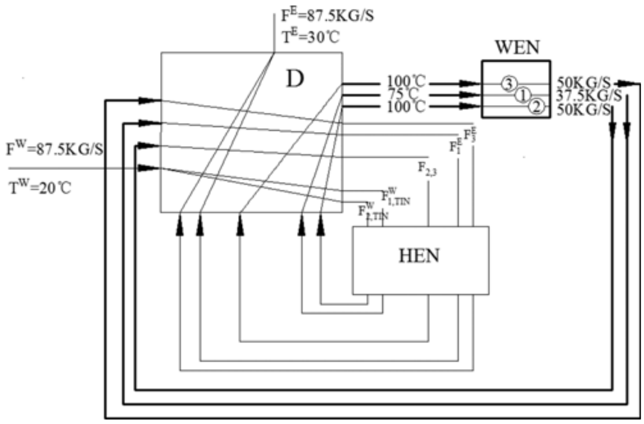

Fig. 6. Solution network of example 2.

Table 5. Comparisons of the results to others' work

Operation	Bagajewicz et al. [8]	Dong et al. [9]	This work
Freshwater ($kg\cdot s^{-1}$)	77.3	87.2	87.5
Cold utility (kW)	491	0	0
Hot utility (kW)	3736.2	3671.4	3675
Heater unit	2	2	1
Cooler unit	1	0	0
Heat exchanger unit	4	1	3

structing the state-space superstructure and solving the MINLP, the optimal structure is generated as shown in Fig. 6. There are three heat exchangers, two heaters and one cooler in the optimized network. In addition, the consumption rates of freshwater and hot utilities are determined to be 87.5 kg/s and 3,675 kW, respectively. Similar to example 1, cold utility is not needed in the obtained network.

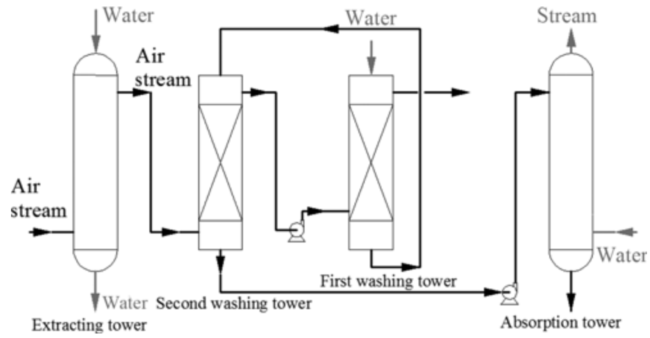

Fig. 8. Flow sheet of the VCM manufacturing process.

Comparisons of the obtained results to others' works are summarized in Table 5. The sequential solution procedure is taken by Bagajewicz et al. [8] to solve example 2. Thus, the consumption of freshwater, 77.3 kg/s, is the lowest, but the utility consumption is the highest among these three works. As both Dong et al. [9] and we chose the simultaneous optimization method, our results are roughly the same as theirs. It means that the simultaneous optimization strategy adopted in our work is effective to handle this kind of problem. In the following example, the method will be used to design a new integrated water allocation and heat exchange network for a PVC plant.

3. Example 3

In the VCM manufacturing process, the vinyl chloride monomer (VCM) is obtained by combining the ethyne and the hydrogen chloride, which is explained in the following equation:

$$CH \equiv CH + HCl \xrightarrow{HgCl_2} CH2 = CHCl$$

In the plant, extra hydrogen chlorides are added in the reactor in order to increase the reaction efficiency of the ethyne. Thus, remaining hydrogen chlorides exist in the reaction product and should be removed in the subsequent procedures. First, the gas stream is piped to the extracting tower and then directed to the first and second washing column in which hydrogen chlorides are absorbed by water. Finally, hydrogen chlorides in the water stream from the second washing column are desorbed in the desorption tower. The simple

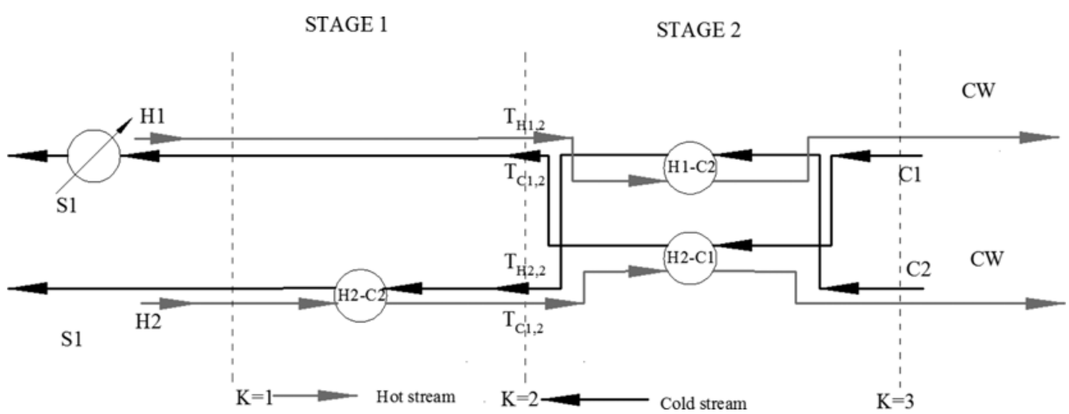

Fig. 7. Heat exchange network of example 2.

Table 6. Process data for example 3

Operation	Number	C_{in} (ppm)	C_{out} (ppm)	$T_{op,\,in}$ (°C)	$T_{op,\,out}$ (°C)	Contaminant mass load (kg/h)
2nd Washing	3	0	1750	30	30	2
1st Washing	2	1800	2000	40	40	6
Extracting tower	1	3000	310000	60	60	200
Desorption tower	4	1000	220000	124	124	158.86

flowsheet of this process is shown in Fig. 8. Consequently, the other contaminants will be ignored and this problem is only treated as a single contaminant problem. The water source is only freshwater at 20 °C and the temperature of the waste water is given as 30 °C. The detailed process data is presented in Table 6.

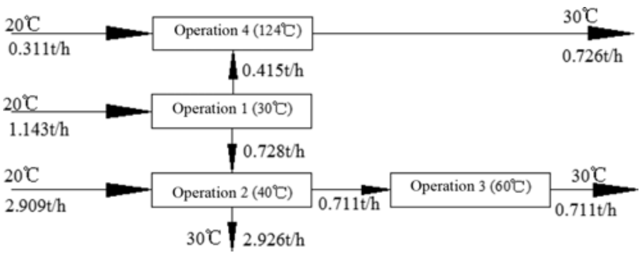

Fig. 9. Water exchange network of example 3.

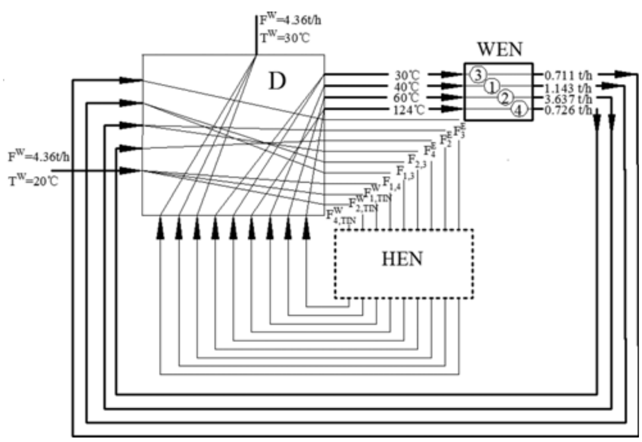

Fig. 10. Solution network of example 3.

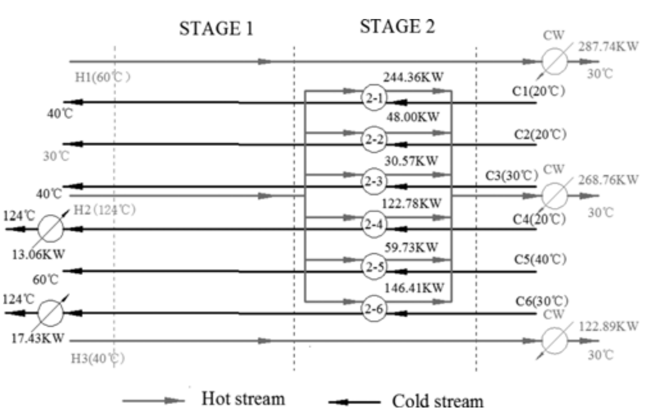

Fig. 11. Heat exchange network of example 3.

After the simultaneous heat and water minimization method is applied to this example, the network structure is obtained, and the details of the water exchange network, the whole network superstructure, and the heat exchange network can be found in Figs. 9, 10, and 11, respectively. In Fig. 9, we found that the freshwater consumption is 4.363 t/h; and Fig. 11 indicates that there are three hot streams and six cold streams, and the hot utility and cold utility consumptions are 30.492 kW and 679.389 kW, respectively. The costs for water and heat networks are 10.9075$/h and 20033.925$/ year.

CONCLUSIONS

A new mathematical model, which consists of three parts, the heat exchange networks, the water exchange networks, and the interactions between heat and water networks, is proposed. Based on it, water allocated heat exchange networks are discussed. More details of the interactions are analyzed to help integrate the water exchange network and the heat exchange network in the mathematical model. To identify that the streams in the heat exchange networks are hot or cold, a new logical method is suggested to conduct the classification procedure. The model is solved via operational software LINGO rather than GAMS. The latter has often been employed to solve such problems [9,11].

Three cases have been presented. The first two are from the literature and the third is from a real PVC manufacturing process. They are analyzed to show the accuracy and the applicability of our approach. Although these results depend on the solving ability of the software and the initial values of the model, the astringency of the model and the theory of simultaneous heat and water optimization have been proved.

The present model is not fit for fixed flow rate problems and is just applicable to the fixed contaminant load problem. As for the problem involving multiple contaminants, the model can be employed to solve such problems after some modifications. These modifications are mainly related to the mass balance equations such as Eqs. (20)-(23) and (27)-(30) in the water exchange networks. In these equations, each kind of contaminant must be discussed once, and the detailed information can be found in the paper proposed by Feng et al. [16] in 2008. Meanwhile, because of the low concentration of contaminant in the water flow, the change of the heat capacity of the stream can be ignored. The multiple contaminants do not bring any impact to the heat exchange model.

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NOMENCLATURE

F^{W} : total freshwater consumption
$F^{W}_{j,IN}$: freshwater flow rate from source to process j
$F^{P}_{j,IN}$: freshwater flow rate at the inlet of process j
$F^{P}_{j,OUT}$: freshwater flow rate at the outlet of process j
$F^{OUT}_{i,j}$: stream flow rate from process i to j
$F^{OUT}_{r,j}$: stream flow rate from regeneration i to process j
$F^{IN}_{j,i}$: stream flow rate from process j to i
$F^{IN}_{j,r}$: stream flow rate from process j to regeneration r
F^{E} : wastewater flow rate from the system
F^{E}_{j} : wastewater flow rate from process j
F^{E}_{r} : wastewater flow rate from regeneration r
$F^{R}_{r,OUT}$: stream flow rate at the outlet of regeneration r
$F^{R}_{r,IN}$: stream flow rate at the inlet of regeneration r
$F^{OUT}_{j,r}$: stream flow rate from process j to regeneration r
$F^{OUT}_{i,j}$: stream flow rate from regeneration r' to r
$F^{IN}_{r,r'}$: stream flow rate from regeneration r to r'
$F^{IN}_{r,j}$: stream flow rate from regeneration r to process j
T^{W} : temperature of freshwater
T^{E} : temperature of wastewater
T^{E}_{j} : temperature of wastewater from process j
T^{E}_{r} : temperature of wastewater from regeneration r
$T^{W}_{j,TIN}$: temperature of freshwater to process j at the inlet of HEN
$T^{W}_{j,TOUT}$: temperature of freshwater to process j at the inlet of HEN
$T^{P}_{j,IN}$: temperature of stream at the inlet of process j
$T^{OUT}_{i,j}$: temperature of stream from process i to j at the inlet of j
$T^{OUT}_{r,j}$: temperature of stream from regeneration r to process j at the inlet of j
$T^{OUT}_{r',r}$: temperature of stream from regeneration r' to regeneration r
$T^{OUT}_{j,r}$: temperature of stream from process j to regeneration r at the inlet of r
$T^{R}_{r,IN}$: temperature of stream at the inlet of regeneration r
$T^{P}_{j,OUT}$: temperature of stream from process j to environment at the outlet of process j
$T^{IN}_{j,i}$: temperature of stream from process j to i at the outlet of process i
$T^{IN}_{j,r}$: temperature of stream from process j to regeneration r at the outlet of j
$T^{IN}_{r,j}$: temperature of stream from regeneration r to process j at the outlet of r
$T_{j,OUT}$: temperature of stream at the outlet of process j
$T^{R}_{r,OUT}$: temperature of stream from regeneration r to the environment at the outlet of r
$T^{IN}_{r,r'}$: temperature of stream from regeneration r to r' at the outlet of r
$T_{r,OUT}$: temperature of stream at the outlet of regeneration r
$C^{IN}_{i,j}$: concentration of stream from process i to j at the outlet of i
$C^{IN}_{r,j}$: concentration of stream from regeneration r to process j at the outlet of r
$C^{PS}_{j,IN}$: concentration of stream at the inlet of process j
$M_{j,s}$: mass load of contaminant s in process j
$C^{PS}_{j,OUT}$: concentration s of stream at the outlet of process j
$C_{j,OUT}$: concentration of stream from process j to environment
$C^{PS}_{j,INMAX}$: limiting inlet concentration s to process j
$C^{RS}_{r,INMAX}$: limiting inlet concentration s to regeneration r
$F_{i,j}$: stream from process i to process j
S_{i} : hot stream
S_{j} : cold stream
T^{IN}_{Si} : inlet temperature of hot stream i
T^{OUT}_{Sj} : outlet temperature of cold stream j
F_{Si} : flowrate of hot stream i
q_{SiSjK} : heat exchanged between hot stream i and cold stream j at stage K
q_{CUSi} : heat exchanged between hot stream i and cold utility
q_{HUSj} : heat exchanged between cold stream j and hot utility
$t_{Si,K}$: temperature of hot stream i at stage K
$t_{Sj,K}$: temperature of cold stream j at stage K
$t_{Si,NOK+1}$: temperature of hot stream i at stage NOK+1
$\Omega_1\Omega_2\Omega_3$: upper bound for temperature difference
$C^{PS}_{j,OUTMAX}$: limiting outlet concentration s to process j
$C^{RS}_{r,OUTMAX}$: limiting outlet concentration s to regeneration r
C_{CU} : unit cost of cold utility
C_{HU} : unit cost of hot utility
C_{FW} : unit cost of fresh water
CO_{WEN} : overall cost for fresh water
CO_{HEN} : overall cost for utility
ΔT_{min} : the minimum temperature difference
TIN_{HU} : inlet temperature of hot utility
$TOUT_{HU}$: outlet temperature of hot utility
TIN_{CU} : inlet temperature of cold utility
$TOUT_{CU}$: outlet temperature of cold utility

Binary Variables

Z_{ijk} : existence of heat exchanger for match (i, j) in stage k
Z_{cui} : existence of heat exchanger for match (i, cold utility)
Z_{huj} : existence of heat exchanger for match (hot utility, j)

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