

Heat Integrated Water Regeneration Networks with Variable Regeneration Temperature

Shweta Kamat^{a,*}, Santanu Bandyopadhyay^a, Anurag Garg^b, Dominic C.Y. Foo^c
 Gopal C. Sahu^{a,d}

^aDepartment of Energy Science and Engineering, IIT Bombay, Powai, Maharashtra, 400076, India

^bCentre for Environmental Science and Engineering, IIT Bombay, Powai, Maharashtra, 400076, India

^cDepartment of Chemical and Environmental Engineering/Centre of Excellence for Green Technologies, University of Nottingham Malaysia, Broga Road, 43500 Semenyih, Selangor, Malaysia

^dAditya Birla Science & Technology Centre, PFIC (unit of Grasim Industries Limited), Plot No. 1 & 1- A/1, MIDC Taloja, Tal Panvel, Dist. Raigad 410208, India

shweta.kam263@gmail.com, 153170003@iitb.ac.in

Process industries need to efficiently utilize energy and water for the reduction in the operating cost as well as to contribute towards achieving sustainability. The heat integrated water regeneration network (HIWRN) reduces the energy and water requirements together. Typically, HIWRN is optimized by maximizing heat exchange between processes including the regeneration unit that operates at a predetermined temperature. A superstructure based (non-)linear programming framework has been proposed to synthesize a HIWRN. In literature, regeneration flow rate and contaminant concentration were optimized along with energy and water, but the temperature of regeneration unit was considered as a constant. This paper focuses on the simultaneous optimization of energy and water consumption in HIWRN by varying the regeneration temperature as well. The effect of varying the regeneration temperature on the water and energy consumption and consequently on the operating cost is discussed with the help of an illustrative example. The proposed methodology minimizes the operating cost by reducing energy and water requirement simultaneously and thereby improves the overall sustainability.

1. Introduction

Energy and water are crucial resources required in a process industry. It is essential to conserve these resources due to its scarcity and rising prices. Maximizing the heat exchange and water re-use within the industry reduces the energy and water requirements. Water to be re-used may be treated partially in the regeneration units to conserve additional fresh water. The regeneration units are classified into a fixed outlet type and a fixed removal ratio type (Foo, 2012). The outlet contaminant concentration of the former type of regeneration unit is constant. The removal ratio, which is the ratio of the contaminant load removed to the contaminant load entering, is constant for the latter. In many process applications, water/steam serves as process fluid (e.g., steam stripping) as well as a medium for heat transfer (e.g., steam tracing). It is important to combine the minimization of water along with energy with the help of Process Integration Methodology (Klemeš et al., 2013). One of the techniques is the synthesis of heat integrated water regeneration networks (HIWRN).

Recently, a pinch-based technique was proposed to obtain a HIWRN graphically (Shen et al., 2017). This method cannot be implemented in case of multiple contaminants, thereby requiring a mathematical programming approach. Ahmetović et al. (2014) proposed a two-step strategy in which a superstructure-based model minimized either freshwater or total annualized cost (TAC); while the energy target and heat exchanger network were obtained by minimizing the energy-related TAC. Both these methods do not provide the energy and water targets simultaneously. Ibrić et al. (2014) minimized the total operating cost (TOC), which served as the initial guess for the overall TAC minimization problem. Ibrić et al. (2016) simplified this HIWRN formulation through a set of pre-screening rules. Ibrić et al. (2017a) improved the energy saving opportunity by including the non-water using processes for heat integration; while Ibrić et al. (2017b) included piping costs in the TAC.

The TOC minimization problem for HIWRNs was mainly solved as a MINLP problem through binary variables for the identification of hot or cold streams (Jagannath and Almansoori, 2016) or as a non-linear programming (NLP) problem using pinch location method (Ibrić et al., 2017a). The MINLP model is complex due to the integer variables; while the pinch location method involves discontinuous derivatives. This paper intends to simplify the HIWRN targeting through linear and non-linear programming formulations depending on the type of regeneration units used, fixed outlet and fixed removal ratio types.

All processes in the above-mentioned studies operated at constant temperatures. However, the desired output can be achieved by operating a process over a range of temperatures. This was highlighted by Tan et al. (2014) by optimizing a heat integrated water network based on the concept of floating pinch. However, the process outlet temperature needed to be known a priori. Also, this technique could not optimize water and energy requirements simultaneously as all the flow requirements for processes needed to be determined before heat integration. An NLP formulation optimized the regeneration temperature through TOC minimization (Ataei et al., 2009). However, the energy cost in the TOC was the cost required to heat only the fresh water. There is no methodology in the literature that considers the overall Heat Integration along with a variable regeneration temperature. A novel model is proposed to simultaneously optimize the freshwater and energy consumption by considering a variable regeneration temperature. The applicability of this technique is demonstrated with the help of an illustrative example for water networks with multiple contaminants.

2. Problem Definition

Figure 1 represents schematic of a typical HIWRN.

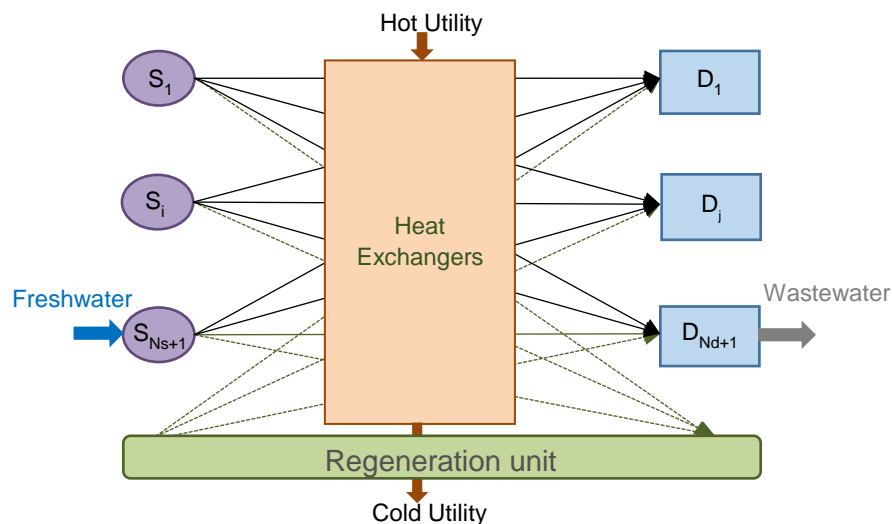


Figure 1: A generalized HIWRN

- A set of N_s internal sources and a set of N_d internal demands are given.
- Every internal source i ($1, 2, \dots, N_s$) provides a flow of F_{si} , at a temperature of T_{si} . There are Z contaminants. The concentration of v^{th} contaminant present in the i^{th} source is denoted by $C_{si,v}$.
- Each demand j ($1, 2, \dots, N_d$) accepts a flow of F_{dj} , at a temperature of T_{dj} . The maximum concentration of the v^{th} contaminant that the j^{th} demand can accept is given by $C_{dj,v}$.
- N_u single pass regeneration units are considered.
- The regeneration flow, F_{ur} , and temperature, T_{ur} , need to be optimized for r ($1, 2, \dots, N_u$) regeneration units. $C_{ur,v}$ (the outlet concentration of the v^{th} contaminant from the r^{th} regeneration unit) needs to be optimized for fixed removal ratio type of interception units.
- Due to the quality restriction and/or shortfall of source flows, all demands might not be met by the existing sources. An optimum amount of external source, F_{Ns+1} (fresh water) is required. Freshwater is available at a contaminant concentration of $C_{Ns+1,v}$ and a temperature of T_{Ns+1} .
- The unallocated sources are allocated to an external demand (waste), which has a flow rate of F_{Nd+1} . There is a limit on contaminant concentration, $C_{Nd+1,v}$, and temperature, T_{Nd+1} , of the waste to be disposed and wastewater may be treated in the regeneration unit prior to discharge.

- Maximum heat exchange between streams to be heated (cold streams) and cooled (hot streams) is carried out to achieve the demand temperatures. In case of unmet temperature requirements, hot utility or cold utility is used.

The objective is to simultaneously optimize fresh water and energy requirements along with the regeneration flow rate, contaminant concentration (for regeneration unit with a fixed removal ratio) and temperature. The optimization model is as follows.

3. Model for HIWRN with variable temperature

The flow transferred from i^{th} source to j^{th} demand is denoted by f_{ij} . Similarly, f_{rj} is the flow from r^{th} regeneration unit to j^{th} demand and f_{ir} is the flow from i^{th} source to r^{th} regeneration unit. The flow balances for all the internal sources, internal demands, and regeneration units are given by Eq(1) - Eq(3).

$$\sum_{j=1}^{N_d+1} f_{ij} + \sum_{r=1}^{N_u} f_{ir} = F_{si} \quad \forall i \in \{1, 2, \dots, N_s\} \quad (1)$$

$$\sum_{i=1}^{N_s+1} f_{ij} + \sum_{r=1}^{N_u} f_{rj} = F_{dj} \quad \forall j \in \{1, 2, \dots, N_d\} \quad (2)$$

$$\sum_{i=1}^{N_s+1} f_{ir} = \sum_{j=1}^{N_d+1} f_{rj} \quad \forall r \in \{1, 2, \dots, N_u\} \quad (3)$$

For a given removal ratio, RR_{ur} , the outlet contaminant concentration is given in Eq(4), where $\epsilon (=10^{-6})$ ensures that the denominator is not zero. The quality load constraint is expressed as Eq(5).

$$C_{ur,v} = \frac{(1-RR_{ur}) \sum_{i=1}^{N_s+1} f_{ir} \times C_{si,v}}{\sum_{j=1}^{N_d+1} f_{rj} + \epsilon}, \quad \forall v \in \{1, 2, \dots, Z\}, \forall r \in \{1, 2, \dots, N_u\} \quad (4)$$

$$\sum_{i=1}^{N_s+1} f_{ij} C_{si,v} + \sum_{r=1}^{N_u} f_{rj} C_{ur,v} \leq F_{dj} C_{dj,v} \quad \forall j \in \{1, 2, \dots, N_d + 1\}, \forall v \in \{1, 2, \dots, Z\} \quad (5)$$

Bade and Bandyopadhyay (2014) proposed a method to minimize the thermal oil used for heat integration in multiple plants based on the principle of thermodynamically equivalent heat exchangers. The hot streams can provide heat to the cold streams as long as the difference between their respective temperatures is greater than or equal to the minimum approach temperature (ΔT_{\min}) for heat exchangers. Consider a pseudo hot stream which provides heat to a cold stream in an imaginary heat exchanger. The heat capacity rates, CP, (product of specific heat capacity, c_p , and flow rate) for both the streams are equal. A minimum temperature difference of ΔT_{\min} has to be maintained between the inlet (or exit) of hot stream and exit (or inlet) of the cold stream. This procedure transforms the entire problem into pseudo streams which are allowed to mix with each other. The enthalpies of pseudo streams (with appropriate ΔT_{\min} corrections) can directly be added while ensuring isothermal mixing of streams. The temperatures of all sources and demands, excluding the regeneration units, are known. A binary variable y_{rj} is introduced to identify the role of streams between r^{th} regeneration unit and j^{th} demand as shown in Eq(8) and Eq(9), where M is a large number (10^6). Similarly, a binary variable, x_{ir} , can be introduced to identify the hot and cold streams between i^{th} source and r^{th} regeneration unit.

$$T_{dj} - T_{ur} - M \times y_{rj} \leq 0 \quad \forall r \in \{1, 2, \dots, N_u\} \text{ and } j \in \{1, 2, \dots, N_d + 1\} \quad (8)$$

$$T_{dj} - T_{ur} + M \times (1 - y_{rj}) \geq 0 \quad \forall r \in \{1, 2, \dots, N_u\} \text{ and } j \in \{1, 2, \dots, N_d + 1\} \quad (9)$$

Each water source-demand match is a heat exchanger stream. Thus, there are $(N_s+N_u+1) \times (N_d+N_u+1)$ heat exchanger sources and demands. The problem size can be reduced by dividing each water source into two sources- the first source consists of only the cold streams and the second source consists of hot streams. Similarly, each water demand is divided based on hot and cold streams.

- Now, the number of heat exchanger sources and demands is $2(N_s+N_u+1)$ and $2(N_d+N_u+1)$.
 - Heat exchanger source l ($1, 2, \dots, 2(N_s+N_u+1)$) provides a capacity flow rate of CP_{sl} at a temperature of $\overline{T_{sl}}$.
 - Heat exchanger demand m ($1, 2, \dots, 2(N_d+N_u+1)$) needs a capacity flow rate of CP_{dm} at a temperature of $\overline{T_{dm}}$.
- The capacity flow balances at heat exchanger demands, CP_{dm} , are expressed by Eq(10) to Eq(13) and its temperatures ($\overline{T_{dm}}$) are given by Eq(14) to Eq(17). Similar equations can be obtained for CP_{sl} and $\overline{T_{sl}}$.

$$CP_{dm} = [\sum_{i=1}^{N_s+1} f_{ij} + \sum_{r=1}^{N_u} y_{rj} \times f_{rj}] \times c_p \quad \forall T_{dj} > T_{si}, \quad m = j, \quad j \in \{1, 2, \dots, N_d + 1\} \quad (10)$$

$$CP_{dm} = [\sum_{i=1}^{N_s+1} f_{ij} + \sum_{r=1}^{N_u} (1 - y_{rj}) \times f_{rj}] \times c_p \quad \forall T_{dj} \leq T_{si}, \quad m = |N_d + 1| + j, \quad j \in \{1, 2, \dots, N_d + 1\} \quad (11)$$

$$CP_{dm} = [\sum_{i=1}^{N_s+1} x_{ir} \times f_{ir}] \times c_p, \quad m = 2|N_d + 1| + r, \quad \forall r \in \{1, 2, \dots, N_u\} \quad (12)$$

$$CP_{dm} = [\sum_{i=1}^{N_s+1} (1 - x_{ir}) \times f_{ir}] \times c_p, \quad m = 2|N_d + 1| + |N_u| + r, \quad \forall r \in \{1, 2, \dots, N_u\} \quad (13)$$

$$\overline{T}_{dm} = T_{dj} + \Delta T_{min} \quad m = j, \quad \forall j \in \{1, 2, \dots, N_d + 1\} \quad (14)$$

$$\overline{T}_{dm} = T_{si} \quad m = |N_d + 1| + j, \quad \forall j \in \{1, 2, \dots, N_d + 1\} \quad (15)$$

$$\overline{T}_{dm} = T_{ur} + \Delta T_{min} \quad m = 2|N_d + 1| + r, \quad \forall r \in \{1, 2, \dots, N_u\} \quad (16)$$

$$\overline{T}_{dm} = T_{ur} \quad m = 2|N_d + 1| + |N_u| + r, \quad \forall r \in \{1, 2, \dots, N_u\} \quad (17)$$

h_{lm} denotes the heat capacity flow rate from CP_{sl} to CP_{dm} . The heat capacity flow balance has to be satisfied for heat exchanger demands (Eq(18)) and sources (Eq(19)). The energy balance for the heat exchanger demands is given by Eq(20). $Q_{hu,m}$, and $Q_{cu,m}$ are the hot and cold utility requirements for the m^{th} demand.

$$\sum_{l=1}^{2|N_s+1|+2|N_u|} h_{lm} = CP_{dm} \quad \forall m \in \{1, 2, \dots, 2|N_d + 1| + 2|N_u|\} \quad (18)$$

$$\sum_{m=1}^{2|N_d+1|+2|N_u|} h_{lm} = CP_{sl} \quad \forall l \in \{1, 2, \dots, 2|N_s + 1| + 2|N_u|\} \quad (19)$$

$$\sum_{l=1}^{2|N_s+1|+2|N_u|} h_{lm} \times \overline{T}_{sl} + Q_{hu,m} - Q_{cu,m} = CP_{dm} \times \overline{T}_{dm} \quad \forall m \in \{1, 2, \dots, 2|N_d + 1| + 2|N_u|\} \quad (20)$$

This utility targeting problem is analogous to the freshwater targeting problem. C_{fw} , C_{reg} , C_{hu} , and C_{cu} are the costs of fresh water, regenerated water, hot utility, and cold utility. The objective is to minimize the TOC, given by Eq(21), subject to Eqs(1) - (20) along with the equations for (1) binary variable for source to regenerator matches; (2) water source to heat exchanger source allocation; and (3) modified source temperatures, \overline{T}_{sl} . The three sets of equations, being similar to the equations expressed for demands, have been excluded for brevity.

$$\text{Min TOC} = C_{fw} \sum_{j=1}^{N_d} f_{(N_s+1)j} + C_{reg} \sum_{r=1}^{N_u} \sum_{j=1}^{N_d+1} f_{rj} + C_{hu} \sum_{m=1}^{2|N_d+1|+2|N_u|} Q_{hu,m} + C_{cu} \sum_{m=1}^{2|N_d+1|+2|N_u|} Q_{cu,m} \quad (21)$$

This is a MINLP model due to the non-linear constraints that are given by Eq(4), Eq(5), and Eq(20) and mixed integer constraints given by Eq(10) to Eq(13) along with the similar equations obtained for heat exchanger sources. If the temperature of regeneration unit is predetermined, then the model will be simplified to an NLP for fixed removal ratio type of regeneration unit with the non-linear constraints given by Eq(4) to Eq(5). The model will be further simplified to a linear programming (LP) formulation if a fixed outlet type of regeneration unit is used as $C_{ur,v}$ is known (Eq(4) is not required), making Eq(5) linear. The proposed methodology simplifies the existing mathematical programming formulations, where all the temperatures are specified. A method is developed to optimize the regeneration temperature, which ensures a minimum TOC. This is demonstrated through an example adapted from literature. GAMS 24.2.2 software is used for optimization with the solvers BARON (version 12.7.7) for NLP and MINLP models, and CONOPT 3 (version 3.15N) for the LP model.

4. Illustrative Example

The limiting process data for this example are shown in Table 1 (Ahmetović et al., 2014). Freshwater is available at 80 °C and waste is discharged at 60 °C. The c_p of water is 4.2 kJ/(kg °C). The cost of fresh water, regenerated water, hot utility, and cold utility is \$ 0.45/t, \$ 0.0067/t, \$ 377/kW, and \$ 189/kW and the yearly working hours of the plant are 8,000 h. ΔT_{min} is considered to be 10 °C. A single regeneration unit is used. The freshwater (and wastewater), hot utility, and cold utility requirements without regeneration were reported as 70 kg/s, 1,260 kW, and 7,140 kW by Ibrić et al. (2013) and the TOC is obtained as \$ 2.7 M.

Table 1: Limiting Process Data (Ahmetović et al., 2014)

Sources (Si)	Flow rate (kg/s)	Contaminant concentration (ppm)			Temperature (°C)	Demands (Dj)	Flow rate (kg/s)	Contaminant concentration (ppm)			Temperature (°C)
		A	B	C				A	B	C	
S1	30	100	80	60	100	D1	30	0	0	0	100
S2	40	150	115	105	75	D2	40	50	40	15	75
S3	20	125	80	130	35	D3	20	50	50	30	35

The removal ratios for contaminants A, B, and C are 90 %, 70 %, and 98 % (Ahmetović et al., 2014). The discharge limit is given to be 30 ppm for all the contaminants. A fixed regeneration temperature of 60 °C is considered. The freshwater (and wastewater), regenerated water, hot, and cold utility requirements are obtained to be 30 kg/s, 73.57 kg/s, 1,260 kW, and 3,780 kW from the proposed NLP. TOC of \$ 1.6 M is achieved. TOC drops by 41 % upon the incorporation of regeneration unit. These results are comparable to the results obtained through sequential (Ahmetović et al., 2014) as well as simultaneous (Ibrić et al., 2014) optimization. Apart from the amount of regeneration (76.82 kg/s) and consequently the TOC, identical results were obtained by Ibrić et al. (2016). The NLP was solved by varying the regeneration temperature within the range of process operation (35 °C to 100 °C). The variation in water cost, energy cost, and consequently the TOC with the regeneration temperature is shown in Figure 2. With the increase in regeneration temperature, the water cost remains the same; while the energy cost and TOC remain constant (minimum) from 35 °C to 75 °C, and then increase. The optimum temperature range is achieved to be 35 °C to 75 °C. A MINLP is solved to optimize fresh water and energy consumption considering a variable regeneration temperature. The optimum regeneration temperature is found to be 75 °C (within the range obtained previously). The water allocation network is given in Table 2 for this case. The fresh water, regenerated water, hot utility, and cold utility requirements are found to be same as compared to the case where regeneration temperature is 60 °C.

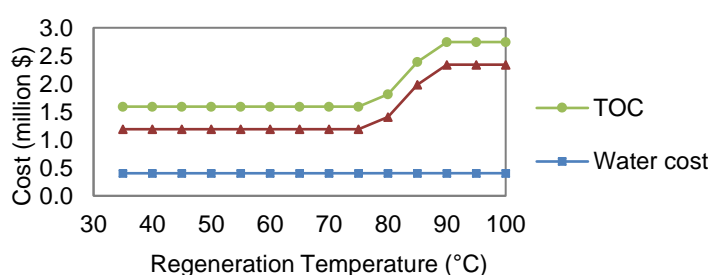


Figure 2: Variation in water cost, energy cost and TOC with the regeneration temperature

Table 2: Water allocation network for fixed RR type of regeneration unit (flow rates given in kg/s)

	D1	D2	D3	D4	R
S1	-	8.19	6.76	-	15.05
S2	-	-	-	-	40
S3	-	-	1.31	0.17	18.52
S4	30	-	-	-	-
R	-	31.81	11.93	29.83	-

Consider a fixed outlet type of regeneration unit that provides water at a contaminant concentration of $C_A = 60$ ppm, $C_B = 80$ ppm, $C_C = 30$ ppm, which is also the upper limit on the contaminant to be discharged. The LP model is solved for a regeneration temperature of 60 °C. The freshwater (and wastewater), regenerated water, the hot utility and cold utility are found to be 57.5 kg/s, 83.75 kg/s, 1,260 kW, and 6,090 kW. The TOC is \$ 2.4 M (11 % TOC reduction through regeneration). The LP model is solved for temperatures within the range of process temperatures. A trend similar to that obtained in Figure 2 is observed. The optimum range of operation is found to be 35 °C to 75 °C. The optimum temperature is found to be 75 °C from the MINLP by considering variable regeneration temperature. The freshwater (and wastewater), regeneration water, and utility requirements are identical to the results from a fixed regeneration temperature of 60 °C. The water allocation network (for $T_U = 75$ °C) is shown in Table 3. The utility targets for the water allocation network are verified as shown in Table 4.

Table 3: Water allocation network for fixed outlet type of regeneration unit (flow rates given in kg/s)

	D1	D2	D3	D4	R
S1	-	-	6.25	-	23.75
S2	-	-	-	-	40
S3	-	-	-	-	20
S4	30	20	7.5	-	-
R	-	20	6.25	57.5	-

Table 4: Energy targeting for water network in Table 3

T_H (°C)	F_{13}	F_{1R}	F_{42}	F_{43}	F_{R3}	F_{R4}	Q_H (kW)	T_C (°C)	F_{3R}	F_{41}	Q_C (kW)	Q (kW)
kg/s→	6.25	23.75	20	7.5	6.25	57.5			20	30		
110							0	100		↑		1,260 (Q_{hu})
100	↓	↓					1,260	90		↑	1,260	0
90	↓	↓					630	80		↑	0	0
85	↓	↓					630	75	↑		420	630
80	↓	↓	↓	↓			1,207.5	70	↑		420	840
75	↓	↓	↓	↓	↓	↓	4,882.5	65	↑		1,260	1,627.5
60	↓			↓	↓	↓	1,260	50	↑		1,260	5,250
45	↓			↓	↓		840	35	↑		0	5,250
35	↓			↓	↓			25				6,090 (Q_{cu})

5. Conclusions

A simultaneous solution strategy is proposed for the optimization of HIWRN. The formulations are based on the principle of thermodynamically equivalent heat exchangers. An NLP model for fixed removal ratio type and an LP model for fixed outlet type regeneration unit are developed to minimize the TOC. The LP/NLP models are solved for different regeneration temperatures to find out an optimum range of operating temperatures. A novel MINLP formulation optimizes the energy and water through variable regeneration temperature. The future research will be directed towards the improvement of the MINLP model. The model needs to be extended to optimize HIWRNs with variable process temperatures and include non-isothermal mixing.

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