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Targeting minimum waste treatment flow rate

Santanu Bandyopadhyay *

Energy Science and Engineering, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India

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ABSTRACT

Due to various environmental regulations, it is important to minimize the cost associated with treatment of different industrial wastes prior to its discharge to the environment. In this paper, an algebraic methodology, based on the principles of process integration, is proposed to target the minimum waste treatment flow rate to satisfy environmentally safe discharge limit. An associated graphical representation of the optimization problem is also provided to gain physical insight. In the proposed methodology, the treatment units are modelled either as unit with constant outlet concentration or as a unit with fixed removal ratio. There is flow loss associated with the treatment unit. The flow loss is assumed to be proportional to the inlet flow rate. Applicability of the proposed methodology is demonstrated through examples from water management, volatile organic compound treatment and flue gas desulphurization.

1. Introduction

The cost of treating different waste streams is increasing steadily as environmental regulations are becoming more and more stringent. It is, therefore, important to minimize the cost associated with treatment of these wastes while satisfying the environmental norms. Targeting and designing waste allocation network for optimal treatment can be effectively addressed through process integration techniques. Techniques of process integration are primarily used for process design (both grassroots and retrofits) with special emphasis on efficient utilization of resources and reducing environmental pollution. Techniques of process integration were originally developed for analyzing heat exchanger networks [1,2] and integration of energy intensive equipments [3,4]. Later, these techniques are evolved to address mass exchanger networks [5,6] and water networks [7–9]. Recently, the techniques of process integration have been applied for design and optimization of various energy systems [10–17]. Bandyopadhyay [18] demonstrated the applicability of targeting tools for waste reduction. Primary objective of this paper is to propose an algebraic methodology, based on the principles of process integration, for targeting the minimum waste treatment flow rate to satisfy environmentally safe discharge limit.

Techniques of process integration may be classified into two broad categories: graphical pinch analysis-based approaches and approaches based on mathematical optimization techniques. Graphical pinch analysis-based approaches help in getting a physical insight of the problem through its graphical representations and simplified tableau-based calculation procedures. On the other hand, mathematical optimization-based methodologies are preferred to address issues like multiple contaminants, controllability, flexibility, cost-optimality, etc. In this paper, an algebraic approach based on tableau-based calculation procedure is proposed and associated graphical representation is also provided to gain physical insight of the problem. However, the proposed methodology is restricted to single contaminant only.

In a seminal paper, Takama et al. [19] solved the complete water management problem using superstructure-based non-linear optimization technique. Wang and Smith [20] have developed a systematic approach for designing distributed effluent treatment systems. This procedure has been extended by Kuo and Smith [21] for multiple treatment processes. Mathematical optimization techniques have also been used to design distributed effluent treatment systems [22,23]. Freitas et al. [24] proposed the use of the hierarchical design approach [25], supplemented with a database and expert system to determine the best sequence of treatment processes. However, such a method cannot guarantee the optimality. Statyukha et al. [26] proposed a hybrid approach for designing wastewater treatment networks. The insight-based technique is employed to obtain an initial solution and then superstructure-based non-linear optimization is solved. Zhelev and Bhaw [27] introduced combined water and oxygen pinch analysis for designing optimum wastewater treatment network. The minimum oxygen requirement for waste degradation was targeted in combination of the water pinch analysis. Interaction between operations that use water and effluent treatment systems have also been addressed [8,28–33]. Alva-Argáez et al. [34,35] addressed the entire water

* Tel.: +91 22 25767894; fax: +91 22 25726875.
E-mail address: santanu@me.iitb.ac.in.

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management problem through superstructure-based MINLP formulation.

In literature, treatment units are either modelled as unit with constant outlet concentration (e.g., filtration, and membrane separation systems) or as a unit with fixed removal ratio (e.g., scrubber). These units are typically modelled without any flow loss. Most treatment units such as membrane separation systems (e.g., microfiltration, ultrafiltration, reverse osmosis, etc.), flotation systems (e.g., dissolved air flotation, induced air flotation, etc.), gravity and settling systems (e.g., coagulation, flocculation, clarification, etc.), filtration systems (e.g., granular bed, vacuum drum, press, belt filter, etc.), etc. have flow loss associated with them. For example, a membrane-based treatment system separates a feed stream into two product streams; a lower concentration permeate and a higher concentration retentate (or reject) streams. In literature such treatment units with two product streams are termed as partitioning treatment units [36,37]. Typically, higher concentrate reject stream form a partitioning unit is not reused in the process and is sent for treatment separately. Mathematical optimization-based methodology has been proposed in the context of water regeneration and reuse [36]. In this paper, treatment units are assumed to have flow loss and applied to satisfy the environmental discharge norms. An algebraic targeting methodology is developed to incorporate such treatment units with flow loss in the process design to satisfy the environmental regulations. Applicability of the proposed methodology is demonstrated through different illustrative examples.

2. Problem statement

The general problem of targeting the minimum waste treatment flow rate using waste composite curve may be mathematically stated as follows. In a process, a set of N_w waste sources is given. Each waste source produces a flow F_{wi} with a given contaminant concentration of C_{wi}. As the environmental regulations imposed on the overall plant, C_e denotes the concentration below which waste may be discharged to the environment. These waste streams have to be treated and contaminant has to be removed in the treatment plant. The objective of this work is to develop an algorithmic technique with graphical representation to target the minimum effluent flow rate to be treated in the treatment plant. In this paper, we assume that only one treatment plant is sufficient for the purpose and the proposed methodology is restricted to single contaminant.

An effluent treatment unit with flow loss may be modelled in two ways: constant outlet concentration and constant removal factor. Furthermore, there may be an added constraint on the maximum inlet concentration to a treatment unit. For both kinds of treatment units, the outlet flow rate from the treatment unit (F_{Tout}) is assumed to be proportional to the inlet flow rate to the treatment unit (F_{Tin}).

$$F_{Tout} = \alpha F_{Tin} \tag{1}$$

Eq. (1) suggests that $(1-\alpha)$ times the inlet flow rate to the treatment unit (F_{Tin}) is lost during treatment and α may be called the flow factor of the treatment unit. It may be noted that treatment units are not modelled as partitioning treatment units [36,37] in this paper. A partitioning treatment unit produces a highly concentrated reject stream that has to be treated separately in another treatment unit. In this paper, treatment units are simply modelled with flow loss and it is assumed that the lost flow cannot be recovered as a separate stream. However, a partitioning treatment unit can also be modelled as a treatment unit with flow loss and higher concentration reject stream has to be treated separately or may be converted into by-product. Treatment of such reject streams or production of saleable by-products are beyond the scope of the proposed algebraic methodology.

For a treatment unit with constant outlet concentration (C_{Tout}), the treated waste comes out of the treatment unit at a fixed concentration of C_{Tout} and this is independent of the inlet concentration (C_{Tin}). On the other hand, for a treatment unit with constant removal factor, the outlet concentration (C_{Tout}) of the treated effluent depends on the inlet concentration of the effluent to the treatment unit (C_{Tin}). The removal ratio (r) of the treatment unit is defined as

$$r = \frac{F_{Tin}C_{Tin} - F_{Tout}C_{Tout}}{F_{Tin}C_{Tin}} \tag{2}$$

Additional constraint in the form of the maximum inlet concentration to the treatment unit may also be imposed for overall optimization.

The objective is to minimize the inlet flow rate to the waste treatment plant (F_{Tin}) such that the concentration of the remaining waste, after mixing with the treated one, is less than the specified environmental discharge limit (C_e).

3. Targeting minimum effluent flow rate

Bandyopadhyay et al. [8] have proposed a novel limiting composite curve, called the source composite curve, to simultaneously target the minimum freshwater requirement, the maximum water reuse, the minimum wastewater generation, and the minimum effluent to be treated to meet environmental norms. To target the minimum effluent to be treated to meet the environmental regulation, a wastewater composite curve was proposed [8]. It may be noted that the wastewater composite curve is equivalent to the original source composite curve without any internal demand. The wastewater composite curve is plotted on contaminant load (M) vs. concentration (C) diagram. Generation of the waste composite curve (equivalent to the wastewater composite curve) for a given set of waste sources is discussed briefly before developing the targeting methodologies. Formulae for each step are tabulated in Table 1.

Step 1: Concentrations of all waste sources including the environmental limit are tabulated in decreasing order in the first column. If value of a particular concentration occurs more than once, the same need not be repeated. Without loss of generality, it can be said that the concentration for kth row is denoted as C_k such that

$$C_1 > C_2 > \cdots > C_k > \cdots > C_n \tag{3}$$

In may be noted that the last entry of this column should be zero ($C_n = 0$).

Step 2: Net waste flows (i.e., sum of waste flow rates corresponding to a particular concentration) are tabulated in second column. For kth row, net flow rate is denoted as F_k (Table 1).

Step 3: Cumulative waste flow rates are tabulated in the third column. Summation of net waste flow rates for all previous rows ($\sum_{l=1}^{k} F_l$) denotes the cumulative flows for kth row. Last entry in this column suggests the total waste available (F_T) for a given problem.

Step 4: Fourth column represents the contaminant load (m_k) for each concentration interval. Contaminant load is defined as the product of the concentration with the flow rate. First entry in fourth column is assigned to be 0. For all subsequent rows, the difference between the last two concentrations is multiplied by the cumulative flow rates, tabulated in third column, to calculate the concentration load. Mathematically, concentration load (m_k) for each concentration

Table 1
Tabular representation for generation of waste composite curve.

	First column Concentration	Second column Net waste flows	Third column Cumulative flows	Fourth column Contaminant load	Fifth column Cumulative contaminant load
First row	C_1	F_1	F_1	$m_1=0$	$M_1=m_1=0$
Second row	C_2	F_2	F_1+F_2	$m_2=F_1\ (C_1-C_2)$	$M_2=m_1+m_2$ $=F_1\ (C_1-C_2)$
...	...	...	...	...	...
kth row	C_k	F_k	$\sum_{l=1}^{k} F_l$	m_k $=(C_{k-1}-C_k)(\sum_{l=1}^{k-1} F_l)$	M_k $=\sum_{l=1}^{k} m_l=\sum_{l=1}^{k-1} F_l(C_l-C_k)$
...	...	...	...	...	...
nth (last) row	$C_n=0$	F_n	$\sum_{l=1}^{n} F_l=F_T$	m_n $=C_{n-1}(\sum_{l=1}^{n-1} F_l)$	$M_T=\sum_{l=1}^{n} m_l$ $=\sum_{l=1}^{n-1} F_l C_l$

interval can be calculated using the following formula.

$$\begin{aligned} m_k &= 0 && \text{for } k=1 \\ &= (C_{k-1}-C_k)\left(\sum_{l=1}^{k-1} F_l\right) && \text{for } k>1 \end{aligned} \tag{4}$$

Step 5: Cumulative contaminant loads are calculated by summing contaminant loads for all previous rows ($M_k=\sum_{l\le k} m_l$) and tabulated in the fifth column. Using Eq. (4), cumulative contaminant load for kth row may be expressed as

$$\begin{aligned} M_k &= 0 && \text{for } k=1 \\ &= \sum_{l=1}^{k-1} F_l(C_l-C_k) && \text{for } k>1 \end{aligned} \tag{5}$$

Last entry in this column suggests the total contaminant load available (M_T) for a given problem.

$$M_T=\sum_{l=1}^{n} m_l=\sum_{l=1}^{n-1} F_l C_l \tag{6}$$

Now fifth column (cumulative contaminant load) may be plotted against the first column (concentration) to obtain the waste composite curve.

3.1. Treatment unit with constant outlet concentration

The outlet concentration of the waste, treated in a treatment unit with constant outlet concentration, is always fixed at C_{Tout}. The relation between the outlet flow rate (F_{Tout}) from the treatment unit and the inlet flow rate (F_{Tin}) to the treatment unit is given by Eq. (1). Total contaminant load removed (M_R) by the treatment unit is expressed as follows:

$$M_R=F_{Tin}C_{Tin}-F_{Tout}C_{Tout}=F_{Tin}(C_{Tin}-\alpha C_{Tout}) \tag{7}$$

Rearranging the above equation, the inlet concentration to the treatment unit can be expressed as follows:

$$C_{Tin}=\frac{M_R}{F_{Tin}}+\alpha C_{Tout} \tag{8}$$

For targeting the minimum effluent flow rate to be treated in the treatment without any flow loss ($\alpha=1$), treatment line is rotated on the contaminant load (M) vs. concentration (C) diagram. The minimum treatment flow rate is targeted by rotating the treatment line with point (M_R, C_{Tout}) as the pivot point such that it just touches the waste composite curve. The point at which the treatment line touches the waste composite curve represents the treatment pinch point and the point at which it touches the concentration axis represents the inlet concentration to the treatment unit. However, the same methodology cannot be applied directly due to the flow loss associated with the treatment unit. For a treatment unit with constant outlet concentration and flow loss, the treatment line on a contaminant load (M) vs. concentration (C) diagram must pass through the points (0, C_{Tin}) and ($F_{Tin}\ \{C_{Tin}-C_{Tout}\}$, C_{Tout}). Using Eq. (8), $F_{Tin}\ (C_{Tin}-C_{Tout})$ can be simplified as $M_R-(1-\alpha)\ F_{Tin}\ C_{Tout}$. Therefore, the treatment line must pass through the points (0, C_{Tin}) and ($M_R-\{1-\alpha\}\ F_{Tin}\ C_{Tout}$, C_{Tout}). If the point (M_k, C_k) on the source composite curve holds the treatment pinch, the effluent flow rate at the inlet of the treatment unit is calculated to be:

$$f_{Tk}=\frac{M_R-M_k}{C_k-\alpha C_{Tout}} \tag{9}$$

After treating a portion of the waste in the treatment unit, remaining waste, including the treated one, may be discharged to the environment. Therefore, a total of $F_T-(1-\alpha)\ f_{Tk}$ waste is discharged with a contaminant load of M_T-M_R. To satisfy the environmental discharge limit, following equation must be satisfied.

$$\frac{M_T-M_R}{F_T-(1-\alpha)f_{Tk}}\le C_e \tag{10}$$

Eliminating M_R form Eqs. (9) and (10), the treatment flow rate can be expressed as

$$f_{Tk}\ge\frac{M_T-F_TC_e-M_k}{C_k-\alpha C_{Tout}-(1-\alpha)C_e} \tag{11}$$

The above inequality can be applied to target the minimum waste flow rate to be treated in the treatment unit. Algorithmic step, in continuation of the previous steps, is described below to target the minimum waste treatment flow rate.

Step 6: Waste flow rates corresponding to the contaminant concentrations (tabulated in the first column) and the cumulative contaminant loads (tabulated in the fifth column), are calculated applying the following equation and tabulated in the sixth column.

$$\begin{aligned} f_{Tk} &= \frac{M_T-F_TC_e-M_k}{C_k-\alpha C_{Tout}-(1-\alpha)C_e} && \text{when } C_k\ge C_{Tout} \\ &= 0 && \text{otherwise} \end{aligned} \tag{12}$$

Maximum entry in this column defines the minimum waste flow rate to be treated in the treatment unit.

For some treatment unit, an additional constraint in the form of the maximum allowable inlet concentration ($C_{Tin\max}$) to the treatment unit is also specified. The minimum waste flow rate to the treatment unit that satisfy the additional constraint may be calculated directly using the following equation:

$$f_T=\frac{M_T-F_TC_e}{C_{Tin\max}-\alpha C_{Tout}-(1-\alpha)C_e} \tag{13}$$

The minimum waste treatment flow rate to be treated in the treatment unit is the maximum of the flow rates obtained using Eqs. (12) and (13).

3.2. Treatment unit with constant removal ratio

For a treatment unit with constant removal factor, the relation between the outlet concentration (C_{Tout}) of the treated waste and the inlet concentration (C_{Tin}) to the treatment unit is given by Eq. (2). Combining Eq. (1) with the definition of the removal ratio, the inlet concentration to the treatment unit can be expressed as a function of the outlet concentration.

$$C_{Tin} = \frac{\alpha}{1-r} C_{Tout} \tag{14}$$

Total contaminant load removed (M_R) by the treatment unit is simplified as follows:

$$M_R = F_{Tin} C_{Tin} - F_{Tout} C_{Tout} = F_{Tin} C_{Tin} r \tag{15}$$

For targeting the minimum waste flow rate to be treated in the treatment unit without any flow loss ($\alpha = 1$), treatment line is rotated on the contaminant load (M) vs. concentration (C) diagram. The pivot point for targeting the minimum treatment flow rate is (M_R/r, 0). It may be noted that the pivot points are different for different types of treatment units. Similar to the previous section, the point at which the treatment line touches the waste composite curve represents the treatment pinch point and the point at which it touches the concentration axis represents the inlet concentration to the treatment unit. Due to flow loss associated with the treatment unit, the same methodology cannot be applied directly.

Similar to the previous section, the treatment line on a contaminant load (M) vs. concentration (C) diagram must pass through the points $(0, C_{Tin})$ and $(F_{Tin}\{C_{Tin} - C_{Tout}\}, C_{Tout})$. Using Eqs. (14) and (15), F_{Tin} $(C_{Tin} - C_{Tout})$ can be simplified as M_R $(1-\alpha-r)/r\,\alpha$. Therefore, the treatment line must pass through the points (0, C_{Tin}) and (M_R $(1-\alpha-r)/r\,\alpha$, C_{Tout}). The waste flow rate at the inlet of the treatment unit, if the point (M_k, C_k) on the waste composite curve holds the treatment pinch, is calculated to be:

$$f_{Tk} = \frac{M_R/r - M_k}{C_k} \tag{16}$$

Similar to the previous section, after treating a portion of the waste in the treatment unit, remaining waste, including the treated one, may be discharged to the environment. To satisfy the environmental discharge limit, Eq. (10) has to be satisfied. Eliminating M_R from Eqs. (10) and (16), the treatment flow rate can be expressed as

$$f_{Tk} \geq \frac{M_T - F_T C_e - rM_k}{rC_k - (1-\alpha)C_e} \tag{17}$$

Similar to Eq. (11), Eq. (17) can be applied to target the minimum waste flow rate to be treated in the treatment unit having constant removal ratio. An algorithmic step is described below to target the minimum waste treatment flow rate.

Step 6: Waste flows corresponding to the contaminant concentrations (tabulated in the first column) and the cumulative contaminant loads (tabulated in the fifth column), are calculated applying the following equation and tabulated in the sixth column.

$$f_{Tk} \begin{cases} = \dfrac{M_T - F_T C_e - rM_k}{rC_k - (1-\alpha)C_e} & \text{when } M_k \leq M_c \\ = 0 & \text{otherwise} \end{cases} \tag{18}$$

where the critical contaminant mass load (M_c) is calculated as follows:

$$M_c = \frac{(M_T - F_T C_e)(\alpha + r - 1)}{r\alpha - (1-\alpha)(1-r)(C_e/C_k)} \tag{19}$$

Eq. (19) is equivalent to the condition that $C_k \geq C_{Tout}$. Maximum entry in this column defines the minimum waste flows to be treated in the treatment unit.

In absence of the additional constraint of the maximum allowable inlet concentration ($C_{Tin\,max}$) to the treatment unit, Eq. (18) targets the minimum waste flow rate to be treated in the treatment unit. Similar to Eq. (13), the minimum waste flow rate to the treatment unit that satisfy the additional constraint of the maximum allowable inlet concentration ($C_{Tin\,max}$) to the treatment unit, may be calculated directly using the following equation:

$$f_T = \frac{M_T - F_T C_e}{rC_{Tin\,max} - (1-\alpha)C_e} \tag{20}$$

The minimum waste treatment flow rate to be treated in the treatment unit is the maximum of the flow rates obtained using Eqs. (18) and (20).

For a low value of both removal ratio and flow factor, the environmental discharge concentration controls the pinch point. In such cases, treated waste from the treatment unit has to be recycled across the treatment unit. However, due to flow loss associate with the treatment unit, there exists a minimum value of flow factor for which the targeting step is physically meaningful. The minimum value of the flow factor is expressed as follows:

$$\alpha_{min} = \frac{M_T(1-r)}{M_T(1-r) - rF_T C_e} \tag{21}$$

The limiting flow rate to the treatment unit is given as

$$f_{T\,max} = F_T \frac{M_T(1-r)}{rC_e} \tag{22}$$

If the actual alpha is lower than the minimum, the entire waste to the treatment unit is lost and no waste is produced. It suggests that such a simple model cannot be used and a more realistic model has to be used.

Application of the proposed algorithm is demonstrated through the following illustrative examples.

4. Illustrative examples

In this section different illustrative examples are considered to demonstrate the applicability of the proposed methodology. Examples are considered from the field of water management, treatment of volatile organic compounds (VOCs), and desulphurization of flue gases.

4.1. Example 1: Water treatment through a treatment unit with constant outlet concentration

This example is taken from the field of wastewater treatment. The wastewater and treatment unit data for this example are given in Table 2. There are two wastewater sources. The outlet concentration of the treatment unit is fixed at 25 ppm. In the first case, no restriction related to the inlet concentration to the treatment unit is imposed. Later on, an additional constraint on the maximum allowable inlet concentration of 500 ppm to the treatment unit is imposed. The objective is to target the minimum amount of effluent to be treated in the treatment unit to satisfy the environmental discharge limit of 30 ppm.

The steps of the proposed algorithm are shown in Table 3. In the first column of Table 3, concentrations of all water sources, including the environmental limit, are tabulated in decreasing order (step

Table 2
Wastewater and treatment unit data for example 1.

#	Contaminant concentration (ppm)	Flow rate (t/h)
1	800	50
2	400	100

Environmental limit for discharge concentration, C_e = 30 ppm. Characteristics of the treatment unit, α = 0.8, C_{Tout} = 25 ppm, and $C_{Tin\,max}$ = 500 ppm.

Table 3
Generation of waste composite curve and targeting for minimum effluent flow rate to be treated for example 1.

Contaminant concentration (ppm)	Net flow rate (t/h)	Cumulative flow rate (t/h)	Contaminant mass load (kg/h)	Cumulative mass load (kg/h)	Treatment flow rate (t/h)
800	50	50	0	0	97.55
400	100	150	20	20	148.40
30	0	150	55.5	75.5	0
25	0	150	0.75	76.25	0
0	0	150	3.75	80	0

1). Net waste flows, corresponding to each concentration in column one, is tabulated in the second column of Table 3 (step 2). Cumulative waste flow rates, as described in step 3 of the proposed algorithm, are tabulated in the third column. Contaminant mass loads, calculated using Eq. (4), are tabulated in the forth column of Table 3. Cumulative contaminant mass loads, calculated using step 5 of the proposed algorithm, are tabulated in column five of Table 3. For this example, the outlet concentration of the treatment unit is specified to be 25 ppm. Applying Eq. (12), treatment flow rates, corresponding to different contaminant concentrations, are calculated and tabulated in the sixth column of Table 3 (step 6).

The sixth column of Table 3 suggests that 148.4 t/h of effluent to be treated in the treatment unit to satisfy the environmental norm. Waste composite curve, shown in Fig. 1, is obtained by plotting fifth column against the first column. The treatment line is also shown in Fig. 1. Form Table 3 as well as from Fig. 1, the treatment pinch is identified to be 400 ppm. According to the pinch principles [20], any wastewater with concentration higher than the pinch concentration has to be treated in the treatment unit. Therefore, 50 t/h of wastewater at 800 ppm and 98.4 t/h of wastewater at 400 ppm must be put to the treatment unit. The inlet concentration of the wastewater to the treatment unit is 534.8 ppm. Remaining 1.6 t/h of wastewater at 400 ppm bypasses the treatment unit and mixed with the treated water to satisfy the discharge limit of 30 ppm. The wastewater allocation network is shown in Fig. 2a.

Without considering the flow loss associated with the treatment unit, the target for the minimum effluent flow rate to be treated in the treatment unit would have been 148 t/h. Due to flow loss associate with the treatment unit, the minimum flow rate of the effluent to be treated in the treatment unit is increased by 0.27% and the total wastewater discharged to the environment is reduced by 19.8%.

If the maximum allowable inlet concentration to the treatment unit is restricted to 500 ppm, Eq. (13) may be used to target the minimum effluent to be treated in the treatment unit. Treatment flow rate of 159.28 t/h satisfies the environmental limit. The treatment line for this case is not shown for brevity. Due to restriction on the maximum allowable inlet concentration to the treatment unit, the minimum flow rate of the effluent to be treated in the treatment unit is increased by 7.3% and the total wastewater discharged to the environment is reduced by 1.8%. It may be noted that there is no treatment pinch for this example. It may also be noted that the minimum effluent flow rate to be treated in the treatment unit is more than the total wastewater available. To satisfy the environmental norm, output from the treatment unit has to be recycled across it. The wastewater allocation network is shown in Fig. 2b. It may be noted that the entire wastewater at 400 ppm is not passed on to the treatment unit, while some portion of the treated water at 25 ppm is recycled across the treatment unit. Usual rule of designing wastewater allocation network cannot be applied to such problems. However, once the targets are set, nearest neighbor algorithm [38] may be applied to design the wastewater allocation network.

Variation of the minimum effluent treatment flow rate as a function of flow factor for different values of treatment unit outlet concentration is presented in Fig. 3. It may be noted that the constraint related to the minimum allowable inlet concentration to the treatment is relaxed while generating Fig. 3. It may be concluded that for this particular example, flow factor does not play a significant role in increasing the minimum effluent flow rate to be treated in the treatment unit. For this particular example, application of different existing algebraic and graphical methodologies [8,20,21,28,31], neglecting flow loss associated with the treatment unit, may not lead to any significant error. However, this may not be the general case and moreover, the total waste discharged to the

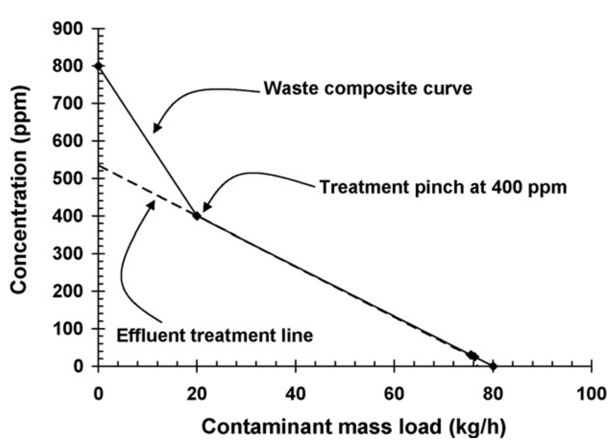

Fig. 1. Waste composite curve for example 1 and effluent treatment line for unconstraint case.

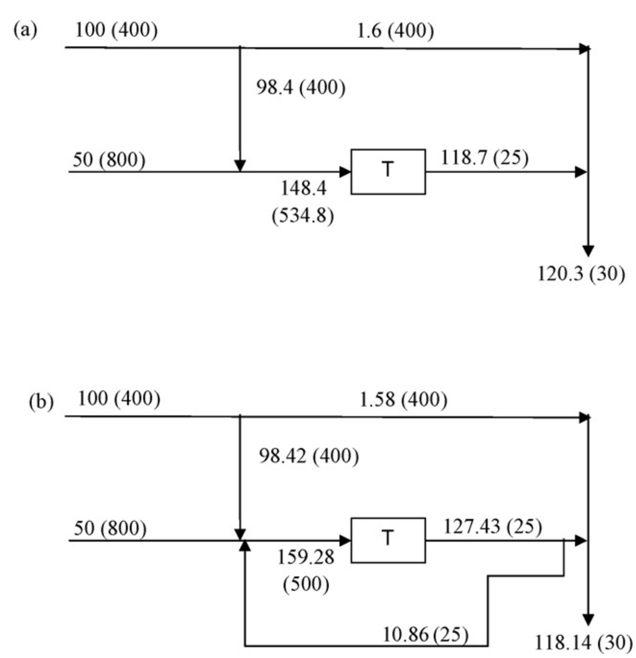

Fig. 2. Wastewater allocation networks for example 1: (a) without any restriction on the inlet concentration to the treatment unit, and (b) the maximum allowable inlet concentration to the treatment unit is restricted to 500 ppm. (The values show flow rate in t/h with contaminant concentrations in ppm within parenthesis.)

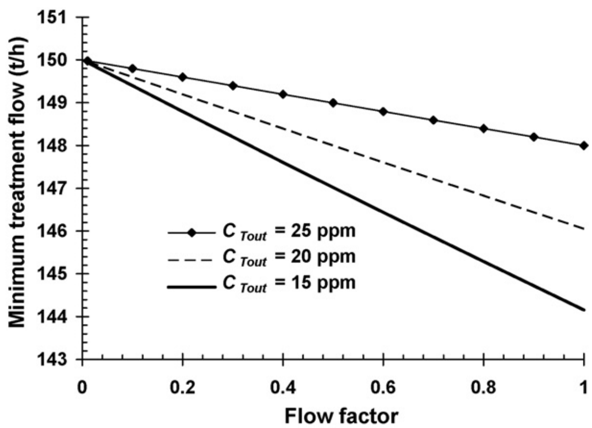

Fig. 3. Variation of the minimum effluent treatment flow rate as a function of flow factor for different values of treatment unit outlet concentration.

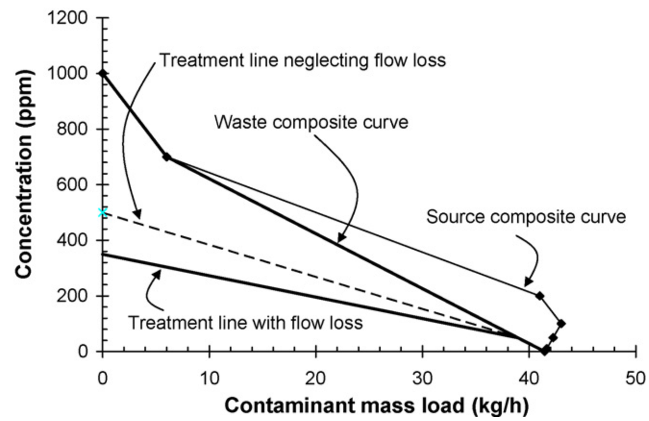

Fig. 4. Source composite curve, waste composite curve, and treatment line for example 2.

environment reduces drastically due to higher flow loss (i.e., lower flow factor).

4.2. Example 2: Total water management of a specialty chemical plant

This example is also taken from the field of waste management of a specialty chemical plant. Limiting process data for this example are given in Table 4 [8,20]. The removal ratio and the flow factor of the effluent treatment unit are assumed to be 0.9 and 0.7, respectively. Furthermore, it has been assumed that the treated water cannot be recycled across the water-using processes. Bandyopadhyay et al. [8] have targeted the minimum requirement of 90.64 t/h of freshwater and 50.64 t/h of wastewater generation. Corresponding freshwater pinch is determined to be 700 ppm. In this example, wastewater is generated at two concentration levels: 20 t/h of wastewater is generated at 1000 ppm and 30.64 t/h of wastewater is generated at 700 ppm.

Based on the proposed algorithm (Table 5), the minimum effluent treatment flow rate is targeted to be 129.72 t/h. Source composite curve, waste composite curve, and the treatment line are shown in Fig. 4. Inlet concentration to the treatment unit is calculated to be 350 ppm and the treatment pinch is identified to be 400 ppm. The minimum effluent flow rate to be treated in the treatment unit is more than the total wastewater available. Therefore, to satisfy the environmental norm, output from the treatment unit has to be recycled across the treatment unit. 79.08 t/h of treated water has to be recycled across the treatment unit. Since this is a pinched problem, rules of pinch technology applies and waste allocation network can be designed accordingly (not shown for brevity). Targets for the minimum effluent treatment flow rate, corresponding to the neglected flow loss, is only 86.48 t/h. Application of different existing algebraic and graphical methodologies [8,20,21,28,31], neglecting flow loss associated with the treatment unit, underestimates the minimum effluent flow rate to be treated by 33.3%. Treatment line neglecting flow loss is shown in Fig. 4 for visual comparison with the treatment line with flow loss.

Variation of the minimum effluent treatment flow rate as a function of flow factor for different values of removal ratio is presented in Fig. 5. It may be concluded that for this particular example, flow factor as well as the removal factor play a significant role in determining the minimum effluent flow rate to be treated in the treatment unit.

4.3. Example 3: Reduction of emissions of volatile organic compounds

This example is related to the reduction of emissions of volatile organic compounds (VOCs) and VOCs are responsible for producing urban smog. VOCs are emitted from different sources in a process plant: condenser vents, purges, dryers, combustion processes, spillages, tank loading, fugitive emissions from gaskets,

Table 4
Limiting process data for example 2.

Processes	Inlet/demand		Outlet/source	
	Contaminant concentration (ppm)	Flow rate (t/h)	Contaminant concentration (ppm)	Flow rate (t/h)
Reactor/thickener	100	80	1000	20
Cyclone	200	50	700	50
Filtration	0	10	100	40
Steam system	0	10	10	10
Cooling system	10	15	100	5

Concentration of the freshwater, $C_{fw} = 0$ ppm. Environmental limit for discharge concentration, $C_e = 50$ ppm. Characteristics of the treatment unit, $\alpha = 0.7$ and $r = 0.9$.

Table 5
Waste composite curve and targeting for minimum effluent flow rate for example 2.

Contaminant concentration (ppm)	Net flow rate (t/h)	Cumulative flow rate (t/h)	Contaminant mass load (kg/h)	Cumulative mass load (kg/h)	Treatment flow rate (t/h)
1000	20	20	0	0	43.97
700	30.64	50.64	6	6	54.50
50	0	50.64	32.92	38.92	0
0	0	50.64	2.53	41.45	0

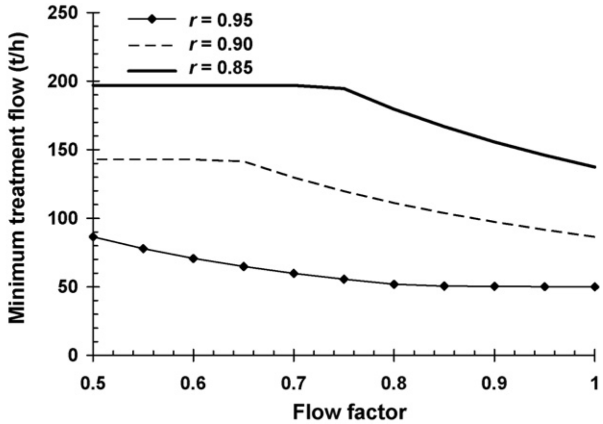

Fig. 5. Variation of the minimum effluent treatment flow rate as a function of flow factor for removal factors.

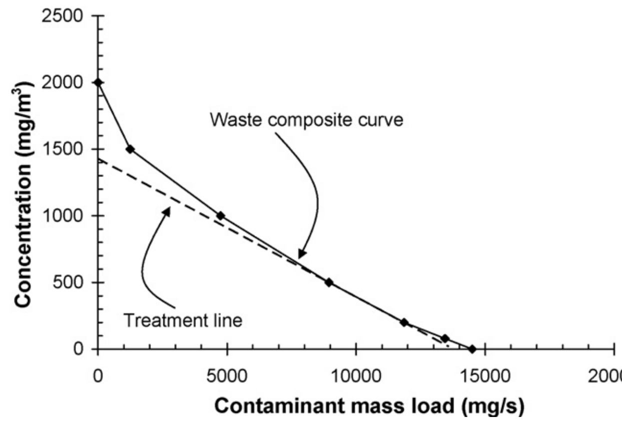

Fig. 6. Waste composite curve and treatment line for example 3.

Table 6
Process data for example 3.

#	Concentration (mg/m^3)	Flow rate (m^3/s)
1	2000	2.5
2	1500	4.5
3	1000	1.4
4	500	1.3
5	200	3.5

Environmental limit for discharge concentration, $C_e = 80\,\text{mg/m}^3$. Characteristics of the treatment unit, $\alpha = 0.75$, and $r = 0.99$.

Table 8
Process data for example 4.

#	Concentration (mg/N m^3)	Flow rate (N m^3/h)
1	5000	900,000
2	4500	105,000
3	500	1,500,000

Environmental limit for total discharge of SO_2, $M_e = 700 \times 10^6$ mg/h. Characteristics of the treatment unit, $\alpha = 0.98$, and $r = 0.90$.

shaft seals, sewers, etc. Significant reductions in VOC emissions can usually be achieved by controlling tank venting, condensers and purges and by thorough inspection and maintenance of gaskets and shaft seals. Methods such as condensation, membranes, absorption and adsorption are generally adopted to recover VOC from different source streams. After minimizing VOC emissions from different sources, different recovery processes may be implemented. Recovery, allocation and recycle/reuse of the VOC not only reduce environmental pollution, but also provide significant economic and environmental benefits to the process. Parthasarathy and El-Halwagi [39] presented optimum mass integration strategies for the maximum VOC recovery. After recovery, different treatment units must be considered for reduction in VOC emission. For treatment and reduction in VOCs, incineration in flares, thermal incinerators, catalytic incinerators, biological scrubbers, etc. may be employed. In this example, the minimum VOC laden stream flow rate to be treated in the treatment unit is determined to achieve the environmental norm.

Process data for this example are given in Table 6 [40]. Incineration, as the treatment process, removes 99% of the contaminant with a flow factor of 0.75 (assumed). Based on the proposed algorithm (Table 7), the minimum effluent treatment flow rate is targeted to be $9.65\,\text{m}^3/\text{s}$, which is 4.2% higher due to flow loss. Waste composite curve and the treatment line are shown in Fig. 6. Inlet concentration to the treatment unit is calculated to be $1427.5\,\text{mg/m}^3$ and the treatment pinch is identified to be $500\,\text{mg/m}^3$.

To avoid fire and explosion hazards in vent headers, vent gases are diluted by air or nitrogen. In practice, flammable mixtures are diluted to 30% or less of the flammability limit [40]. By diluting these gases with air or nitrogen, environmental discharge limit, in terms of concentration, can easily be achieved without any treatment unit. Therefore, it may be more meaningful to set environmental limit as terms of total discharge of waste in the environment. Proposed procedure of targeting cannot be applied directly for such cases. Alternate problem definition and targeting procedure are described below.

5. Targeting for specified total discharge

The general problem of targeting the minimum waste treatment flow rate for specified total discharge may be mathematically stated as follows. In a process, a set of N_w waste sources is given. Each waste source produces a flow F_{wi} with a given contaminant concentration of C_{wi}. As the environmental regulations imposed on the overall plant, M_e denotes the total mass flow rate of the contaminant below which waste may be discharged to the environment. Rest of the problem statement is similar to that described in Section 2.

The total contaminant load available (M_T) for a given problem can be obtained using Eq. (6). As the environmental discharge limit is known (M_e), total contaminant load removed (M_R) by the

Table 7
Waste composite curve and targeting for minimum waste treatment flow rate for example 3.

Contaminant concentration (mg/m^3)	Net flow rate (m^3/s)	Cumulative flow rate (m^3/s)	Contaminant mass load (mg/s)	Cumulative mass load (mg/s)	Treatment flow rate (m^3/s)
2000	2.5	2.5	0	0	6.86
1500	4.5	7	1250	1,250	8.33
1000	1.4	8.4	3500	4,750	9.01
500	1.3	9.7	4200	8,950	9.65
200	3.5	13.2	2910	11,860	9.57
80	0	13.2	1584	13,444	2.27
0	0	13.2	1056	14,500	0

Table 9
Waste composite curve and targeting for minimum flow rate to FGD unit for example 4.

Contaminant concentration (mg/N m^3)	Net flow rate (10^6 N m^3/h)	Cumulative flow rate (10^6 N m^3/h)	Contaminant mass load (10^6 mg/h)	Cumulative mass load (10^6 mg/h)	Treatment flow rate (10^6 N m^3/h)
5000	0.9	0.9	0	0	1.116
4500	0.105	1.005	450	450	1.140
500	1.5	2.505	4020	4470	2.221
0	0	2.505	751.5	5722.5	2.005

treatment unit is expressed as follows:

$$M_R = M_T - M_e \tag{23}$$

For a treatment unit with constant outlet concentration, Eq. (9) can be used directly to target the minimum waste flow rate to be treated in the treatment unit. In this case, first five steps for generating waste composite curve remain same. However, Eq. (12) in step six should be modified as follows:

$$\begin{aligned} f_{Tk} &= \frac{M_R - M_k}{C_k - \alpha C_{Tout}} \quad \text{when } C_k \geq C_{Tout} \\ &= 0 \quad \text{otherwise} \end{aligned} \tag{24}$$

For a treatment unit with constant removal factor, Eqs. (18) and (19) should be changed suitably to target the minimum waste flow rate to be treated in the treatment unit. For the specified total contaminant flow, the critical contaminant mass load (M_c) is calculated using the following formula:

$$M_c = \frac{M_R(\alpha + r - 1)}{r\alpha} \tag{25}$$

It may be noted that unlike Eq. (19), the value of the critical mass load is independent of the concentration C_k. To target the minimum flow rate to be treated in the treatment unit with fixed removal ratio and specified total mass load of the contaminant, Eq. (18) should be modified as follows:

$$\begin{aligned} f_{Tk} &= \frac{M_R - rM_k}{rC_k} \quad \text{when } M_k \leq M_c \\ &= \frac{M_R(1-r)/(\alpha r)}{C_{k-1} - (C_{k-1} - C_k)(M_c - M_{k-1})/(M_k - M_{k-1})} \quad \text{when } M_{k-1} \leq M_c < M_k \\ &= 0 \quad \text{otherwise} \end{aligned} \tag{26}$$

Applicability of the proposed algorithm is demonstrated through the following flue gas desulphurization example.

5.1. Example 4: Flue gas desulphurization

Combustion of fuels, containing significant amounts of sulphur, is one of the primary sources of sulphur dioxide (SO_2) emission. SO_2 causes severe damage to the environment and to human health such as urban and industrial decay, acid rain, and pulmonary disease. Environmental regulations are formulated to reduce SO_2 emission. For example, the US Clean Air Act Amendments of 1990 set a goal of reducing annual SO_2 emissions by 10 million tons below 1980 levels. There are many methods available for controlling the emission of SO_2 from boilers. One such method is removal of SO_2 by scrubbing the flue gas with a calcium compound to precipitate calcium sulphate. However, the chloride ion builds up in recirculated scrubbing liquid in the desulphurization unit, should be controlled to reduce corrosion.

Sulphur dioxide (SO_2) emissions from three utility boilers in a chemical process plant are given in Table 8. A wet scrubber-based desulphurization unit with a removal factor of 0.9 and a flow factor of 0.98 has been employed to satisfy the environmental discharge limit of 700×10^6 mg/h. First five steps for generating the waste composite curve are shown in Table 9. Last entry of the fifth column suggests that these three utility boilers produce 5722.5×10^6 mg/h of SO_2. Therefore, applying Eq. (23), it may be determined that 5022.5×10^6 mg/h of SO_2 has to be removed by the desulphurization unit. Results of the targeting step of the proposed algorithm, after replacing Eqs. (18) and (19) with Eqs. (25) and (26), are reported in column six of Table 9. The minimum treatment flow rate of the flue gas is targeted to be 2.221×10^6 N m^3/h to satisfy the discharge limit. The treatment pinch point may be identified to be 500 mg/N m^3. The waste composite curve and the treatment line are not shown for brevity. It may be noted that conservative performance parameters, related to the removal factor and flow factor, are considered in this example. Removal factors in the range of 0.9–0.98, and flow factors in the range of 0.95–0.99 have been reported based on the actual performance of wet flue gas desulphurization unit [41,42]. Finally, SO_2 removed from the flue gas is converted in the form of saleable byproduct, gypsum, a material commonly used in the manufacturing of wallboard. Gypsum is also used, to a lesser extent, as a soil amendment and as an additive in cement [43]. A forced oxidation system is usually employed to oxidize the main reaction product, calcium sulphite, to gypsum.

6. Conclusions

Recently, environmental concerns have extended to the control of macro- as well as micro- or hazardous pollutants. These pollutants, including globally significant pollutants such as green house gasses, cause significant damage to the ecosystem. Environmental problems span a continuously growing range of pollutants, hazards and ecosystem degradation over wider areas. In this paper, a methodology is proposed to target the minimum waste flow to the treatment unit to satisfy the environmental discharge condition. In the proposed methodology, the conventional models of a treatment unit, with constant outlet concentration and fixed removal ratio, are extended with flow loss that is proportional to the inlet flow rate. Applicability of the proposed methodology is demonstrated through illustrative examples from the domain of water management, volatile organic compound treatment and flue gas desulphurization. The environmental safe limits for discharge for various pollutants are defined either as concentration or total mass flow rate. Based on the ecosystem degradation potential of various pollutants, regulation norms for safe discharge may be defined and accordingly the proposed methodology may be generalized.

The proposed methodology is based on an algebraic approach, calculated on a tableau. An associated graphical representation is also provided to gain physical insight of the targeting problem. However, the proposed methodology is restricted to single contaminant only. Current research is directed towards developing appropriate targeting technology for multiple contaminants. The proposed methodology is also restricted for a single treatment unit. Due to stringent environmental regulations, it may not always be possible to satisfy them with a single treatment unit. Multiple treatment units may have to be employed to satisfy such stringent environmental safe discharge limits. Current research is also directed towards developing appropriate targeting technology for optimal networks of multiple treatment units.

References

[1] M.M. El-Halwagi, Process Integration, Academic Press, Elsevier, 2006.
[2] I.C. Kemp, Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy, Elsevier, 2007.
[3] S. Bandyopadhyay, M. Mishra, U.V. Shenoy, Energy-based targets for multiple-feed distillation columns, AIChE J. 50 (2004) 1837–1853.
[4] J. Varghese, S. Bandyopadhyay, Targeting for energy integration of multiple fired heaters, Ind. Eng. Chem. Res. 46 (2007) 5631–5644.
[5] M.M. El-Halwagi, V. Manousiouthakis, Synthesis of mass exchange networks, AIChE J. 8 (1989) 1233–1244.
[6] N. Hallale, D.M. Fraser, Capital cost targets for mass exchange networks. A special case: water minimization, Chem. Eng. Sci. 53 (1998) 293–313.
[7] Y.P. Wang, R. Smith, Wastewater minimization, Chem. Eng. Sci. 49 (1994) 981–1006.
[8] S. Bandyopadhyay, M.D. Ghanekar, H.K. Pillai, Process water management, Ind. Eng. Chem. Res. 45 (2006) 5287–5297.
[9] H.K. Pillai, S. Bandyopadhyay, A rigorous targeting algorithm for resource allocation networks, Chem. Eng. Sci. 62 (2007) 6212–6221.
[10] G.N. Kulkarni, S.B. Kedare, S. Bandyopadhyay, Determination of design space and optimization of solar water heating systems, Solar Energy 81 (2007) 958–968.
[11] A. Roy, P. Arun, S. Bandyopadhyay, Design and optimization of renewable energy based isolated power systems, SESI J. 17 (2007) 54–69.
[12] P. Arun, R. Banerjee, S. Bandyopadhyay, Sizing curve for design of isolated power systems, Energy Sustain. Dev. 11 (2007) 21–28.
[13] G.N. Kulkarni, S.B. Kedare, S. Bandyopadhyay, Design of solar thermal systems utilizing pressurized hot water storage for industrial applications, Solar Energy 82 (2008) 686–699.
[14] G.N. Kulkarni, S.B. Kedare, S. Bandyopadhyay, Optimization of solar water heating systems through water replenishment, Energy Convers. Manage. 50 (2009) 837–846.
[15] R.R. Tan, D.C.Y. Foo, Pinch analysis approach to carbon-constrained energy sector planning, Energy 32 (2007) 1422–1429.
[16] S.C. Lee, D.K.S. Ng, D.C.Y. Foo, R.R. Tan, Extended pinch targeting techniques for carbon-constrained energy sector planning, Appl. Energy 86 (2009) 60–67.
[17] P. Arun, R. Banerjee, S. Bandyopadhyay, Optimum sizing of battery integrated diesel generator for remote electrification through design-space approach, Energy 33 (2008) 1155–1168.
[18] S. Bandyopadhyay, Source composite curve for waste reduction, Chem. Eng. J. 125 (2006) 99–110.
[19] N. Takama, T. Kuriyama, K. Shiroko, T. Umeda, Optimal water allocation in petroleum refinery, Comput. Chem. Eng. 4 (1980) 251.
[20] Y.P. Wang, R. Smith, Design of distributed effluent treatment systems, Chem. Eng. Sci. 49 (1994) 3127.
[21] W.C.J. Kuo, R. Smith, Effluent treatment system design, Chem. Eng. Sci. 52 (1997) 4273.
[22] B. Galan, I.E. Grossmann, Optimal design of distributed wastewater treatment networks, Ind. Eng. Chem. Res. 37 (1998) 4036.
[23] R. Hernández-Suaïrez, J. Castellanos-Fernández, J.M. Zamora, Superstructure decomposition and parametric optimization approach for the synthesis of distributed wastewater treatment networks, Ind. Eng. Chem. Res. 43 (2004) 2175.
[24] I.S.F. Freitas, R.A.R. Boaventura, C.A.V. Costa, Conceptual design of industrial wastewater treatment processes: a hierarchical approach procedure, in: Proceedings of the Second Conference on Process Integration, Modeling and Optimization for Energy savings and Pollution Reduction (PRESS'99), Budapest, Hungary, 1999.
[25] J.M. Douglas, Conceptual Design of Chemical Processes, McGraw-Hill, New York, 1988.
[26] G. Statyukha, O. Kvitka, I. Dzhygyrey, J. Jeżowski, A simple sequential approach for designing industrial wastewater treatment networks, J. Clean. Prod. 16 (2008) 215–224.
[27] T.K. Zhelev, N. Bhaw, Combined water–oxygen pinch analysis for better wastewater treatment management, Waste Manage. 20 (2000) 665–670.
[28] W.C.J. Kuo, R. Smith, Designing for the interactions between water use and effluent treatment, Trans. Inst. Chem. Eng. 76 (1998) 287.
[29] C.-T. Chang, B.-H. Li, Improved optimization strategies for generating practical water-usage and -treatment network structures, Ind. Eng. Chem. Res. 44 (2005) 3607–3618.
[30] M. Gunaratnam, A. Alva-Argaĭ ez, A. Kokossis, J.-K. Kim, R. Smith, Automated design of total water systems, Ind. Eng. Chem. Res. 44 (2005) 588–599.
[31] D.K.S. Ng, D.C.Y. Foo, R.R. Tan, Targeting for Total Water Network. Part 2. Waste treatment targeting and interactions with water system elements, Ind. Eng. Chem. Res. 46 (2007) 9114–9125.
[32] S. Bandyopadhyay, C.C. Cormos, Water management in process industries incorporating regeneration and recycle through single treatment unit, Ind. Eng. Chem. Res. 47 (2008) 1111–1119.
[33] D.K.S. Ng, D.C.Y. Foo, R.R. Tan, Y.L. Tan, Ultimate flowrate targeting with regeneration placement, Chem. Eng. Res. Design 85 (9) (2007) 1253–1267.
[34] A. Alva-Argáez, A.C. Kokossis, R. Smith, Automated design of industrial water networks. American Institute of Chemical Engineering Annual Meeting, Paper 13f, Miami, FL, 1998.
[35] A. Alva-Argáez, A.C. Kokossis, R. Smith, Wastewater minimisation of industrial systems using an integrated approach, Comput. Chem. Eng. 22 (1998) S741–S744.
[36] R.R. Tan, D.K.S. Ng, D.C.Y. Foo, K.B. Aviso, A superstructure model for the synthesis of single-contaminant water networks with partitioning regenerators, Process Saf. Environ. Protect. 87 (2009) 197–205.
[37] D.K.S. Ng, D.C.Y. Foo, R.R. Tan, C.H. Pau, Y.L. Tan, Automated targeting for conventional and bilateral property-based resource conservation network, Chem. Eng. J. 149 (2009) 87–101.
[38] R. Prakash, U.V. Shenoy, Targeting and design of water networks for fixed flowrate and fixed contaminant load operations, Chem. Eng. Sci. 60 (2005) 255–268.
[39] G. Parthasarathy, M.M. El-Halwagi, Optimum mass integration strategies for condensation and allocation of multicomponent VOCs, Chem. Eng. Sci. 55 (2000) 881–895.
[40] C.-W. Hui, R. Smith, Targeting and design for minimum treatment flowrate for vent streams, Trans. Inst. Chem. Eng. 79 (2001) 13–24.
[41] C. Erickson, M. Jasinski, L. VanGansbeke, Wet flue gas desulfurization (WFGD) upgrade at the trimble county generating station unit 1, in: Proceedings of the MEGA Symposium, Baltimore, Maryland, August 28–31, 2006.
[42] M. Quitadamo, C. Erickson, J. Langone, SO_2 removal enhancement to the vectren, culley generating station units 2&3 wet flue gas desulfurization system, in: Proceedings of the ICAC Forum 05', Baltimore, Maryland, March 7–10, 2005.
[43] C.L. Kairies, K.T. Schroeder, C.R. Cardone, Mercury in gypsum produced from flue gas desulfurization, Fuel 85 (17–18) (2006) 2530–2536.