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Rigorous Targeting Approach for Water Reuse and Wastewater Minimization in Industrial Processes

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Abstract

Water reuse/recycle is one of the key strategies in reducing the freshwater flow rate in the process industries. The problem involves the allocation of internal water and freshwater sources to process units considered as demands with the objective of minimizing freshwater feed and wastewater discharge. However, several graphical and numerical techniques have been developed to target freshwater flow rate. In this paper, we present a new rigorous numerical targeting approach to minimize the utilization of freshwater and identify wastewater streams ahead of detailed design of the recycle/reuse network. First, the problem is formulated mathematically to establish rigorous rules for targeting and designing water network. Then, targeting algorithm is elaborated to make this methodology more practical. The numerical technique is useful in locating pinch point, which provides insightful information on the utilization of freshwater, identification and discharge of wastewater streams. In fact, examples for both models of fixed flow rate and fixed load problems are solved to illustrate the ease, rigor, and applicability of the developed targeting technique. Hence, this technique is extended to deal with a combined problem of fixed flow and fixed load.

1. Introduction

Water has become a crucial resource particularly in the process industry and its allied industries due to increasingly higher demand for water use that may expose plants to supply disruptions in the future. Furthermore, in recent years, stringent emission legislation and the increased cost of raw material as well as wastewater treatment [1-4] have motivated the process and manufacturing industries to emphasis on water minimization in their daily operations. In particular, *water network synthesis*, often known as *water minimization*, has gained good attention in both industrial and research communities [5].

The analogy between heat and mass transfer led to the evolution of *mass exchanger network synthesis* in thethe beginning of theeighties [6-8]. Within the framework of mass integration, water network synthesis appearsas a special case for the area. Considerably amount of work has been presented the water network can be designed through two approaches known asinsight-based using *water pinch analysis*[9-11]and mathematical-basedusing optimization approach; in which the success of the insight-based approach has been reported for *single contaminant systems*.Robin Smith and his co-workers [12-14] initiated the insight-based approach on pinch analysis techniquein the mid-nineties.Severalauthors consideredthe technology to have achieved a mature stage after the publication of specific reviews [15,16] at the end of the last century. However, the technology appears to be once again renewed with the various recent published papers addressing the limitation of the techniques methods employed in the 20th century. In fact, Pinch-targeting methods can be mostly classified into two classes: graphical and numerical methods. Although graphical methods provide physical insight and intuitive[17-23], they are tedious and not accurate solution for complex problem. On the other side, numerical methods look at algebraic accuracy and are amendable for computer programming [24-26].

Processes and their utility systems generate wastewater. The processes generate wastewater when water is contacted with process materials like steam stripping and many washing operations. Also, wastewater is generated by the utility system like boiler feed water treatment processes, boiler blowdown and cooling tower blowdown. Apart from making fundamental changes for the process operations, options for minimizing the water demand of a process may be done via water *reuse*, *recycle*, and *regeneration*. Reuse means that the effluent from a water-using operation is sent to other operation and does not re-enter to the operation where it was emitted. On the other hand, a recycle scheme permits the effluent to re-enter to the operation where it is generated. In regeneration schemes, effluent is partially treated by water purification unit before reuse or recycle takes place.

The tasks of water network synthesis are subdivided into two stages involving *flow rate targeting* and *network design*. Flow rate targeting aims to set the minimum fresh water and wastewater flow rates for a network based especially on concentration and flow rate restrictions. Using this basic data, water pinch analysis is in its ability to locate simultaneously the minimum flow rate targets of both fresh water feed and wastewater generation prior to detailed network design this offers a base line for any water network to be synthesized. Then, the processes are matched in the network design stage to achieve minimum flow rates obtained in the targeting stage. Indeed,the problems of water network design includedoperations that may be categorised into two broad problems as discussed below:

Fixed load problems (FL): The operations, in this category, are *quality controlled* [26] and may be modelled as mass transfer units (e.g., washing, scrubbing, and extraction) with water being used as the only mass separating agent [12,28]. Each operation has a fixed contaminant load and the maximum allowable inlet and outlet concentrations specified. The flow rate $F$of water entering and leaving the unit is the same, and is determined by$\Delta m = F(C_{out} - C_{in})$where$\Delta m$is the mass load of the contaminant and $C_{in}$and $C_{out}$are the inlet and outlet concentrations of contaminant in the water stream. The values of these concentrations should not exceed their specified maximum values.The *limiting composite curve*presented by Wang and Smith [12] is the most known targeting graphical technique for water pinch analysis. Based on the mass transfer model, water is used as a mass separating agent in removing contaminant load from *water-using process*. To construct the limiting composite curve, the *limiting water profile* of each individual process is plotted on a contaminant concentration versus load diagram (Figure 1a). The limiting water profiles are plotted according to their maximum limiting inlet and outlet concentrations which define the concentration intervals. The contaminant load is then added within each concentration interval to form the limiting composite curve (Figure 1b). The limiting composite curve may be viewed as the representation of the overall water network system. The minimum flow rate for a fresh water feed to the entire water system may then be targeted by drawing a *water supply line*from the origin and rotated counter-clockwise until it touches the limiting composite curve, where a pinch point is achieved (Figure 1b). The inverse slope of the water supply line defines the minimum flow rate of thefresh water from external source that can be purchased to satisfy the contaminant removal requirement of the system.

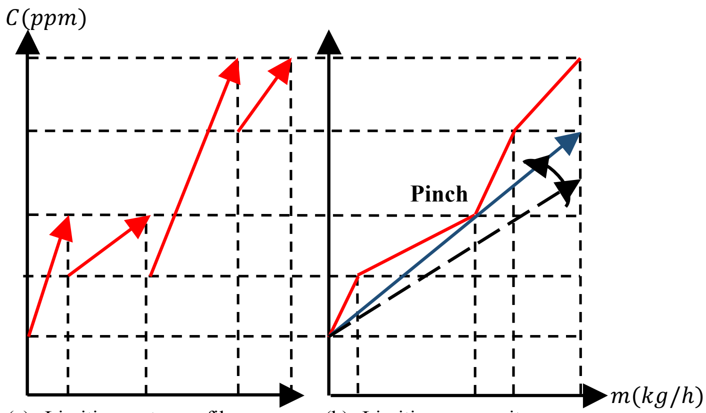

Figure 1: Construction of the limiting water profiles and limiting composite curve

Fixed flowrate problems (FF): The operations, in this category, are quantity controlled [27] that does not involve any mass transfer, and may include water-using units like boilers, cooling towers and reactors. One typical characteristic for this model is that the inlet and outlet flow rates of the water-using processes may not be uniform, which is different from that of the fixed load problems. The outlet streams have a fixed flow rate and fixed concentrations of contaminants, while the inlet streams also feature a fixed flow rate but the contaminant concentrations are variables, although they are limited by given maximal values. In this case, the external fresh water source is available to be purchased to satisfy the requirement of inlet streams.

Both graphical and numerical methods were initially developed for FL problems such as, limiting composite curve [12] and mass load table [16,29] under the condition that inlet and outlet water flow rate are the same for a given operation. Although this condition was relaxed by Wang and Smith [13] in their later work, the proposed approach needs tedious procedure to locate a true target. Improved concentration interval table [30] is the extended version of mass load tablein order to cope with FF problems. To use this method, limiting data must be converted fromFL intoFFproblems. Thus, for highly integrated processes, these approaches are very cumbersome.Dhole et al. [31] developed the source-sink composite curve to overcome this limitation and suggested that all the inlet streams are similar as sink and all the outlet streams as sources and proposed a targeting method for FF problems.However, Sorin et al. [32] proposedevolutionary table method because they pointed outthat source-sink composite curve approach results in several local pinch points and not necessarily guarantees the global pinch point location. The water surplus diagram [33] was the first promising tool able to deal with the FL and FF problems. However, water surplus diagram requires an iterative procedure before the target can be achieved.To correct this deficiency, graphical targeting method such as material recovery pinch diagramwas developed [34,35]. On the other hand, several other numerical methods were also proposed, such as, water cascade analysis [36] Method. Furthermore, two hybrids, non-iterative methods were also put forward known as composite table algorithm [37]andsource composite curve [38].

Indeed, these techniques can be mostly classified into two categories: iterative targeting and detailed network design. Iterative targeting involves the use of multistep graphical approaches to evolve the fresh water flow rate into a minimum target. On the other hand, detailed network design involves the matching of sources and sinks and the configuration of a network that provides minimum fresh water flow rate. Multiple networks can be configured to give the same minimum of fresh water. In many cases, it is important to identify the targetof wastewater streams ahead of detailed design and without commitment to the final network configurations. Therefore, the identification of individual wastewater streams is important, because smaller wastewater stream flow rate lead to lower cost in the distributed wastewater treatment system [39,40]. It serves as a good guideline in identifying regeneration placement unit as well as for final treatment for discharge.

However, in this work, the objective for both kinds of problems reside in minimizing fresh water and wastewater flow rates by formulation the rigorous rules using pinch analysis technique, on the other hand identifying wastewater streams, so long as the limiting water data for both models are converted correctly. In principle, the water inlet and outlet of a water-using process of the fixed load problem are taken as water demand and source in the fixed flow rate problem, respectively.For a water-using process in the fixed load problem, its maximum inlet concentration corresponds to the highest concentration limit of the water demand in the fixed flow rate problem; while its outlet concentration corresponds to the source concentration, in order to achieve maximum water recovery among water-using process. Savelski and Bagajewicz [41,42] have shown that it is necessary that inlet and outlet concentrations of a process should be set at their maximum allowable values for an optimal water network. This allows lower quality outlet stream from other water-using process to be reused. Hence, if the flow rate of the process is to be minimized, the water supply line will always take the steepest slope. In this case, the water supply line is known as the limiting water profile, i.e. minimum water supply flow rate for a given set of the inlet and outlet concentration; this situation is only applicable for single contaminant problems.

To transform the FL problem into the FF problem, the minimum water supply flow rate of the water-using process is extracted along with its inlet and outlet concentration for each water demand and source, respectively.Inlet and outlet streams of each water-using process are considered as separate entities, i.e. with the inlet flow rate taken as the water demand and the outlet as the water source. Similarly, transformation steps are necessary to convert the limiting data for a FF problem into a FL problem, with necessary adjustment to cater for water losses and gains [13]. The limiting water data for both FL and FF problems are interchangeable. However, it should be noted here is that, when many water demand and sources exist for a complex FF problem, analyzing the case with a FL model may be cumbersome, as effort is needed to pair the water demand and sources into water-using processes. In this case, the FF problem is more convenient to use.

The purpose of this paper is to develop a systemicprocedure for rigorously targeting the minimum of freshwater flow rate and identifying wastewater streams. First, we describe theproblem through amathematical formulation. Then, we prove the rigorous rules that must be considered for targeting and designing the water network. Next, based ontheserulesa targetingalgorithmwill be elaborated. This approachalso aimsto identify the individual wastewater streams and their respective flow rates. Three case studies from literature are solved to illustrate the applicability and merits of the developed numerical procedure.

2. Problem statement and mathematical formulation

As shown inFigure 2, the general problem of water minimization may be formulated asfollows:

- Given a number n of internal water-generating streams designated as:$sources = \{s_{1,}s_2, s_{3,\dots,}s_n\}$, each source has a given flow rate F_i^s and a contaminant concentration ofC_i^s.
- Given a number $m$of internal water-using processes designated as: $demands = \{d_{1,}d_2, d_{3,\dots,}d_m\}$, each demand accepts a flow rate F_j^d with a concentration of targeted contaminant that must be less or equal to predetermined maximum limitC_j^d.

- There is an external water source s_0 with a flow rate of F_0^s and a concentration C_0^s, such as: $freshwater = \{s_0\}$.
- There is an external water demand d_0 with a flow rate of F_0^d and a concentration C_0^d, such as: $wastewater = \{d_0\}$, It requires any maximum concentration limit or any flow rate limitation.

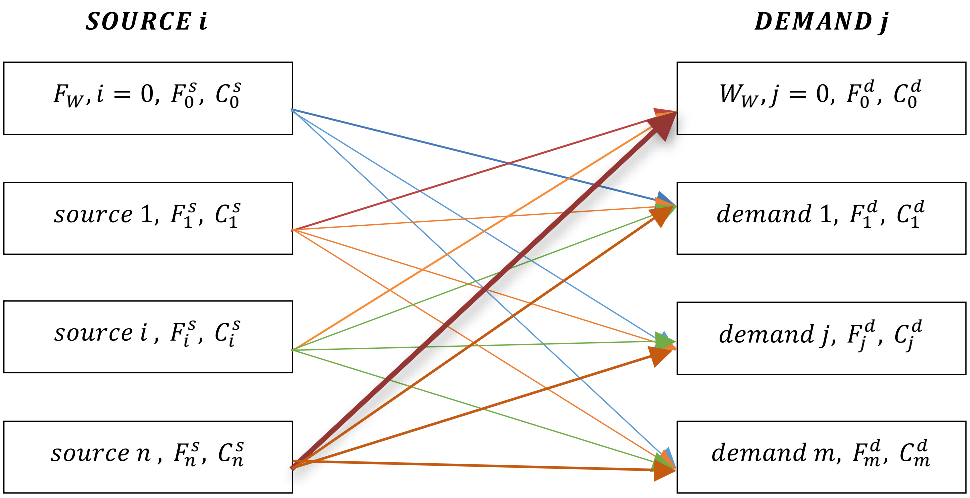

Figure 2: Fresh water minimization problem presented as a network flow rate optimization problem

Before developing an appropriate formulation for the above problem, the equations of conservation of mass must be defined. Conservation of mass means that mass is neither created nor destroyed during ordinary physical, chemical, and biological activities. In fact, two streams with flow rates F_a and F_b and concentrations C_a and C_b, respectively, may be mixed to produce a stream with flow rate F_c and concentration C_c. Commonly, using the law of conservation of mass is referred to as making a mass balance expressed by the next equations:

$$F_a + F_b = F_c \qquad \text{Eq.1}$$

$$F_a C_a + F_b C_b = F_c C_c \qquad \text{Eq.2}$$

3. Formulation of rigorous rules for using pinch analysis technique

3.1 Equivalence between water and wastewater minimization

Let $F_{i,j}^{s,d}$ denotes the flow transferred from internal source s_i to internal demand d_j. Similarly, $F_{0,j}^{s,d}$ and $F_{i,0}^{s,d}$ represent, respectively, the flow rate of fresh water transferred from the external source to internal demandand flow rate of wastewater transferred from internal source to external demand, the flow rate balance for every internal source and internal demand can be formulated as shown in Eq.3 and Eq.4 according to Eq.1.

$$\sum_{j=1}^{m} F_{i,j}^{s,d} + F_{i,0}^{s,d} = F_i^s \qquad \text{Eq.3}$$

$$F_{0,j}^{s,d} + \sum_{i=1}^{n} F_{i,j}^{s,d} = F_j^d \qquad \text{Eq.4}$$

Taking summation over all internal sources and demands inEq.3 and Eq.4, the overall flow rate balance across the processes can be established:

$$\sum_{j=1}^{m} F_{0,j}^{s,d} + \sum_{i=1}^{n} F_i^s = \sum_{j=1}^{m} F_j^d + \sum_{i=1}^{n} F_{i,0}^{s,d} \qquad \text{Eq.5}$$

This equation illustrates that the total flow rate of freshwater requirement expressed as $F = \sum_{j=1}^{m} F_{0,j}^{s,d}$ and the total flow of rate wastewater generation quantified as $W = \sum_{i=1}^{n} F_{i,0}^{s,d}$. Using these expressions, overall flow rate balance across the processcan be simplified as follows:

$$\sum_{i=1}^{n} F_i^s - \sum_{j=1}^{m} F_j^d = W - F = \Delta_1 \qquad \text{Eq.6}$$

Where Δ_1 is a constant for a given system and signifies overall flow rate loss or gain in the system.Positive Δ_1 signifies that there is flow rate gain in the system and a negative Δ_1 implies the loss of flow rate in the system. Note that wastewater generation and fresh water requirement are dependent; Eq.6 implies that they are related by a constant. This result can be formulated in the following rule:

Rule 1: The Minimization of fresh water requirement is equivalent to the minimization of wastewater generation

On the other hand, considering Eq.2, the mass balances for contaminant over the total system give the net system mass load (Δ_2) that is also constant for a given problem and expressed by the following equation:

$$\sum_{i=1}^{n} F_i^s C_i^s - \sum_{j=1}^{m} F_j^d C_j^d = WC_W - FC_F = \Delta_2 \quad \text{Eq.7}$$

3.2 Water transfer possibility from below to above pinch

A pinch concentration (C_{pinch}) is defined as the minimum concentration at which wastewater is generated at optimum. In other words,$F_{i,0}^{s,d} = 0$ if$C_i^s < C_{pinch}$. This implies that$F_{i,0}^{s,d} \neq 0$ if$C_i^s = C_{pinch}$. It should be noted that this definition does not imply that wastewater must be generated from all sources whose concentration is more than the pinch concentration. A pinch divides the system into two parts; the one is above pinch and the other is below pinch.All internal sources and demands with concentrations greater than the pinch concentration are located at above pinch, the rest of internal sources and demands are located at below pinch. On the other hand, external demand (wastewater) is situated at above pinch contrary to external source (fresh water) that is positioned at below pinch.

Suppose at optimum there exists an above pinch demand($C_a^d > C_{pinch}$), where a flow rate F_b^s is transferred from a below pinch source ($C_b^s < C_{pinch}$). Assume that a maximum flow rate$F_{a,max}^s$ with a given concentrationC_a^s, such that ($C_a^s > C_{pinch}$)is also transferred to this demand as a combined flow rate from different above pinch sources. Flow rate and mass load balances for this demand can be written as follows:

$$F_{a,max}^s + F_b^s = F_a^d \quad \text{Eq.8}$$

$$F_{a,max}^s C_a^s + F_b^s C_b^s = F_a^d C_a^d \quad \text{Eq.9}$$

From Eq.8 and Eq.9, we find:

$$F_{a,max}^s = F_a^d \frac{C_a^d - C_b^s}{C_a^s - C_b^s} \quad \text{Eq.10}$$

However, flow rate transferred from a source with pinch concentration to wastewater is positive. If a flow rate of $F_{pinch}$with a pinch concentrationtransferred to the above pinch demand, only a maximum flow rate$f_{a,max}^s < F_{a,max}^s$ with a concentration C_a^s is sufficient to satisfy the flow rate and mass load equations for the demand:

$$f_{a,max}^s + F_b^s + F_{pinch} = F_a^d \quad \text{Eq.11}$$

$$f_{a,max}^s C_a^s + F_b^s C_b^s + F_{pinch} C_{pinch} = F_a^d C_a^d \quad \text{Eq.12}$$

From Eq.11 and Eq.12 we get:

$$f_{a,max}^s = F_a^d \frac{C_a^d - C_b^s}{C_a^s - C_b^s} - F_{pinch} \frac{C_{pinch} - C_b^s}{C_a^s - C_b^s} \quad \text{Eq.13}$$

Consequently, only $f_{a,max}^s$ can be transferred to the demand and the remaining flow rate ($F_{a,max}^s - f_{a,max}^s$) is diverted. Total change in flow rate of wastewater may be calculated as follows:

$$F_{pinch} - (F_{a,max}^s - f_{a,max}^s) = F_{pinch} \frac{C_a^s - C_{pinch}}{C_a^s - C_b^s} > 0 \quad \text{Eq.14}$$

Eq.14 suggests that by introducing flow rate with pinch concentration, wastewater flow rate can be further reduced. This leads to a contradiction as it violates the original optimality criterion. It should be noted that in the definition of pinch concentration, optimal condition is assumed. This implies that for an appropriate pinch point, the fresh water requirement and wastewater generation are at their respective minimum. It is not possible to reduce them further. We shall refer to this as the optimality criterion. In the other word,
$F_{i,j}^{s,d} = 0$ if$C_i^s < C_{pinch}$and$C_j^d > C_{pinch}$. This result can be formulated as follows:

Rule 2: no flow rate is transferred from below pinch sources to above pinch demand.

Based on the above rule, it can easily be seen that the fresh water cannot be used for any above pinch demand ($F_{0,j}^{s,d} = 0$ if$C_j^d > C_{pinch}$).This observation may be expressed as follows:

Rule 3: fresh water cannot be used for above pinch demands.

3.3. Water transfer possibility fromabove to below pinch

Suppose at optimum there exists a below pinch demand($C_b^d < C_{pinch}$), where a flow rate F_a^s is transferred from above pinch source ($C_a^s > C_{pinch}$). Assume that a maximum flow rate$F_{b,max}^s$ with a concentrationC_b^s, such that$C_b^s < C_{pinch}$ is also transferred to this demand as a combined flow rate from different below pinch sources. Flow rate and mass load balances for this demand can be written as follows:

$$F_{b,max}^{s} + F_{a}^{s} = F_{b}^{d} \quad \text{Eq.15}$$

$$F_{b,max}^{s} C_{b}^{s} + F_{a}^{s} C_{a}^{s} = F_{b}^{d} C_{b}^{d} \quad \text{Eq.16}$$

From Eq.15 and Eq.16, we find the maximum combined flow rate that may be transferred from the below pinch sources.

$$F_{b,max}^{s} = F_{b}^{d} \frac{C_{b}^{d} - C_{a}^{s}}{C_{b}^{s} - C_{a}^{s}} \quad \text{Eq.17}$$

If a flow ofF_{pinch} with a pinch concentration is transferred to the below pinch demand, only a flow rate $f_{b,max}^{s} < F_{b,max}^{s}$with a concentration C_{a}^{s} is sufficient to satisfy the flow rate and mass load equations for the demand:

$$f_{b,max}^{s} + F_{a}^{s} + F_{pinch} = F_{b}^{d} \quad \text{Eq.18}$$

$$f_{b,max}^{s} C_{b}^{s} + F_{a}^{s} C_{a}^{s} + F_{pinch} C_{pinch} = F_{b}^{d} C_{b}^{d} \quad \text{Eq.19}$$

FromEq.18 and Eq.19 we get the maximum flow rate ($f_{b,max}^{s}$) that may be transferred from the below pinch sources is given by Eq.20.

$$f_{b,max}^{s} = F_{b}^{d} \frac{C_{b}^{d} - C_{a}^{s}}{C_{b}^{s} - C_{a}^{s}} - F_{pinch} \frac{C_{pinch} - C_{a}^{s}}{C_{b}^{s} - C_{a}^{s}} \quad \text{Eq.20}$$

Since, only $f_{b,max}^{s}$ can be transferred to the demand the remaining flow rate ($F_{b,max}^{s} - f_{b,max}^{s}$)is diverted. The total change in flow rate of wastewater may be calculated as expressed by the following equation.

$$F_{pinch} - (F_{b,max}^{s} - f_{b,max}^{s}) = F_{pinch} \frac{C_{b}^{s} - C_{pinch}}{C_{b}^{s} - C_{a}^{s}} > 0 \quad \text{Eq.21}$$

Eq.21 suggests that by injecting water with pinch concentration, wastewater flow rate can be more reduced. This leads to a contradiction as it violates the original optimality criterion. In the other word, $F_{i,j}^{s,d} = 0$ if$C_{i}^{s} > C_{pinch}$ and$C_{j}^{d} < C_{pinch}$. In this sense, the following rule can be formulated as:

Rule 4: no flow rate is transferred from an above pinch source to a below pinch demand.

4. Wastewater streams identification

As discussed previously, a pinch divides the entire processes into two parts: an above pinch portion and a below pinch portion. As proved in rule 3, all below pinch demands are satisfied by fresh water and below pinch sources. In this sense, below pinch portion is a flow rate deficit region that is satisfied by the fresh water. On the other hand, as proved in rule 4, all above pinch sources feed all above pinch demands and remaining flow rate is discharged as wastewater. Above pinch portion is a flow rate surplus region that is transferred to the wastewater discharge.Accordingly, the water network will be divided into two separate regions at the pinch concentration. Fresh water is used in the lower-concentration region after the available water sources for reuse/recycle to the demands have been exhausted. On the other hand, in the higher-concentration region, the available water sources exceed what is required by the demands; hence, the unused sources are discharged as wastewater. During streams segregation, all water demands and sources located in their respective regions, either in the higher or lower-concentration regions. For the sources that lies at the pinch concentration, its water allocation targets are to beidentified to determine the distribution between the higher and lower-concentration regions.

In the higher-concentration region, the cleanest available water source is supplied at the pinch concentration, i.e., by the pinch-causing source because no fresh water is used in this region. The quality of the excess water in this region can be maximized by utilizing streams that will just meet the concentration limits of the demands. It is noted that all wastewater streams are generated from sources in the higher concentration region and can determined by rewritingequation Eq.6 just in this region to express wastewater generation as shown in Eq.22:

$$W = \sum_{C_{i}^{s} \geq C_{pinch}} F_{i}^{s} - \sum_{C_{j}^{d} \geq C_{pinch}} F_{j}^{d} \quad \text{Eq.22}$$

Then, the flow rates of wastewater streams emitted from sources in the higher-concentration region can be identified. One ofthese will always be the pinch-causing source, because of the excessive flow rate that is supplied to this region, whereas the others will be the flow rates of wastewater sources with higher concentration. By using the mass balance, this flow rates can be determinedby solving by the following equations system with two unknownsF_1 andF_2; where F_1 denotes the flow rate of wastewater from pinch-causing source and F_2 denotes the total of flow rates of wastewater sources with higher concentration. LetC_{ds} denote the concentration of dirtiest source.

$$\begin{cases} F_1 + F_2 = W \\ F_1 C_{pinch} + F_2 C_{ds} = W C_W \end{cases} \quad \text{Eq.23}$$

5. Fresh water and wastewater targeting algorithm

Based on the recommended rules, the following algorithm with nine steps described below proposed to target minimum fresh water requirementand wastewater streams identification. Numerical results, calculated from step 1 to step 5, may be tabulated in the form of a Table 1that can be usedto generate the limiting composite curve and water supply line.

Table 1: Tabular representation of fresh water targeting

	1st Column	*2nd Column*	*3td Column*	*4td Column*	*5td Column*
	Concentration	Net Flow Rate	Net Mass Load	Cumulative Mass Loads	Fresh Water
	$C_k(ppm)$	$F_k\ (t/h)$	$m_k(kg/h)$	$\sum_1^k m_k\ (kg/h)$	$\frac{\sum_1^k m_k}{C_k - C_0^s}\ (t/h)$
1st row	C_1	$F_1 = 0$	$m_1 = 0$	m_1	0
2nd row	C_2	F_2	$m_2 = (C_2 - C_1)F_2$	$m_1 + m_2$	$\frac{m_1 + m_2}{C_2 - C_0^s}$
...	…	…	…	…	…
kth row	C_k	F_k	$m_k = (C_k - C_{k-1})F_k$	$m_1 + m_2 + \cdots + m_k$	$\frac{m_1 + m_2 + \cdots + m_k}{C_k - C_0^s}$
	…	…	…	…	…
nth row	C_n	F_n	$m_n = (C_n - C_{n-1})F_n$	$m_1 + \cdots m_k + \cdots + m_n$	$\frac{m_1 + \cdots m_k + \cdots + m_n}{C_n - C_0^s}$

The steps required for the targeting algorithm are described as follows:

Step 1: The problem of FL must be converted into FF problem and the concentrations of all internal sources and demands are tabulated in increasing order in the first column. If the value of such concentration occurs more than once, it is not repeated.

Step 2: Tabulate the net flow rates in the second column. The sum of the flow rates of the sources is subtracted from the sum of the flow rates of the demands present in each concentration interval and entered against the higher concentration limit of the interval. The net flow rate corresponds to the reciprocal of the slope of a segment on the limiting composite curve. The first entry in the second column is set to zero.

Step 3: Tabulate the net mass loads in the Third column. Multiply the net flow rate by the concentration difference of the corresponding interval to obtain the net mass load. The first entry in the third column is set to zero.

Step 4: Cumulative mass loads are calculated by summing the net mass loads for all previous rows and tabulated in the fourth column. The concentration column may be plotted against the cumulative mass load column to obtain the limiting composite curve.

Step 5: Tabulate the possible water supply flow rates in the fifth column. Divide the cumulative mass load by $(C_k - C_0^s)$ to obtain the possible water supply flow rate. Here, $C_k$is theupperlimit of eachconcentrationintervaland C_0^s is the initial concentration of the water supply. In the case of freshwater: $C_0^s = 0$. The possible water supply flow rate corresponds to the reciprocal of the slope of a line originating fromC_0^s on the vertical axis to the limiting composite curve. The first entry in the fifth column is set to zero.

Step 6: calculatethe constant Δ_1 using Eq.6 and deduct the overall flow rate of wastewater.

Step 7: locate the pinch-causing sources, then separate all internal sources and demands between above and below pinch regions.

Step 8: presentseparatelythe limiting water data for each region of concentration and calculate the wastewater flow rate generated from higher-concentration region using Eq.22.

Step 9: applyEq.7 anddeduce the concentration of total wastewater streams, then use Eq.23 to identify each water stream.

6. Illustrative cases studies

6.1. Case study 1: Targeting for fixed flow rate problems

To illustrate the new targeting approach, an example of a fixed flowrate problem is considered [27]. The data for four internal demands streams and four internal sources streams are given in Table 2. The objective is to reduce freshwater requirement which have been calculated and tabulated in Table 3. Demands and sources are arranged in increasing order of contaminant concentration for the calculation of net flow rate and net mass load for each interval of concentration, then the cumulative mass loads and water supply flow rates are calculated as shown in Table 3.

Subsequently, the maximum value in the last column gives the minimum freshwater flow rate target of *70 t/h*, because the water supply line can never be above the limiting composite, and the corresponding pinch concentration of *150 ppm* corresponding to pinch-causing source s_3. Knowing that total source and demand flow rates are *280* and *300 t/h*, respectively, therefore, for thisproblem$\Delta_1 = -20\ t/h$according to Eq.6. On other hand, the minimum wastewater flow rate target is$W = \Delta_1 + F = -20 + 70 = 50\ t/h$, according also to Eq.6. In fact, fresh water and wastewater flow rates are not be equal, the wastewater flow rate is less than fresh water flow rate, that there is a loss offlow rate in the overallsystem of *20 t/h*. this result is consistent with that obtained by Prakash and Shenoy [35], and Alwi and Manan [42] using graphical methods.

Since the pinch concentration is *150 ppm*, it is observed from Table 2 that demands d_1, $d_2$and $d_3$are below the pinch, and d_4 is the only demand above the pinch. However, sources s_1 and s_2 are below the pinch, source s_3 is at the pinch, and source s_4 is above the pinch. Therefore, the water allocation targets of the pinch-causing sources correspond to a flow rate of *10 t/h* that sent to the lower-concentration region and a flow rate of*60 t/h* that goes to higher-concentration region. The amount of source $s_3$below the pinch is 10 t/h obtained by subtracting the freshwater target of *70 t/h* from the net flow rate of *80* t/h at the pinch concentration (*150 ppm*) according to Table 3. Consequently, the limiting water data for each demand and source can be presented separately between the lower and higher-concentration regions as shown in Table 4.

Table 2: Limiting water data for example 1

d_j	F_j^d (t/h)	C_j^d (ppm)	s_j	F_i^s (t/h)	C_i^s (ppm)
d_1	50	20	s_1	50	50
d_2	100	50	s_2	100	100
d_3	80	100	s_3	70	150
d_4	70	200	s_4	60	250

Table 3: Generation of composite curve and fresh water targeting for example 1

C_k (ppm)	F_k (t/h)	m_k (kg/h)	$\sum_1^k m_k$ (kg/h)	$\frac{\sum_1^k m_k}{C_k - C_0^s}$ (kg/h)
20	0	0.0	0.0	0
50	50	1.5	1.5	30
100	100	5.0	6.5	65
150	80	4.0	**10.5**	(*Pinch*) **70**
200	10	0.5	11.0	55
250	80	4.0	15.0	60

Table 4: Distribution of limiting water data for example 1 between lower and higher concentration regions

	d_j	F_j^d (t/h)	C_j^d (ppm)	s_j	F_i^s (t/h)	C_i^s (ppm)
Lower-concentration region	d_1	50	20	s_1	50	50
	d_2	100	50	s_2	100	100
	d_3	80	100	s_3	10	150
Higher-concentration region	d_4	70	200	s_3	60	150
				s_4	60	250

From the datalistedin Table 4 andusing Eq.22 we find the wastewater flow rate generated from higher concentration region equal at *50 t/h*, it is noted that it is the same as that which was calculated using Eq.6 for all the system. This result means that the entire wastewater stream is generated from higher-concentration region.

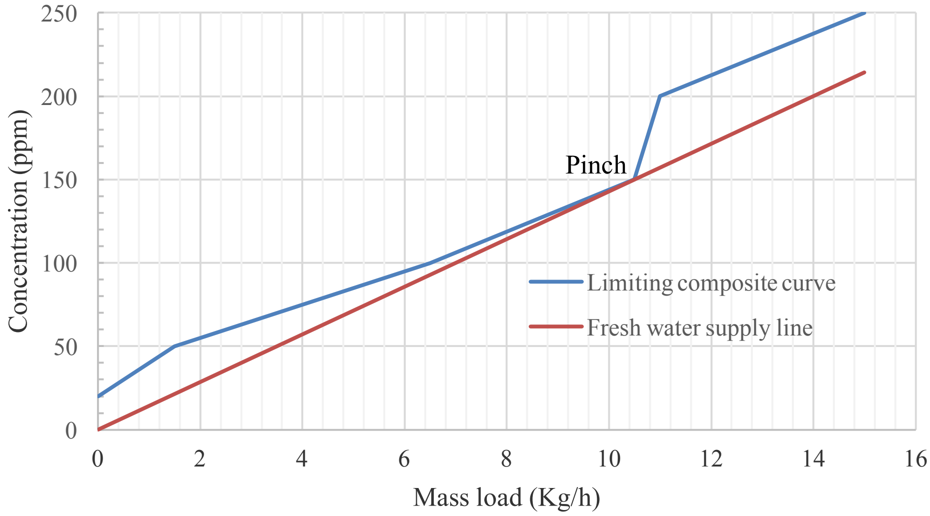

Figure 3: Limiting composite curve and water supply line for example 1

However, the fresh water is used only in lower-concentration region. On the other hand, applying Eq.7 in this region, we get$FC_F = 0$; this means that the fresh water enters in thesystemwithzero concentration($C_F = 0$). In higher-concentration region Eq.7 gives $\Delta_2 = WC_W = 1\,000 g/h$and consequently the global concentration of wastewater streams mixed together will be equal at $C_W = 200\ ppm$corresponds wastewater streams from pinch-causing source and sources with higher concentration mixed together. Thisresult is consistentwithwhich is obtainedbyAgrawal and Shenoy [37],but they are not identified the flow rates at pinch and dirtiest source concentrations in first stage of targeting. Todetermine these flow rates, the Eq.23 should be applied, we have $F_1 + F_2 = 50\ t/h$and $150F_1 + 250F_2 = 10\,000\ g/h$ which give the wastewater flow rate at pinch concentration of *25 t/h* and wastewater flow rate at dirtiest source concentration of*25 t/h*.
Limiting composite curve can be constructed based on the results ofTable 3as shown inFigure 3.Fresh water supply line starts from origin as a pivot and is rotated anticlockwise until touches limiting composite curve in the pinch point. Inverse slope of water supply line determines the minimum fresh water requirement.

6.2 Case study 2: Targeting for fixed contaminant load problems

The new targeting approach is illustrated next for a fixed contaminant load problem through example 2 [12]. The limiting water data for the four water-using processes in this example are given in Table 5.
To convert the fixed load problem into the fixed flow rate problem, the minimum water supply flow rate of the water-using processes is extracted along with its maximum inlet and outlet concentrations ($C_{i,in}^{max}$ and$C_{i,out}^{max}$) for each water demand and source, respectively. Indeed, Table 5 shows the mass load (Δm_i) to be removed from each water-using process in column 2 and the maximum inlet $C_{i,in}^{max}$ and outlet $C_{i,out}^{max}$ concentrations in columns 3 and 4, respectively. Each water-using process (P_i) has an equal inlet and outlet flow rates ($F_{i,in}^{lim} = F_{i,out}^{lim} = F_i^{lim}$). The final column of the table lists the minimum limiting water flow rate $\left(F_i^{lim}\right)$for each water-using process dictated by the limiting water profile. To transform this problem into an equivalent fixed flow rate problem, inlet and outlet streams of each water-using process are regarded as separate entities, with the inlet flow rates taken as the water demands and the outlet as the water sources. As shown in Table 6, the demand and source flow rates (columns 2 and 5) are essentially equal to the minimum water flow rate dictated by the limiting water profile of the fixed load problem in Table 5 (column 5).
Demands and sources are arranged in increasing order of contaminant concentration for the calculation of net flow rate and net mass load for each interval of concentration, then the cumulative mass loads and water supply flow rates are calculated as shown in Table 7. The maximum value in the last column gives the minimum freshwater flow rate target of *90 t/h* and the corresponding pinch concentration of *100 ppm* corresponding to pinch-causing sources $P_{1,out}$ and $P_{2,out}$. The pinch occurs at a contaminant load of *9 kg/h*. this result is consistent with that obtained by Wang and Smith [12] using a graphical method. On the other hand, the minimum wastewater flow rate target is *90 t/h*, because total source and demand flow rates are both are equal to *170 t/h;* then $\Delta_1 = 0\ t/h$according to Eq.6. In fact, fresh water and wastewater flow rates are equal because the water is used as the lean stream to remove a certain amount of impurity load from the rich stream.

Since the pinch concentration is *100 ppm*, it is observed from Table 6 that demands $P_{1,in}$, $P_{2,in}$and $P_{3,in}$are below the pinch and $P_{4,in}$ is the only demand above the pinch. However, sources $P_{1,out}$and $P_{2,out}$are at the pinch and $P_{3,out}$ and $P_{4,out}$are above the pinch. Therefore, the water allocation targets of the pinch-causing sources correspond to a flow rate of *70 t/h* that sent to the lower-concentration region and a flow rate of*50 t/h* that goes to higher-concentration region, according to Table 7. In other words, the demand $P_{1,out}$flow rate of *20 t/h* is fully used in lower-concentration region and the demand $P_{2,out}$ flow rate is distributed in an equal manner between lower and higher-concentration regions, *50 t/h* for each other. Consequently, the limiting water data for each demand source can be presented separately between the lower and higher-concentration regions as shown in Table 8.

From the datalistedin Table 8 andusing Eq.22 we find the wastewater flow rate generated from higher concentration region equal at *90 t/h*, it is noted that it is the same as that which was calculated using Eq.6 for all the system. This result means that the entire wastewater stream is generated from higher-concentration region. However, the fresh water is used only in lower-concentration region. On the other hand, applying Eq.7 in this region, we get $FC_F = 0$; this means that the fresh water enters in thesystemwithzero concentration($C_F = 0$). In higher concentration region Eq.7 gives $\Delta_2 = WC_W = 41\,000\ g/h$ that represent the final cumulative mass load calculating in Table 7 (column 4) and consequently the global concentration of wastewater stream will be equal at $C_W = 455.5\ ppm$corresponds to wastewater streams from pinch-causing sources and sources with higher concentration mixed together. Todetermine these flow rates, Eq.23 should be applied, we have $F_1 + F_2 = 90\ t/h$ and $100F_1 + 800F_2 = 40995\ g/h$ which give the wastewater flow rate at pinch concentration of *44.3 t/h* and wastewater flow rate at dirtiest source concentration of*45.7 t/h*. Thisresult corresponds precisely at which obtained by Wang and Smith [12] using Graphical method. For illustration, limiting composite curve and fresh water supply line can be plotted based on the results of Table 7 as shown in Figure 4.

Table 5: Limiting water data for example 2 (FL Problem)

P_i	Δm_i (kg/h)	$C_{i,in}^{max}$ (ppm)	$C_{i,out}^{max}$ (ppm)	F_i^{lim} (t/h)
1	2	0	100	20
2	5	50	100	100
3	30	50	800	40
4	4	400	800	10

Table 6: Transformation of limiting water data of example 2 into FF problem

d_j	F_j^d (t/h)	C_j^d (ppm)	s_j	F_i^s (t/h)	C_i^s (ppm)
$P_{1,in}$	20	0	$P_{1,out}$	20	100
$P_{2,in}$	100	50	$P_{2,out}$	100	100
$P_{3,in}$	40	50	$P_{3,out}$	40	800
$P_{4,in}$	10	400	$P_{4,out}$	10	800

Table 7: Generation of composite curve and fresh water targeting for example 2

C_k (ppm)	F_k (t/h)	m_k (kg/h)	$\sum_1^k m_k$ (kg/h)	$\frac{\sum_1^k m_k}{C_k - C_0^s}$ (kg/h)
0	0	0	0	0.00
50	20	1	1	20.00
100	160	8	**9**	*(Pinch)* **90.00**
400	40	12	21	52.50
800	50	20	41	51.25

Table 8: Distribution of limiting water data for example 2 between lower and higher concentration regions

	d_j	F_j^d (t/h)	C_j^d (ppm)	s_j	F_i^s (t/h)	C_i^s (ppm)
	$P_{1,in}$	20	0	$P_{1,out}$	20	100
Lower-concentration region	$P_{2,in}$	100	50	$P_{2,out}$	50	100
	$P_{3,in}$	40	50			
	$P_{4,in}$	10	400	$P_{2,out}$	50	100
Higher-concentration region				$P_{3,out}$	40	800
				$P_{4,out}$	10	800

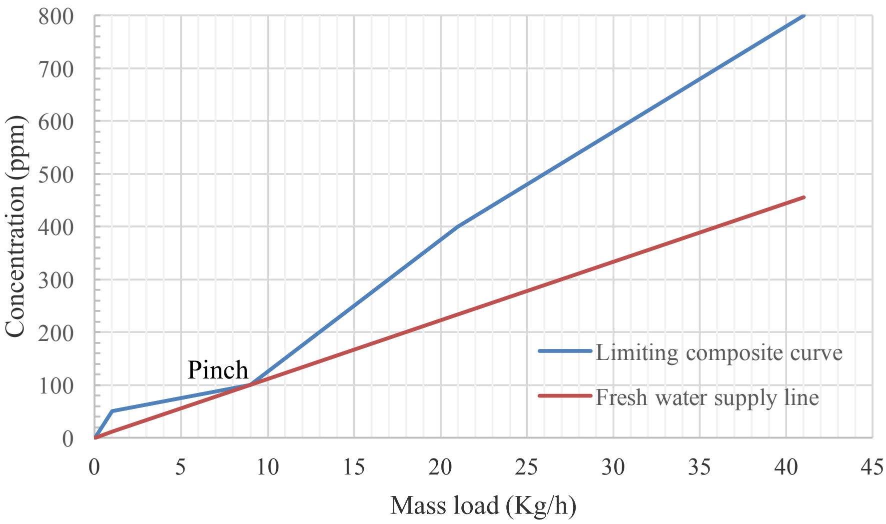

Figure 4: Limiting composite curve and water supply line for example 2

6.3. Case study 3: Combined fixed flow rate and flow load operations

Since the same targeting approach applies to both categories of problems, in example 3, the data of examples 1 and 2 are combined to form the new limiting data presented inTable 9 that shows the complete set of data after conversion of the fixed contaminant load data to demand and source data.

Demands and sources are arranged in increasing order of contaminant concentration for the calculation of net flow rate and net mass load for each interval of concentration, then the cumulative mass loads and water supply flow rates are calculated as shown in Table 10.The maximum value in the last column gives the minimum freshwater flow rate target of *155 t/h.*It should be noted that this value is less than the sum of the individual freshwater targets for the two independent problems. The reduction of *5t/h* in the freshwater target is due to the opportunities that exist for sources from the fixed flowrate problem to satisfy the demands in the fixed contaminant load problem and vice versa. The corresponding pinch concentration of *100 ppm* is equal to pinch-causing sources$P_{1,out}$, $P_{2,out}$, s_2 and demandd_3. The pinch occurs at a contaminant load of *15.5 kg/h*. this result is consistent with that obtained by Prakash and Shenoy [35] using a graphical method.

Knowing that total source and demand flow rates are *450* and *470 t/h*, respectively, therefore, for this problem$\Delta_1 = -20\ t/h$ according to Eq.6. On other hand, the target of minimum wastewater flow rate is$W = \Delta_1 + F = -20 + 155 = 135\ t/h$, according also to Eq.6. In fact, fresh water and wastewater flow rates are not be equal, the wastewater flow rate is less than fresh water flow rate, that there is an overall water loss of *20 t/h*.

Because the pinch concentration is *100 ppm*, it is observed from Table 9 that demands $P_{1,in}$, $P_{2,in}$, $P_{3,in}$ $d_1$and $d_2$are below the pinch, $P_{4,in}$ andd_4 are above the pinch and d_3 is only demand at the pinch. However, sources $P_{1,out}$, $P_{2,out}$and $s_2$are at the pinch while $P_{3,out}$, $P_{4,out}$, s_3 and $s_4$are above the pinch, the only source which below the pinch is s_1. Therefore, the water allocation targets of the pinch-causing sources correspond to a flow rate of *105 t/h* that is sent to the lower-concentration region and a flow rate of *115 t/h* that goes to higher-concentration region, according to Table 10. In other words, the source $P_{2,out}$flow rate of *100 t/h* is fully used with 5 t/h of $P_{1,out}$in lower-concentration region. However, the source $s_2$is fully used with *15 t/h* of $P_{1,out}$ in higher-concentration region. It should be noted that both $P_{2,out}$ and s_2 have same flow rate and same concentration; then both of sources aresubstitutable. Consequently, the limiting water data for each demand and source can be presented separately between the lower and higher-concentration regions as shown in Table 11.

Table 9: Limiting water data for example 3 (hybrid problem)

d_j	F_j^d (t/h)	C_j^d (ppm)	s_j	F_i^s (t/h)	C_i^s (ppm)
$P_{1,in}$	20	0	$P_{1,out}$	20	100
$P_{2,in}$	100	50	$P_{2,out}$	100	100
$P_{3,in}$	40	50	$P_{2,out}$	40	800
$P_{4,in}$	10	400	$P_{3,out}$	10	800
d_1	50	20	$\boldsymbol{s_1}$	50	50
d_2	100	50	$\boldsymbol{s_2}$	100	100
d_3	80	100	$\boldsymbol{s_3}$	70	150
d_4	70	200	$\boldsymbol{s_4}$	60	250

Table 10: Generation of composite curve and fresh water targeting for example 3

C_k (ppm)	F_k (t/h)	m_k (kg/h)	$\sum_1^k m_k$ (kg/h)	$\frac{\sum_1^k m_k}{C_k - C_0^s}$ (kg/h)
0	0	0.0	0.0	0.0
20	20	0.4	0.4	20.0
50	70	2.1	2.5	50.0
100	260	13.0	**15.5**	(*Pinch*) **155.0**
150	120	6.0	21.5	143.3
200	50	2.5	24.0	120.0
250	120	6.0	30.0	120.0
400	60	9.0	39.0	97.5
800	70	28.0	67.0	83.8

Table 11: Distribution of limiting water data for example 3 between lower and higher-concentration regions

	d_j	F_i^d (t/h)	C_i^d (ppm)	s_j	F_i^s (t/h)	C_i^s (ppm)
	$P_{1,in}$	20	0	$P_{1,out}$	5	100
	$P_{2,in}$	100	50	$P_{2,out}$	100	100
Lower-concentration region	$P_{3,in}$	40	50	s_1	50	50
	d_1	50	20			
	d_2	100	50			
	$P_{4,out}$	10	400	$P_{1,out}$	15	100
	d_3	80	100	$P_{3,out}$	40	800
Higher-concentration region	d_4	70	200	$P_{4,out}$	10	800
				s_2	100	100
				s_3	70	150
				s_4	60	250

From the datalistedin Table 11 andusing Eq.22 we find the wastewater flow rate generated from higher concentration region equal at *135 t/h*, it is noted that it is the same as that which was calculated using Eq.6 for all the system. This result means that the entire wastewater stream is generated from higher-concentration region. However, the fresh water is used only in lower-concentration region. On the other hand, applying Eq.7 in this region, we get $FC_F = 0$; this means that the fresh water enters in thesystemwithzero concentration($C_F = 0$). In higher concentration region Eq.7 gives $\Delta_2 = WC_W = 51\,000\ g/h$ and consequently the wastewater stream will be equal at $C_W = 377.78\ ppm$corresponds wastewater streams from pinch-causing and sources with higher concentration mixed together. Todetermine these flow rates, the Eq.23 should be applied, we have $F_1 + F_2 = 135\ t/h$ and $100F_1 + 800F_2 = 51000\ g/h$ which give the wastewater flow rate at pinch concentration of

53.6 t/h and wastewater flow rate at dirtiest source concentration of *81.4 t/h*. Figure 5 illustrates, for this case study, the limiting composite curve and fresh water supply line can be plotted based on the results of Table10.

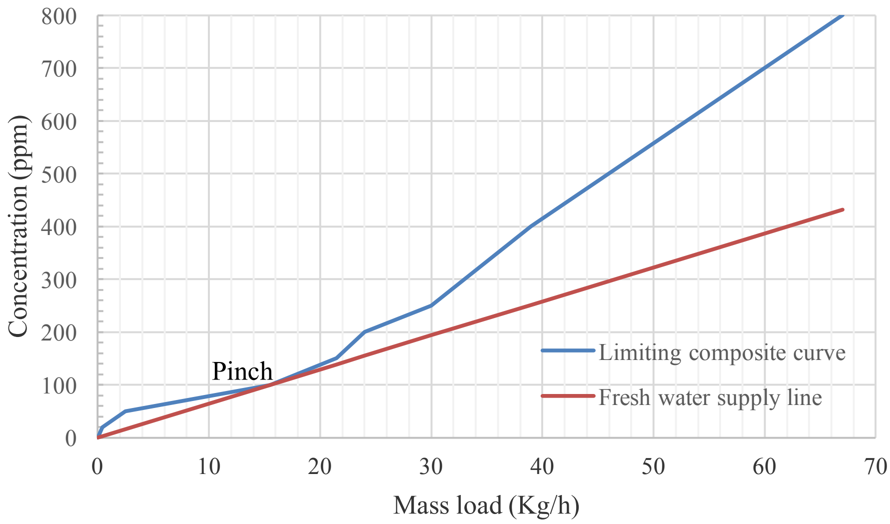

Figure 5: Limiting composite curve and water supply line for example 3

Conclusion

We have developed a first-stage numerical method for identifying rigorous targets for therecycle/reuse water network problem.A methodology has been presented here for targeting the minimum freshwater and to identify individual wastewater streams that are emitted from water network beforethe design stage can bestarted. Note that the summation of the individual wastewater streams flow rates matches the total wastewater flow rate targeted in the reuse/recycle network.

This method provides several advantages than graphical approaches. First, it is not iterative and does not require any initialization. Second, it is computationally very easy to implement in the form of table and generate the limiting composite curve. It does not require any complicated plots or transferring of data from one plot to another. Finally, it can be used with FF operations as well as fixed FL operations. Therefore, combined problems, that haveboth types of operations, can be solved with this unifiedframework.

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