PROCESS DESIGN AND CONTROL

Rigorous Graphical Targeting for Resource Conservation via Material Recycle/Reuse Networks

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Material recycle/reuse is one of the key strategies in reducing the consumption of fresh resources in the process industries. Over the past decade, several techniques have been developed to reduce the consumption of specific material utilities such as water and hydrogen. To date, none of the published techniques provides a noniterative, systematic, and graphical technique for identifying a target for minimum usage of the fresh resources ahead of detailed design of the recycle/reuse network. In this paper, we present a rigorous graphical targeting approach to minimize the use of fresh resources by using segregation, mixing, and direct recycle/reuse strategies. First, the problem is formulated mathematically to provide a systematic basis for its solution. Then, dynamic programming techniques are employed to derive the mathematical conditions and characteristics of an optimal solution strategy. These conditions and characteristics are transformed into a graphical form that can be readily used to identify rigorous targets for minimum usage of fresh resources. The graphical technique is also useful in locating a material recycle/reuse pinch point, which provides insightful information on the use of fresh resources, the discharge of unused materials, and the relationships between process streams (sources) and units (sinks). Several test problems are solved to illustrate the ease, rigor, and applicability of the developed targeting technique.

Introduction

Processing facilities are characterized by the use of enormous amounts of material resources. Such depletion of natural resources poses many economic, social, and ecological challenges. Consequently, the process industries have pursued material conservation as a key approach toward market competitiveness and sustainability. Several strategies can lead to material conservation, including material recycle/reuse, material substitution, reaction alteration, and process modification.

Over the past decade, several design techniques have been developed to minimize the usage of fresh resources using network synthesis and analysis. In 1989, El-Halwagi and Manousiouthakis[1] introduced the problem of synthesizing mass exchange networks (MENs) that seeks to transfer certain species from a set of rich streams to a set of lean streams. They proposed systematic composite representations to identify targets for the maximum extent of mass exchange among process streams and minimum usage of external lean streams. The synthesis of MENs has been successfully used in waste recovery/separation applications. An important variation of MENs, wastewater minimization, was introduced in 1994 by Wang and Smith.[2] They proposed a graphical approach to target the minimum freshwater consumption and wastewater discharged by the transfer of contaminants from process streams to water streams. Both methods use the application of process units as mass exchange applications, and they rely on the basic principle of concentration driving force. Although some process units are mass exchangers, there are many water usage/wastewater discharge problems that are not included in the MEN-based wastewater minimization approach of Wang and Smith.[2] In MEN-based problems, the lean stream (e.g., water) acquires a certain load of mass and then proceeds to be potentially used in other units. There are several cases that are not directly covered by such scenarios. For instance, the lean streams might not leave the units as distinct streams (e.g., due to mixing, reaction, etc.). Another example is when a stream moves into an unrecoverable state. For instance, water might leave in a product stream or wet cake where it will not be recovered. A third case is when the lean stream (e.g., water, hydrogen, etc.) is generated in the process. In this case, no lean stream enters the unit, but a lean stream does leave the unit.

Dhole et al.[3] and El-Halwagi and Spriggs[4] independently observed the limitations of mass exchange networks on the application of wastewater and freshwater minimization methods. Many industrial processes using water and producing wastewater do not meet the criteria of mass exchange units. Instead, they addressed the problem of water usage and discharge through a source (supply) sink (demand) representation. This problem will be referred to as the recycle/reuse problem and is the focus of this paper. The objective of the recycle/reuse problem is to allocate various process sources (or streams) to sinks (units that can employ the sources) so as to minimize the consumption of the fresh resource (e.g., freshwater). Dhole et al.[3] created a new graphical technique that represents concentration versus flow rate and creates a supply composite and a demand composite. When the two composites touch, a bottleneck (water pinch) is identified and can be elimi-

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10.1021/ie030318a CCC: $25.00
Published on Web 08/14/2003

nated by mixing of source streams. Even though the methodology had great impact on the concept for water minimization, it has its drawbacks. The key limitation is that Dhole et al.[3] did not provide a systematic method for elimination of pinch points by mixing. To overcome this limitation, Polley and Polley[5] proposed a set of rules for sequencing mixing and recycle options. Additionally, Sorin and Bedard[6] proposed an algebraic method, called the evolutionary table, that is based on locating the global pinch based on mixing source streams with closer concentration differences first, and then going to the stream with the next nearest concentration. However, the evolutionary table also has its negative aspects. When the process has more than one global pinch, this approach can have drawbacks for process modifications by not discovering the true global pinch, as indicated in a study by Hallale.[7] To address this limitation, Hallale[7] attempted to solve all of the aforementioned limitations by coupling the water surplus diagram with a graphical representation of purity versus flow rate (similar to the Dhole et al.[3] graphical representation). The idea of surplus was first developed by Alves[8] for the application of hydrogen recovery systems in refineries. Both methods rely on extensive calculations to create the surplus diagram to target minimal consumption of resources (water in the case of Hallale[7] and hydrogen in the case of Alves and Towler[9]). Also, the development of this methodology is quite tedious because many calculations are required, and there is a dependence of two graphs to satisfy flow rate and composition for the source−sink structure.

Mathematical programming techniques have also been used to solve the recycle/reuse problems (Savelski and Bagajewicz[10,11]), including multicomponent systems (e.g., Alva-Argaez et al.,[12] Benko et al.,[13] and Dunn et al.[14,15]). Additionally, similar methods have been developed for unsteady-state and batch systems (e.g., Wang and Smith,[16] Almato et al.,[17] and Zhou et al.[18]).

Notwithstanding the usefulness of the aforementioned design procedures for the recycle/reuse problem, none of them presents a single-stage, systematic, and graphical targeting procedure. Indeed, these techniques can be broadly classified into two categories: iterative targeting and detailed network design. Iterative targeting involves the use of multistep graphical approaches to evolve the usage of fresh resource 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 usage of the fresh resource. Multiple networks can be configured to give the same minimum usage of fresh resource. In many cases, it is important to identify the target for minimum usage of fresh resources in a systematic way, ahead of detailed design and without commitment to the final network configurations.

The purpose of this paper is to introduce a systematic, single-stage, and graphical method for rigorously targeting minimum usage of fresh resources through material recycle/reuse techniques. First, we describe the problem through an optimization formulation. Then, we use dynamic programming techniques to determine the mathematical conditions and characteristics of an optimal solution strategy. These conditions and characteristics are transformed into a graphical technique that can be readily used to identify rigorous targets for minimum usage of fresh resources. The devised visualization tool is a novel graph of load versus flow rate constructed in a way that yields the rigorous target without iterations. The graphical technique is also useful in locating material recycle/reuse pinch points, which provides insightful information on the use of fresh resources, the discharge of unused materials, and the maximum extent of mass integration among process streams (sources) and units (sinks). The broad applicability and ease of implementation of this new method are shown and verified through the solution of several previous case studies published in earlier literature.

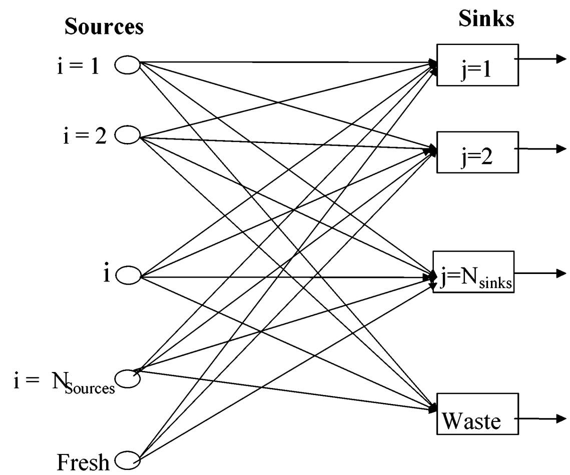

Figure 1. Source/sink allocation.

Problem Statement

Consider a process that consists of a set of process sinks and a set of process sources described as follows:

The set of process sinks (units) is designated SINKS $= \{j = 1, 2, ..., N_{\text{sinks}}\}$. Each sink requires a feed with a given flow rate, G_j, and a composition of a single targeted species, z_j^{in}, that satisfies the following constraint

$$z_j^{\min} \le z_j^{\text{in}} \le z_j^{\max} \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{1}$$

where $z_j^{\min}$ and $z_j^{\max}$ are given lower and upper bounds, respectively, on admissible compositions to unit j.

The set of process sources, designated SOURCES $= \{i = 1, 2, ..., N_{\text{sources}}\}$, can be recycled/reused in process sinks. Each source has a given flow rate, W_i, and a given composition, y_i.

Also available for service is a fresh (external) resource that can be purchased to supplement the use of process sources in sinks.

Given the above-described process, the objective is to develop a noniterative graphical procedure that determines the target for minimum usage of the fresh resource.

Problem Representation

The first step in the analysis is to represent the problem through a source−sink representation, as shown in Figure 1 (e.g., El-Halwagi[19]). Each source is split into fractions (of unknown flow rate) that are allocated to the various sinks. An additional sink is placed to account for unrecycled/unreused material. This sink is referred to as the “waste” sink. The fresh resource is also allowed to split and is allocated to all sinks but the waste sink.

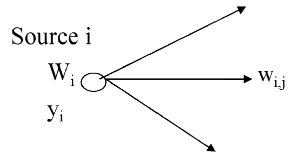

Figure 2. Splitting of sources.

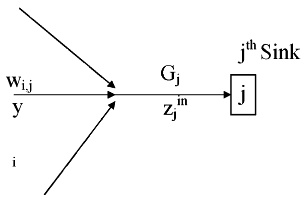

Figure 3. Mixing of sources at inlets of sinks.

Opmization Formulation

The optimization problem is formulated as follows

$$\text{minimize consumption of fresh resource} = \sum_{j=1}^{N_{\text{sinks}}} F_j \tag{2}$$

subject to the following constraints

Splitting of the sources (Figure 2)

$$W_i = \sum_{j=1}^{N_{\text{sinks}}} w_{i,j} + w_{i,\text{waste}} \qquad \text{for } i = 1, 2, ..., N_{\text{sources}} \tag{3}$$

Mixing of the jth sink (Figure 3)

$$G_j = F_j + \sum_{i=1}^{N_{\text{sources}}} w_{i,j} \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{4}$$

where F_j is the amount of fresh resource fed to the jth sink. Considering a fresh source, which has no impurities, we obtain the following component material balance around the mixing point of the feed to the sink

$$G_j z_j^{\text{in}} = \sum_{i=1}^{N_{\text{sources}}} w_{i,j} y_i \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{5}$$

$$z_j^{\min} \le z_j^{\text{in}} \le z_j^{\max} \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{1}$$

As an aside, note that the same equation can be applied even when the fresh source has a nonzero content, y_{fresh}, of the pollutant by defining compositions as differences based on the fresh composition, i.e.

$$z_j^{\text{in}} \le z_j^{\text{in,actual}} - y_{\text{fresh}} \qquad \text{and} \qquad y_i = y_i^{\text{actual}} - y_{\text{fresh}}$$

Nonnegativity of each fraction of source allocated to a sink and of flow of fresh resources

$$w_{i,j} \ge 0 \qquad \text{for } i = 1, 2, ..., N_{\text{sources}} \text{ and } j = 1, 2, ..., N_{\text{sinks}} \tag{6}$$

$$F_j \ge 0 \qquad j = 1, 2, ..., N_{\text{sinks}} \tag{7}$$

The foregoing formulation is a linear program that can be solved globally to identify the optimal target and source−sink matches. However, as mentioned earlier, our objective is to develop a graphical technique that can provide valuable insights into the key characteristics of the problem and not just its solution. These insights can guide many design and operating decisions that extend beyond finding a specific solution.

Derivation of Optimality Conditions via Dynamic Programming

Dynamic programming is an optimization technique that is particularly useful for handling multistage operations. It is based on Bellman's principle of optimality,[20] which states that "an optimal policy has the property that, whatever the initial state and the initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision." In dynamic programming, three elements must be defined:

(1) The first element is the stage (j), which represents the portion of the problem for which a decision is to be made. Hence, we choose each sink as a stage (Figure 4). We rank the sinks in ascending order of maximum allowable composition (i.e., $z_1^{\max} \le \mathbf{z}_2^{\max} \cdots \le z_j^{\max} \cdots \le z_{N_{\text{sinks}}}^{\max}$).

(2) The second element is the return function for each stage, which represents the objective function associated with that stage. For our case, this corresponds to the flow rate of the fresh source used in that stage (i.e., F_j).

(3) The final element is the state of each stage (R_j), which represents the connection between succeeding stages such that, when each stage s is optimized separately, the resulting decision is automatically feasible for the rest of the stages. Here, we define the state of the jth stage as the remaining (unused) flows of the sources up to that stage. Therefore

$$R_j = [R_{1,j}, R_{2,j}, ..., R_{i,j}, ..., R_{N_{\text{sources}},j}] \tag{8}$$

where

$$R_{i,j} = W_i - \sum_{j=1}^{j-1} w_{i,j} \qquad \text{for } i = 1, 2, ..., N_{\text{sources}} \tag{9}$$

Let us start by deriving the optimality conditions for the first subproblem corresponding to stage $j = N_{\text{sinks}}$

$$\min F_{N_{\text{sinks}}} \tag{10}$$

subject to

$$G_{N_{\text{sinks}}} = F_{N_{\text{sinks}}} + \sum_{i=1}^{N_{\text{sources}}} w_{i,N_{\text{sinks}}} \tag{11}$$

$$G_{N_{\text{sinks}}} z_{N_{\text{sinks}}}^{\text{in}} = \sum_{i=1}^{N_{\text{sources}}} w_{i,N_{\text{sinks}}} y_i \tag{12}$$

$$z_{N_{\text{sinks}}}^{\min} \le z_{N_{\text{sinks}}}^{\text{in}} \le z_{N_{\text{sinks}}}^{\max} \tag{13}$$

$$R_{i,N_{\text{sinks}}} = W_i - \sum_{j=1}^{N_{\text{sinks}}-1} w_{i,j} \qquad \text{for i} = 1, 2, ..., N_{\text{sources}} \tag{14}$$

Nonnegativity of each fraction of source allocated to a sink and of flow of fresh resources implies

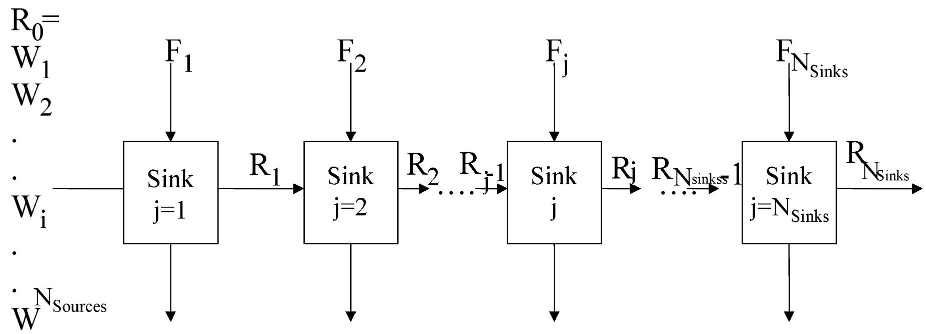

Figure 4. Stage representation.

$$w_{i,N_{\text{sinks}}} \geq 0 \qquad \text{for } i = 1, 2, ..., N_{\text{sources}} \tag{15}$$

$$F_j \geq 0 \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{16}$$

$$R_{i,N_{\text{sinks}}} \geq 0 \qquad \text{for } i = 1, 2, ..., N_{\text{sources}} \tag{17}$$

To derive the optimality conditions for $F_{N_{\text{sinks}}}$, we need to identify optimal parametric values for $z^{\text{in}}_{N_{\text{sources}}}$ *and* $w_{i,N_{\text{sinks}}}$. Let us start with the case of a single process source, i, mixed with a fresh stream. The program then becomes

$$\min F_{N_{\text{sinks}}} \tag{18}$$

subject to

$$G_{N_{\text{sinks}}} = F_{N_{\text{sinks}}} + w_{i,N_{\text{sinks}}} \tag{19}$$

$$G_{N_{\text{sinks}}} z^{\text{in}}_{N_{\text{sinks}}} = w_{i,N_{\text{sinks}}} y_i \tag{20}$$

$$z^{\text{min}}_{N_{\text{sinks}}} \leq z^{\text{in}}_{N_{\text{sinks}}} \leq z^{\text{max}}_{N_{\text{sinks}}} \tag{21}$$

$$R_{i,N_{\text{sinks}}} = W_i - \sum_{j=1}^{N_{\text{sinks}}-1} w_{i,j} \qquad \text{for i} = 1, 2, ..., N_{\text{sources}} \tag{22}$$

By combining constraints 19 and 20, we obtain

$$F_{N_{\text{sinks}}} = G_{N_{\text{sinks}}} - \frac{G_{N_{\text{sinks}}}}{y_i} z^{\text{in}}_{N_{\text{sinks}}} \tag{23}$$

Hence, we can state the following sink-composition rule: To minimize $F_{N_{\text{sinks}}}$, the value of $z^{\text{in}}_{N_{\text{sinks}}}$ should be maximized while satisfying the nonnegativity constraints for the fresh resource and for the ith source

$$F_{N_{\text{sinks}}} \geq 0$$

and

$$R_{i,N_{\text{sinks}}} - w_{i,N_{\text{sinks}}} \geq 0$$

Therefore, when these two nonnegativity constraints are satisfied, we can also state more specifically the following optimality conditions

$$z^{\text{in,optimum}}_{N_{\text{sinks}}} = z^{\text{max}}_{N_{\text{sinks}}} \qquad \text{for } y_i > z^{\text{max}}_{N_{\text{sinks}}} \tag{24a}$$

(implying usage of fresh resource, $F_{N_{\text{sinks}}} > 0$) and

$$z^{\text{in,optimum}}_{N_{\text{sinks}}} = y_i \qquad \text{for } y_i \leq z^{\text{max}}_{N_{\text{sinks}}} \tag{24b}$$

(implying no usage of fresh resource, $F_{N_{\text{sinks}}} = 0$). These two conditions can be summarized by the following specific sink-composition rule: The optimum inlet composition of the sink should be set to its maximum limit unless no fresh resource is to be used in this sink (in which case, the inlet composition of the sink is that of the recycled/reused sources).

It is worth pointing out that, if the recyclable source, i, has been completely recycled (i.e., $R_{i,N_{\text{sinks}}} - w_{i,N_{\text{sinks}}} = 0$), then the minimum amount of fresh resource is given by a simple material balance

$$F^{\text{min}}_{N_{\text{sinks}}} = G_{N_{\text{sinks}}} - R_{i,N_{\text{sinks}}} \tag{25}$$

Consequently

$$z^{\text{in}}_{N_{\text{sinks}}} = \frac{R_{i,N_{\text{sinks}}} y_i}{G_{N_{\text{sinks}}}} \tag{26}$$

Having identified the optimal value of the inlet composition to the sink, we now turn our attention to the optimization of $w_{i,N_{\text{sinks}}}$. Let us start with two sources ($i = 1$ and 2), where, according to our terminology, $y_1 < y_2$. Constraints 11 and 12 can be written as

$$G_{N_{\text{sinks}}} = F_{N_{\text{sinks}}} + w_{1,N_{\text{sinks}}} + w_{2,N_{\text{sinks}}} \tag{27}$$

$$G_{N_{\text{sinks}}} z^{\text{max}}_{N_{\text{sinks}}} = w_{1,N_{\text{sinks}}} y_1 + w_{2,N_{\text{sinks}}} y_2 \tag{28}$$

Combining these two equations, we obtain

$$F_{N_{\text{sinks}}} = w_{1,N_{\text{sinks}}} \left(\frac{y_1}{y_2} - 1 \right) - G_{N_{\text{sinks}}} \left(\frac{z^{\text{max}}_{N_{\text{sinks}}}}{y_2} - 1 \right) \tag{29}$$

Because

$$\left(\frac{y_1}{y_2} - 1 \right) < 0$$

then

$$F^{\text{optimum}}_{N_{\text{sinks}}} \text{ corresponds to } w_{1,N_{\text{sinks}}} = w^{\text{max}}_{1,N_{\text{sinks}}} \tag{30}$$

Therefore, before considering the use of source $i = 2$, the use of source $i = 1$ should be maximized subject to the availability constraint of source i (nonnegative state variable)

$$R_{1,N_{\text{sinks}}} = W_1 - \sum_{j=1}^{N_{\text{sinks}}-1} w_{1,j} \geq 0 \tag{31}$$

If this constraint becomes active (i.e., $R_{1,N_{\text{sinks}}} = 0$), then we move to maximizing the usage of source $i = 2$. By induction, one can reach the same result when more than two process sources are considered.

We now proceed to the use of dynamic programming for the subsequent subproblem ($j = N_{\text{sinks}} - 1$). Hence, the following source prioritization rule can be stated: For a given sink with several remaining sources (unused in previous sinks), recycle/reuse of sources is prioritized on the basis of composition, in ascending order. A source $i + 1$ whose composition is higher than that of source i should not be used until source i is fully recycled/reused.

The next subproblem can be formulated as follows: The objective function is

$$F_{N_{\text{sources}}}^{\text{optimum}} + \min F_{N_{\text{sinks}}-1} \tag{32}$$

subject to

$$G_{N_{\text{sinks}}-1} = F_{N_{\text{sinks}}-1} + \sum_{i=1}^{N_{\text{sources}}} w_{i,N_{\text{sinks}}-1} \tag{33}$$

$$G_{N_{\text{sinks}}-1} z_{N_{\text{sinks}}-1}^{\text{in}} = \sum_{i=1}^{N_{\text{sources}}} w_{i,N_{\text{sinks}}-1} y_i \tag{34}$$

$$z_{N_{\text{sinks}}-1}^{\min} \le z_{N_{\text{sinks}}-1}^{\text{in}} \le z_{N_{\text{sinks}}-1}^{\max} \tag{35}$$

$$R_{i,N_{\text{sinks}}-1} = W_i - \sum_{j=1}^{N_{\text{sinks}}-2} w_{i,j} \qquad \text{for i} = 1, 2, ..., N_{\text{sources}} \tag{36}$$

Because $F_{N_{\text{sources}}}^{\text{optimum}}$ has already been identified by solving the first subproblem, the solution of the second subproblem yields the same source prioritization rules for optimality conditions. Hence, for a sink j and available process sources (with source i being the stream with the lowest composition that has not been fully consumed by previous sinks), we can state the following two fundamental optimization rules for minimizing the use of fresh source:

Rule 1a. If a sink requires the use of fresh source, the inlet composition to the sink should be maximized, i.e.

$$z_j^{\text{in,optimum}} = z_j^{\max} \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{37}$$

unless no fresh resource is to be used in this sink (in which case, the inlet composition of the sink is that of the recycled/reused sources).

Multiply the above condition by the flow rate of the sink, G_j, and recall that the pollutant load entering the sink, M_j^{sink}, is defined as

$$M_j^{\text{sink}} = G_j z_j^{\text{in}} \tag{38}$$

Then, the foregoing rule can be restated as follows:

Rule 1b. If a sink requires the use of fresh source, the inlet pollutant load to the sink should be maximized, i.e.

$$M_j^{\text{in,optimum}} = M_j^{\max} \qquad \text{for } j = 1, 2, ..., N_{\text{sinks}} \tag{39}$$

unless no fresh resource is to be used in this sink (in which case, the inlet load of the sink is that of the recycled/reused sources).

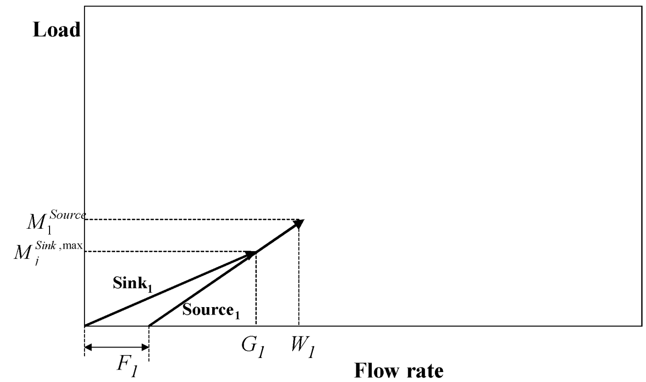

Figure 5. Load versus flow rate graph for one source and one sink.

Rule 2. Maximize the recycle/reuse of the available amount of source (i) until it is fully consumed; then maximize the recycle/reuse of the next source in ascending order of composition ($i + 1$), and so on.

These rules constitute the basis for the following graphical procedure:

(1) Rank the sinks in ascending order of maximum admissible composition

$$z_1^{\max} \le z_2^{\max} \le \cdots \le z_j^{\max} \le \cdots \le z_{N_{\text{sinks}}}^{\max} \tag{40}$$

(2) Rank sources in ascending order of pollutant composition, i.e.

$$y_1 < y_2 < \cdots < y_i < \cdots < y_{N_{\text{sources}}} \tag{41}$$

(3) Start with the first sink, $j = 1$. Recycle/reuse the first source, $i = 1$, until it is fully consumed or until the maximum inlet load to the sink is met. If the first source is fully consumed, recycle/reuse the second source, $i = 2$, until it is fully consumed or until the maximum inlet load to the sink is met (whichever comes first), and so on.

(4) Move on to the second sink, $j = 2$. Repeat the same procedure as in step 3, starting with the remaining source that has the lowest composition. The same procedure is subsequently repeated for the rest of the sinks in ascending order.

Figure 5 illustrates the graphical procedure. The graphical representation is a plot of pollutant load versus flow rate. For each sink, the maximum pollutant load, which is calculated through

$$M_j^{\text{sink,max}} = G_j z_j^{\max} \tag{42}$$

is plotted versus the flow rate required by the sink, G_j. This gives a straight line whose slope is $z_j^{\max}$.

Similarly, the load of each source is given by

$$M_i^{\text{source}} = W_i y_i \tag{43}$$

Hence, the source load is plotted versus its flow rate to give a straight line whose slope is the composition of the pollutant, y_i.

Let us start with the first sink and consider a case where the pollutant load for the first source exceeds the maximum inlet load to the first sink. Therefore, we move the source arrow until it touches the sink arrow with the source completely below the sink in the overlapped region, as shown in Figure 5.

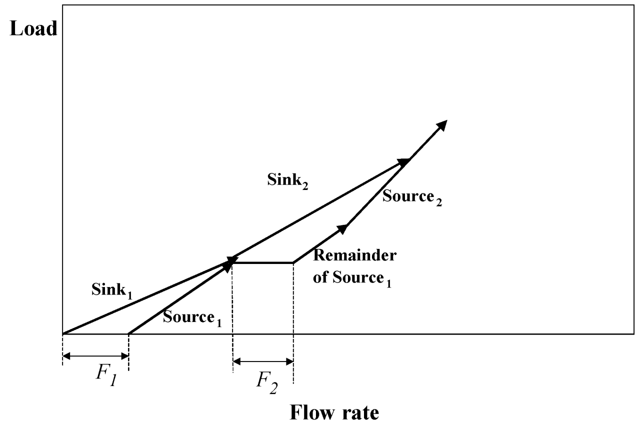

Figure 6. Load versus flow rate graph for two sources and two sinks.

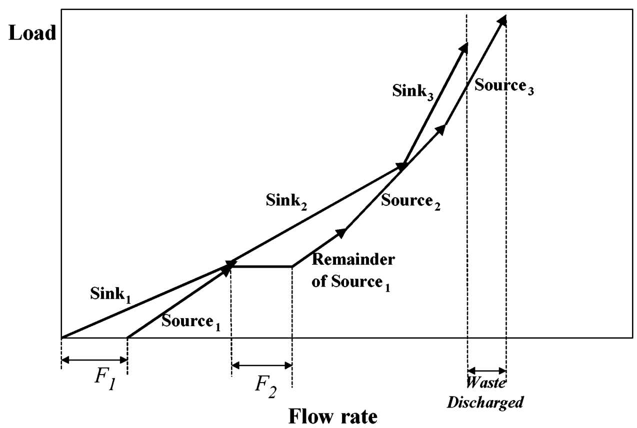

Figure 7. Load versus flow rate graph for three sources and three sinks.

The overlapped flow rate represents the extent of recycle/reuse from the first source to the first sink. The unfulfilled flow rate of the sink must now be provided by a fresh resource. The remaining flow rate of the first source is considered for recycle/reuse in the second sink and is supplemented with fresh source as needed (Figure 6).

The feed requirements for the third sink can be satisfied by a mixture of the remainder of the second source and a fraction of the third source. No fresh source is required in the third sink. With no more sinks in the problem, the rest of the third source is discharged (Figure 7).

By adding the fresh flow rates required in sink$_1$ and sink$_2$, we obtain the total amount of fresh usage. This total amount of fresh usage ($F_1 + F_2$) is plotted along with source$_1$, source$_2$, and source$_3$ in ascending order (lowest to highest concentration) just as for sink$_1$, sink$_2$, and sink$_3$ (Figure 8), with the point of contact between the sources and sinks being the material recycle pinch point. Subsequently, by plotting the sources and sinks in the above-described method, composite curves are generated with the source composite being shifted to the right until it lies completely below the sink composite (Figure 9).

Targeting Procedure

Thus far, we have solved the recycle/reuse problem by identifying optimal recycle/reuse strategies. Nonetheless, the objective is to determine a targeting procedure that provides a value for minimum usage of fresh resource prior to design and without detailing the allocation strategies. Furthermore, whereas there is a single target for fresh resource consumption, there are many (sometimes infinite) alternative source−sink matches that can yield the target. Therefore, it is necessary to extract a targeting procedure from the previous results.

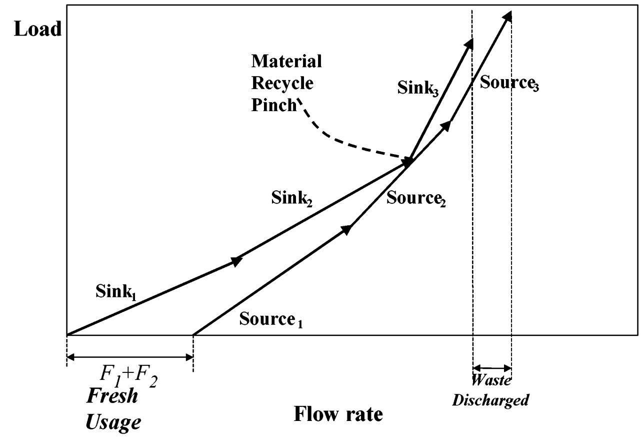

Figure 8. Revised load versus flow rate graph for three sources and three sinks.

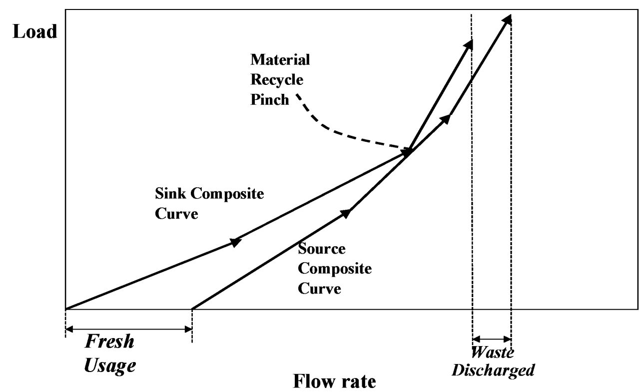

Figure 9. Source/sink composite.

A key insight can be obtained from the preceding graph. There is a point on the graph that distinguishes two zones. Below that point, fresh resource is used in the sinks, and above that point, unused process sources are discharged. This point will be referred to as the "material recycle/reuse pinch point". The key characteristic of this point is based on the following observation: the pinch point is the point where the load of recycled/reused sources matches that of the sink. Therefore, it can be graphically determined through the following procedure:

(1) Rank the sinks in ascending order of maximum admissible composition

$$z_1^{\max} \le z_2^{\max} \le \cdots \le z_j^{\max} \le \cdots \le z_{N_{\text{sinks}}}^{\max}$$

(2) Rank the sources in ascending order of pollutant composition, i.e.

$$y_1 < y_2 < \cdots < y_i < \cdots < y_{N_{\text{sources}}}$$

(3) Plot the maximum load of each sink ($M_j^{\text{sink,max}} = G_j z_j^{\max}$) versus its flow rate. Create a sink composite curve by superimposing the sink arrows in ascending order.

Table 1. Process Information for Example 1

sink	flow (tonne/h)	maximum inlet concentration (ppm)	load (kg/h)
1	120	0	0
2	80	50	4
3	80	50	4
4	140	140	19.6
5	80	170	13.6
6	195	240	46.8

source	flow (tonne/h)	concentration (ppm)	load (kg/h)
1	120	100	12
2	80	140	11.2
3	140	180	25.2
4	80	230	18.4
5	195	250	48.75

(4) Plot the load of each source ($M_i^{\text{source}} = W_i y_i$) versus its flow rate. Create a source composite curve by superimposing the sources in ascending order.

(5) Move the source composite stream until it touches the sink composite stream, with the source composite below the sink composite in the overlapped region. The point where they touch is the material recycle/reuse pinch point. The flow rate of sinks below which there are no sources is the target for minimum fresh discharge. On the other hand, the flow rate of the sources above which there are no sinks is the target for waste discharge.

It is worth noting that the above procedure is geared toward single-component systems. It can also apply to multicomponent systems where there is a limiting component and the solution strategies for the other components are consistent with that of the limiting component. For other multicomponent problems, a more general approach should be developed.

Case Studies

To illustrate the applicability of the devised procedure, we solve four case studies that were published recently with solutions through iterative procedures or detailed analyses encompassing the structure of the recycle/reuse networks.

Example 1. This case study is taken from Sorin and Bedard.[6] Table 1 shows six processes containing a single contaminant. Each process has an inlet and outlet water flow rate and contaminant concentration, with the exception of process 3, which consumes its entire flow rate and therefore has no outlet. Additionally, the process inlet and outlet flow rates have been fixed for all six operations.

To begin the targeting procedure, first the sinks and sources are identified and ranked in terms of ascending concentration levels. In this system, each process inlet is identified as a sink. Additionally, the outlets of processes 1, 2, 4, 5, and 6 are identified as sources. Following the procedure outlined in the Targeting Procedure section, the sinks are cumulatively plotted on a load versus flow rate diagram starting with those with the lowest concentration. Then, the sources are plotted cumulatively on the same graph, also in ascending order of concentration. Finally, the source composite line is shifted to the right by adding freshwater until the entire composite source line lies to the right and below the composite sink line. The resulting plot can be seen below in Figure 10. As shown in Figure 10, the minimum freshwater required is 200 tonnes/h, and the minimum wastewater discharge is 120 tonnes/h. These values agree exactly with those found by Sorin and Bedard[6] using their algebraic evolutionary table method. Additionally, the graph identifies two points where the source composite touches the sink composite.

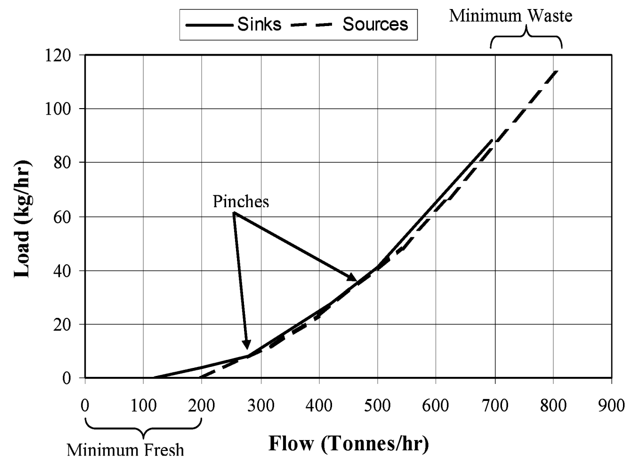

Figure 10. Shifted source/sink composite curves for example 1.

Table 2. Process Information for Example 2

sink	flow (tonne/h)	maximum inlet concentration (ppm)	load (kg/h)
1	50	20	1
2	100	50	5
3	80	100	8
4	70	200	14

source	flow (tonne/h)	concentration (ppm)	load (kg/h)
1	50	50	2.5
2	100	100	10
3	70	150	10.5
4	60	250	15

By examining the graph, two water recycle/reuse pinch points are identified corresponding to compositions of 100 and 180 ppm. Through the evolutionary table method, Sorin and Bedard[13] located a limiting source concentration of 180 ppm that they deemed the global pinch source. The existence of multiple pinch points at 100 and 180 ppm in this case study was discovered by Hallale[14] through an iterative water surplus diagram. Hallale[14] also verified the targets found for freshwater and wastewater by Sorin and Bedard.[13]

Example 2. The second case study is taken from Polley and Polley.[5] This problem involves four sources and four sinks, and relevant information about them is provided in Table 2:

Constructing the cumulative composite curves and shifting the source composite to the right as in the previous example, the shifted source/sink composite graph can be created and is shown below in Figure 11.

Figure 11 shows that the minimum freshwater required by the sinks is 70 tonnes/h, and the minimum wastewater discharged from the process is 50 tonnes/h. Additionally, the pinch concentration is shown to correspond to source 3 (150 ppm). The minimum freshwater and wastewater targets found above are identical to those found by Polley and Polley[5] using their method. Polley and Polley did not locate a pinch point; however, Hallale,[7] using a water surplus diagram, determined the pinch location to be 150 ppm, which is in agreement with the value obtained here.

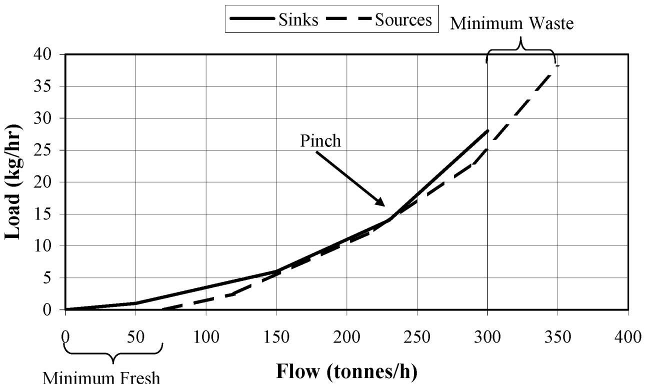

Figure 11. Shifted source/sink composite curves for example 2.

Table 3. Process Source Information for Example 3

source	flow (L/min)	fines concentration (%)	load (L/min)
TMP clear water	25 000	0.07	17.5
TMP cloudy water	39 000	0.13	50.7
inclined screen water	5980	0.5	29.9
press header water	2840	0.49	13.9
save-all clear water	6840	0.08	5.5
save-all clear water	3720	0.1	3.7
silo water	73 000	0.39	284.7
machine chest whitewater	8585	0.34	29.2
vacuum pump overflow	2570	0	0.0
residual showers	1940	0.13	2.5

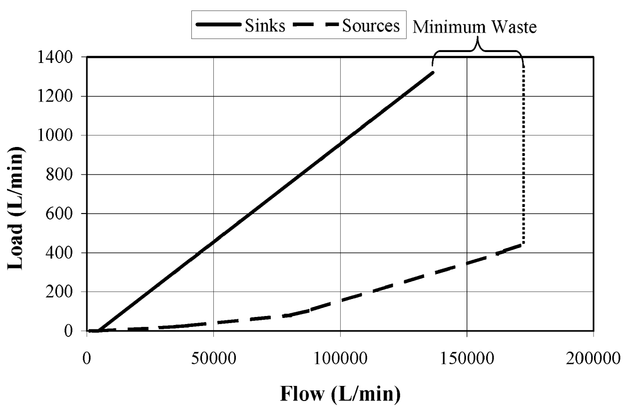

Figure 12. Shifted source/sink composite curves for example 3.

Example 3. To show the applicability of the approach to a large process, the third case study is taken from Jacob et al.[20] The study is of a thermomechanical pulp and newsprint mill consisting of 54 sinks and 10 sources. The source and sink data are presented in Tables 3 and 4.

Upon examination of the sinks, it is clear that there are only four concentration levels of interest. Therefore, the sinks can be lumped into four sinks with fines concentrations of 0, 0.018, 0.02, and 1. The resulting lumped sinks can be seen in Table 5.

Using the information from Tables 3 and 5, the shifted source/sink composite can be constructed and is shown in Figure 12.

From Figure 12, the minimum wastewater discharge can be determined as 34 292 L/min; however, to determine the minimum freshwater requirements and pinch location, the region close to the origin must be examined. In Figure 13, a magnified plot of the area of interest in Figure 12 can be seen.

Analyzing Figure 13, the minimum freshwater required for the process can be found as 1342 L/min, with a pinch located at 0.07% fines. According to Jacob et al.,[21] the minimum freshwater required for this system is 1380 L/min, which is slightly higher than the target we identified.

Example 4. To show the broad applicability of the proposed method, the final case study to be solved involves the recycle and reuse of hydrogen rather than water. The fourth case study is taken from Alves and

Table 4. Process Sink Information for Example 3

sink	flow (L/min)	maximum allowable fines concentration (%)	load (L/min)
1	200	1	2.0
2	400	1	4.0
3	355	0.02	0.1
4	150	1	1.5
5	13 000	1	130.0
6	4250	1	42.5
7	2800	1	28.0
8	4580	1	45.8
9	1950	1	19.5
10	500	1	5.0
11	1000	1	10.0
12	3000	1	30.0
13	435	1	4.4
14	310	1	3.1
15	60	1	0.6
16	1880	1	18.8
17	4290	1	42.9
18	9470	1	94.7
19	6500	1	65.0
20	620	1	6.2
21	55	1	0.6
22	70	1	0.7
23	320	1	3.2
24	1050	1	10.5
25	73 000	1	730.0
26	1765	1	17.7
27	235	1	2.4
28	95	1	1.0
29	20	1	0.2
30	180	0	0.0
31	160	0.018	0.03
32	30	0.018	0.005
33	20	0.018	0.004
34	315	0	0.0
35	315	0	0.0
36	930	0.018	0.2
37	460	0.018	0.1
38	30	0.018	0.005
39	30	0.018	0.005
40	315	0	0.0
41	315	0	0.0
42	110	0.018	0.02
43	110	0.018	0.02
44	190	0	0.0
45	190	0	0.0
46	100	0	0.0
47	20	0	0.0
48	15	0	0.0
49	60	0.018	0.01
50	30	0.018	0.005
51	100	0	0.0
52	20	0	0.0
53	100	0	0.0
54	20	0	0.0

Table 5. Consolidated Process Sink Information for Example 3

sink	flow (L/min)	maximum allowable fines concentration (%)	load (L/min)
1′	2195	0	0.0
2′	1970	0.018	0.4
3′	355	0.02	0.1
4′	132 005	1	1320.1

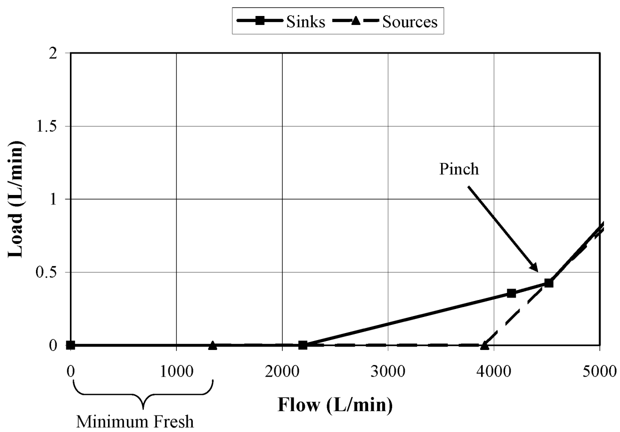

Figure 13. Magnified shifted source/sink composite curves for example 3.

Table 6. Process Information for Example 4

sink	flow (mol/s)	maximum inlet impurity concentration (mol %)	load (mol/s)
1	2495	19.39	483.8
2	180.2	21.15	38.1
3	554.4	22.43	124.4
4	720.7	24.86	179.2

source	flow (mol/s)	impurity concentration (mol %)	load (mol/s)
1	623.8	7	43.7
2	415.8	20	83.2
3	1801.9	25	450.5
4	138.6	25	34.7
5	346.5	27	93.6
6	457.4	30	137.2

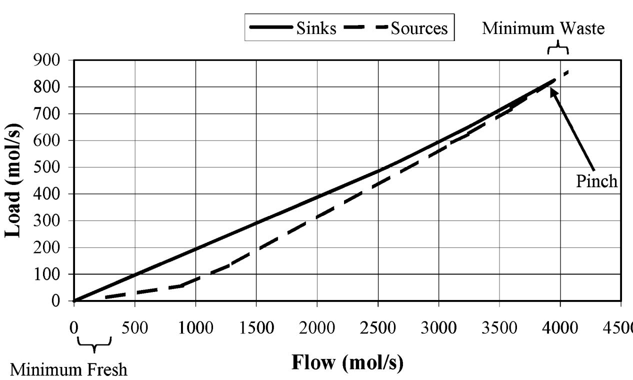

Figure 14. Shifted source/sink composite curves for example 4.

Towler.[9] This case study involves the optimization of a hydrogen distribution system within a refinery, and it comprises four sinks and six sources. The pertinent information regarding these sinks and sources is given in Table 6.

Additionally, in this case study, the fresh resource contains a small quantity of impurity, i.e., the fresh hydrogen has a 5% impurity level. Using the information in Table 6, the shifted source/sink composite curves can be constructed, as shown in Figure 14.

From Figure 14, one can determine that the minimum hydrogen required and waste hydrogen to be discharged are 268.8 and 102.5 mol/s, respectively. Additionally, the pinch point occurs at the last source, which corresponds to a hydrogen impurity of 30%. These values are in agreement with those found by Alves and Towler[9] using the iterative hydrogen surplus diagram approach.

Conclusions

We have developed a single-stage, systematic, and graphical method for identifying rigorous targets for the recycle/reuse problem. The optimality conditions were first derived using a dynamic programming formulation and an analytical solution for parametric optimization. The results of the mathematical analysis were next invoked in developing a new pinch-based graphical representation of composite load versus flow in a way that ensures optimality. The devised visualization tools accurately determine the minimum usage of fresh resources, the minimum discharge of waste, and the maximum recycle/reuse of process streams. Several published case studies were used to illustrate the ease and applicability of this novel graphical technique.

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Received for review April 16, 2003
Revised manuscript received June 24, 2003
Accepted June 24, 2003

IE030318A