CHAPTER SIX

ALGEBRAIC APPROACH TO TARGETING DIRECT RECYCLE

Chapter Three presented the material recycle pinch diagram as a graphical tool to identify targets for direct recycle problems. In spite of the usefulness and insights of the graphical methods, it is beneficial to develop an algebraic procedure which is particularly useful in the following cases:

- Numerous sources and sinks: As the number of sources and sinks increase, it becomes more convenient to use spreadsheets or algebraic calculations to handle the targeting.
- Scaling problems: If there is a significant difference in values of flowrates and/or loads for some of the sources and/or sinks, the graphical representation becomes inaccurate since the larger flows/loads will skew the scale for the other streams.
- If the targeting is tied with a broader design task that is handled through algebraic computations, it is desirable to use consistent algebraic tools for all the tasks.

This chapter presents the algebraic analogue to the material-recycle pinch diagram.

6.1. PROBLEM STATEMENT

The problem can be expressed as follows:

Given a process with a number ($N_{sources}$) of process sources (e.g., process streams, wastes) that may be considered for possible recycle and replacement of the fresh material and/or reduction of waste discharge. Each source, i, has a given flow rate, W_i, and a given composition of a targeted species, y_i. Available for service is a fresh (external) resource that can be purchased to supplement the use of process sources in sinks. The sinks are N_{sinks} process units that employ a fresh resource. Each sink, j, requires a feed whose flow rate, G_j^{in}, and an inlet composition of a targeted species, z_j^{in}, must satisfy the following bounds:

$$0 \le z_j^{in} \le z_j^{max} \quad \text{where } j = 1,2, \ldots, N_{sinks} \qquad (6.1)$$

Fresh (external) resource may be purchased to supplement the use of process sources in sinks. The objective is to develop a non-iterative algebraic procedure aimed at minimizing the purchase of fresh resource, maximizing the usage of process sources, and minimizing waste discharge.

6.2. ALGEBRAIC TARGETING APPROACH

In this section, the algebraic procedure developed by Almutlaq and El-Halwagi (2005) and Almutlaq et al. (2005) is presented. First, it is necessary to recall the two direct-recycle optimality conditions derived in Chapter Three:

Sink Composition Rule: When a fresh resource is mixed with process source(s), the composition of the mixture entering the sink should be set to a value that minimizes the fresh arm. For instance, when the fresh resource is a pure substance that can be mixed with pollutant-laden process sources, the composition of the mixture should be set to the maximum admissible value.

Source Prioritization Rule: In order to minimize the usage of the fresh resource, recycle of the process sources should be prioritized in order of their fresh arms starting with the source having the shortest fresh arm.

These rules constitute the basis for the material-recycle pinch diagram as shown in Fig. 6.1. As described in Chapter Three, the sink composite is a cumulative representation of all the sinks and corresponds to the upper bound on their feasibility region whereas the source composite curve is a cumulative representation of all process streams considered for recycle. The source composite stream may be represented anywhere and is then slid horizontally (in the case of pure fresh) on the flowrate axis until it touches the sink composite stream with the source composite below the sink composite in the overlapped region.

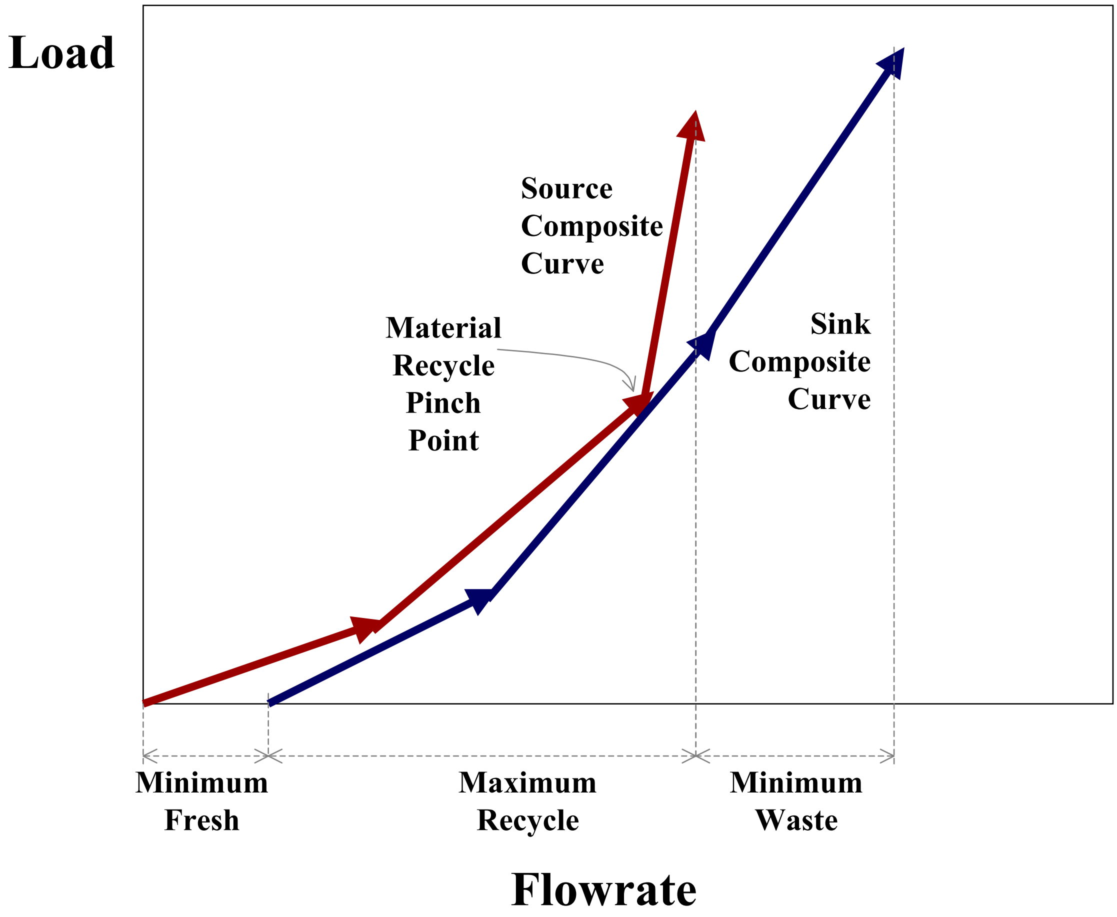

Figure 6.1: Material Recycle Pinch Diagram (El-Halwagi et al., 2003)

Now, suppose that we start plotting both composite streams from the origin point (Fig. 6.2). If the source composite is completely, below the sink composite, then the process does not require a fresh resource. Nonetheless, if there is any portion of the source composite lying above the sink composite, then infeasibilites exist and must be removed by using a fresh resource. Such infeasibility may be described in a couple of ways by looking vertically and horizontally. Looking vertically at a given flowrate, if the source composite lies above the sink composite, then the source composite violates the maximum load admissible to the sink. Alternatively by looking horizontally at a given load, if the source composite lies to the left of the sink composite, then there is a shortage of the flowrate necessary for the sink. The maximum horizontal infeasibility corresponds to the maximum shortage of flowrate which is designated as δ_{max}. Indeed, all infeasibilities are eliminated by sliding the source composite curve to the right a distance equal to δ_{max} (Fig. 6.3). Consequently, the target for minimum fresh usage is equal to the maximum shortage, i.e.

$$\text{Target for Minimum Fresh Consumption} = \delta_{max} \quad (6.2)$$

The targeting question involves the algebraic identification of this maximum shortage without the need to resort to the graphical representation.

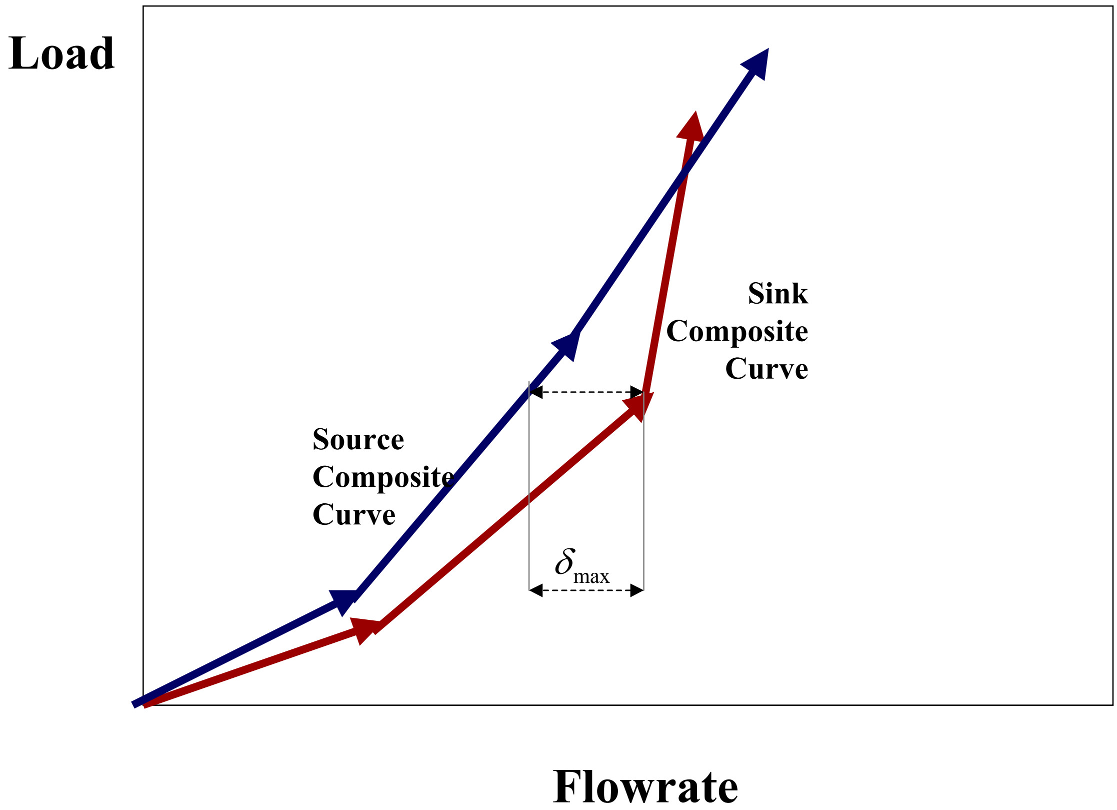

Fig. 6. 2. Sliding the Source Composite to the Left Generates Infeasibility (Almutlaq and El-Halwagi, 2005)

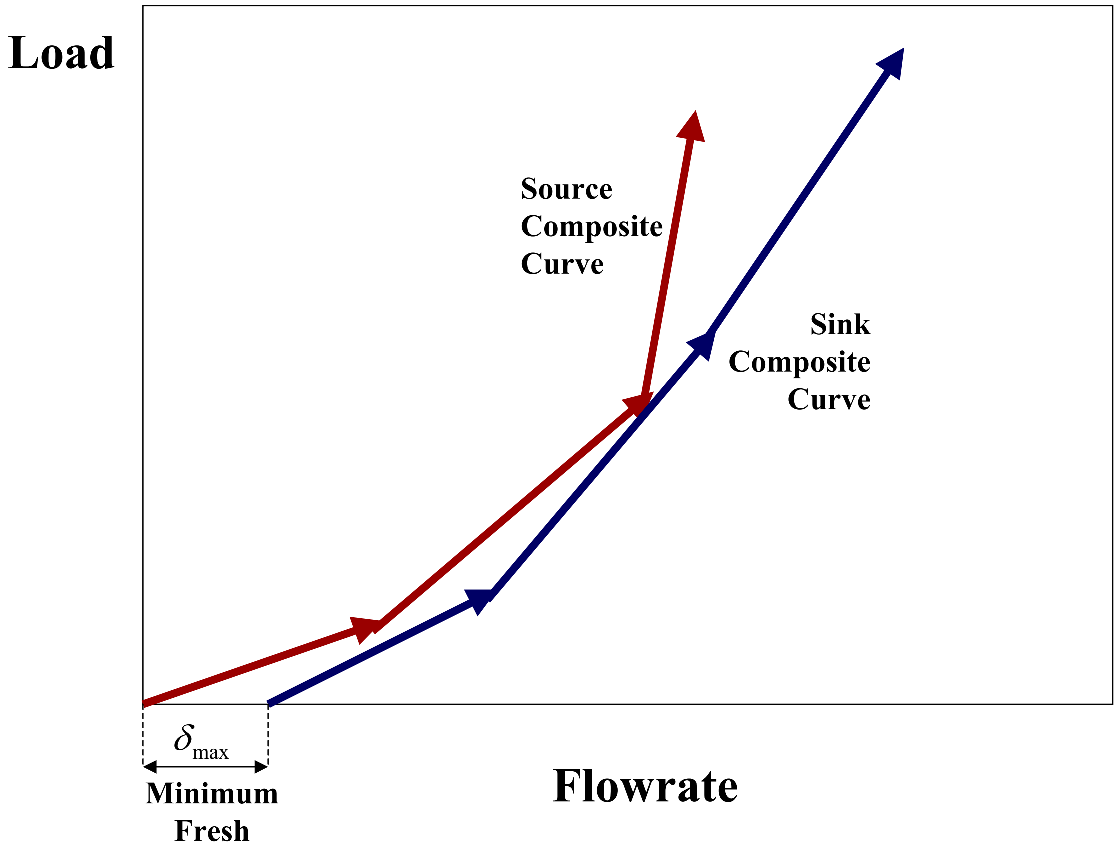

Fig. 6.3. Minimum Fresh Target Corresponds to Maximum Flow Shortage (Almutlaq and El-Halwagi, 2005)

Let us revisit Fig. 6.2 and draw horizontal lines at corner points (kinks) of the source- and sink-composite curves (Fig. 6.4). Let us use an index k to designated those horizontal lines starting with k = 0 at the zero load level and going up at each horizontal level. The load at each horizontal level, k, is referred to as M_k. The vertical distance between each two horizontal lines is referred to as a *load interval* and is given the index k as well. The load within interval k is calculated as follows:

$$\Delta M_k = M_k - M_{k-1} \tag{6.3}$$

The next step is to calculate the flowrates of the source and the sink within each load interval. These flowrates correspond to the horizontal distances on the source- and sink-composite curves contained within the interval. Therefore, the following expressions may be used to calculate the source and sink flowrate (respectively) within the k[th] interval:

$$\Delta W_k = \frac{\Delta M_k}{y_{\text{source in interval k}}} \qquad (6.4)$$

and

$$\Delta G_k = \frac{\Delta M_k}{z^{\max}_{\text{sink in interval k}}} \qquad (6.5)$$

Figure 6.4 illustrates the concepts of a load interval and flowrates of sources and sinks within an interval. Additionally, Fig. 6.4 illustrates is that at any horizontal level ($\bar{k}$), the horizontal distance between the source- and the sink-composite curves is given by:

$$\delta_{\bar{k}} = \sum_{k=1}^{\bar{k}} W_k - \sum_{k=1}^{\bar{k}} G_k \qquad (6.6)$$

Equation 6.6 indicates that at any value of load, the horizontal distance between the source- and the sink-composite curves is the difference in cumulative flowrates. As mentioned earlier, a negative value of δ implies that the source composite lies to the left of the sink composite which is infeasible.

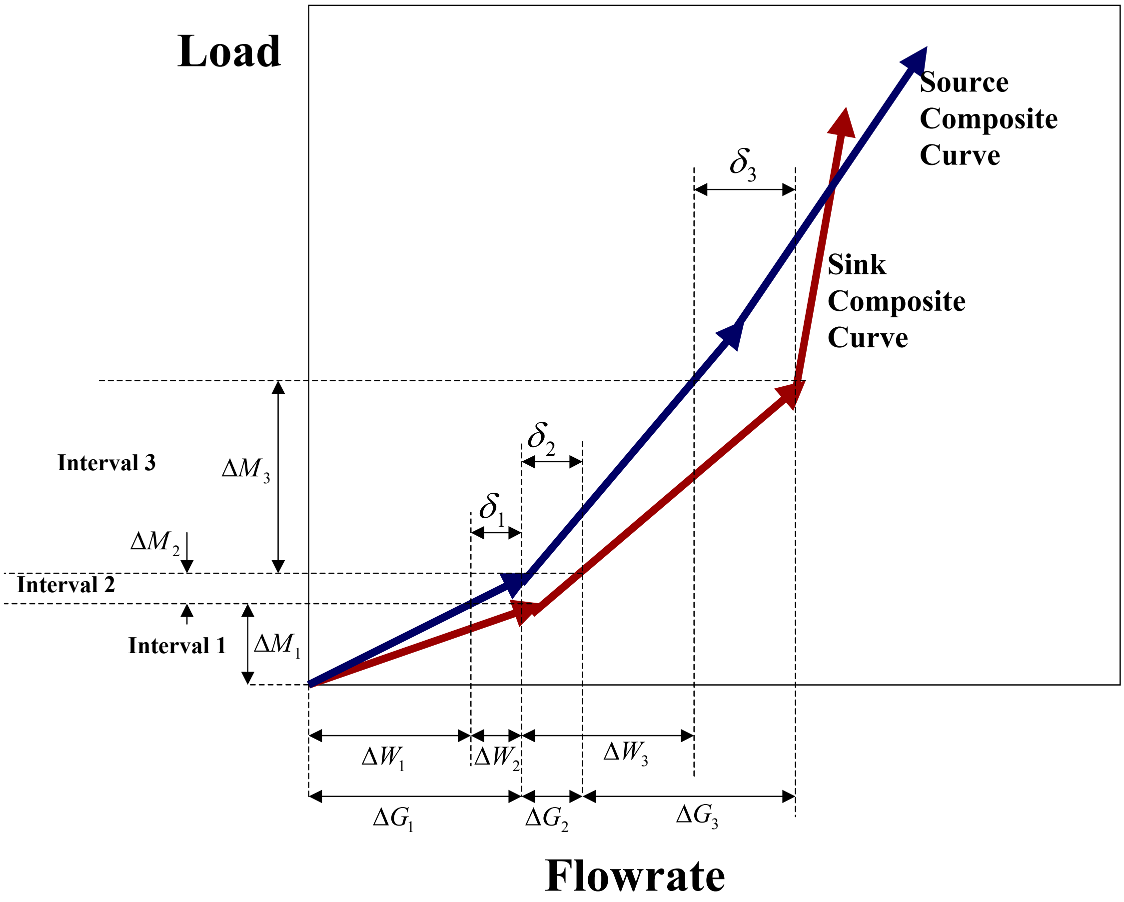

Fig. 6.4. Load Intervals, Flows, and Residuals (Almutlaq and El-Halwagi, 2004)

To illustrate Eq. (6.6), let us apply it to the first interval:

$$\delta_1 = \Delta W_1 - \Delta G_1 \quad (6.7)$$

This result can be verified by Fig. 6.4. Similarly, applying Eq. (6.6) to the second interval, we have:

$$\delta_2 = \Delta W_1 + \Delta W_2 - \Delta G_1 - \Delta G_2 \quad (6.8)$$

Substituting from Eq. (7.7) into Eq. (7.8), we obtain

$$\delta_2 = \delta_1 + \Delta W_2 - \Delta G_2 \quad (6.9)$$

and, for the kth interval:

$$\delta_k = \delta_{k-1} + \Delta W_k - \Delta G_k \quad (6.10)$$

with $\delta_0 = 0$. Equation (6.10) is represented by Fig. 6.5. The flow balances can be carried out for all intervals resulting in the cascade diagram shown on Fig. 6.6. As mentioned earlier, the most negative value of δ on the cascade diagram ($\delta_{\max}$) represents the target for minimum fresh consumption as indicated by Eq. (6.2). In order to remove the infeasibilities a flowrate of the fresh resource equal to $\delta_{\max}$ is added to the top of the cascade (i.e., $\delta_0 = \delta_{\max}$). The residuals are accordingly increased by $\delta_{\max}$, i.e.

$$\delta_k^{'} = \delta_k + \delta_{\max} \tag{6.11}$$

where $\delta_k^{'}$ is the revised residual flow leaving the kth interval. Consequently, the most negative residual becomes zero thereby designating the pinch location. Additionally, the revised residual leaving the last interval is the target for minimum wastewater discharge since it represents the unrecycled/unreused flowrates of sources. Figure 6.7 is an illustration of the revised cascade diagram. As can be seen from this illustration, the following residuals determine the targets:

$$\delta_{\max} = \text{Target for minimum fresh usage} \tag{6.12}$$

$$\delta_n^{'} = \text{Target for minimum waste discharge} \tag{6.13}$$

where n is the last load interval.

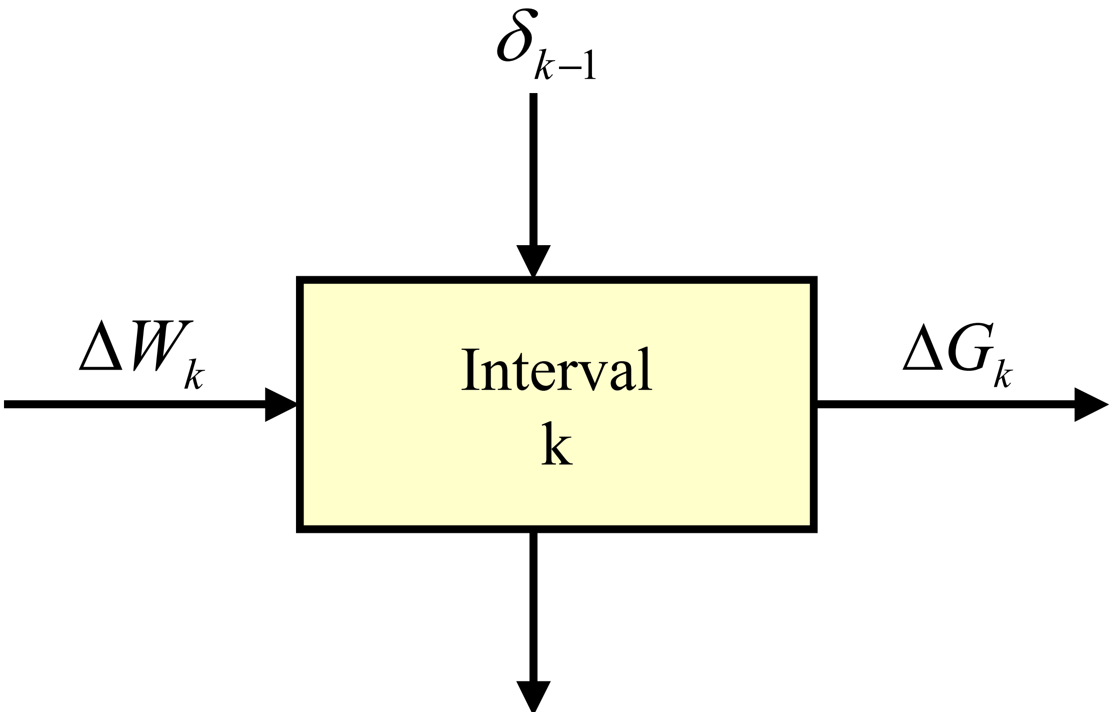

Fig. 6.5. Flow Balance around a Load Interval (Almutlaq and El-Halwagi, 2005)

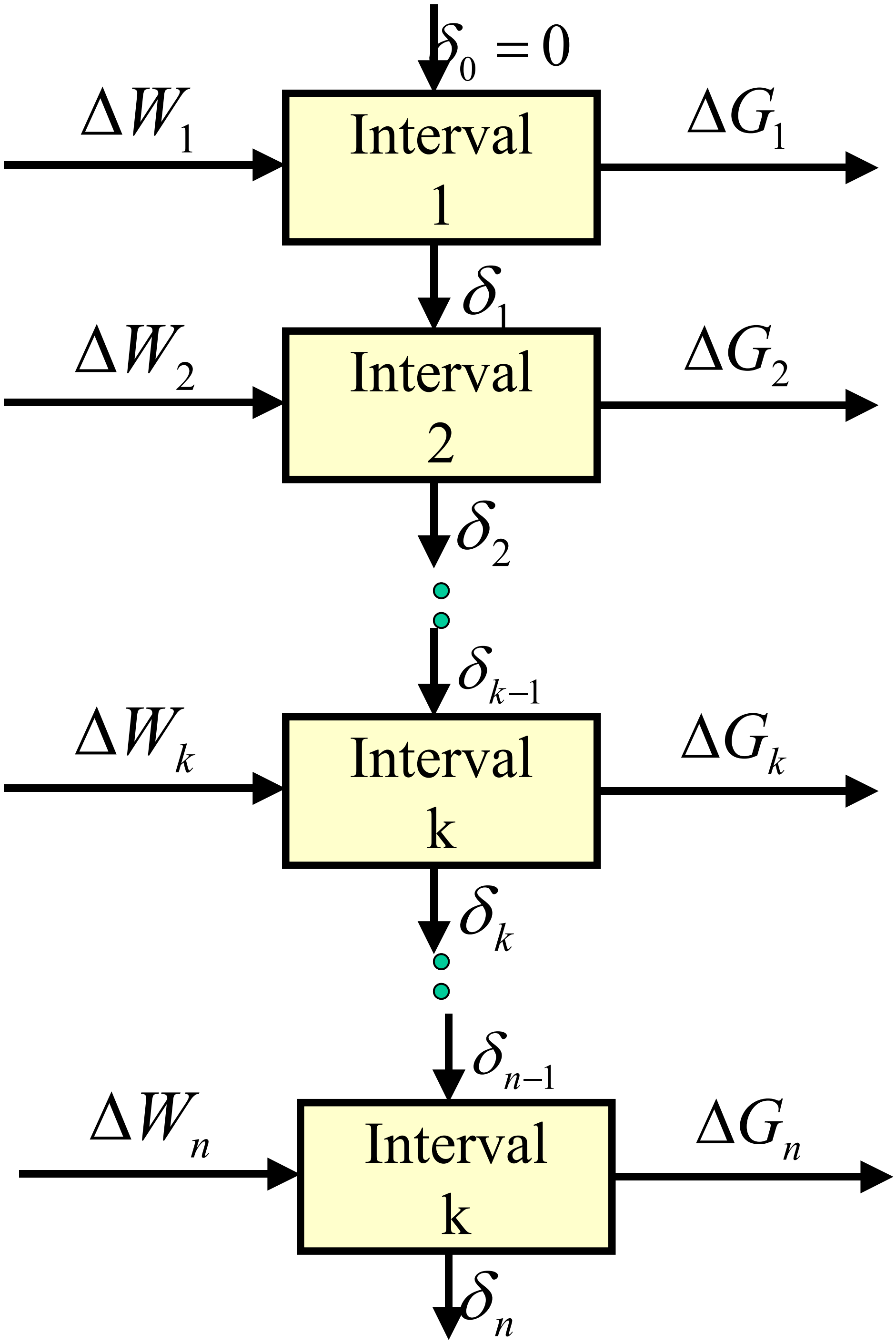

Fig. 6.6. Cascade Diagram (Almutlaq and El-Halwagi, 2005)

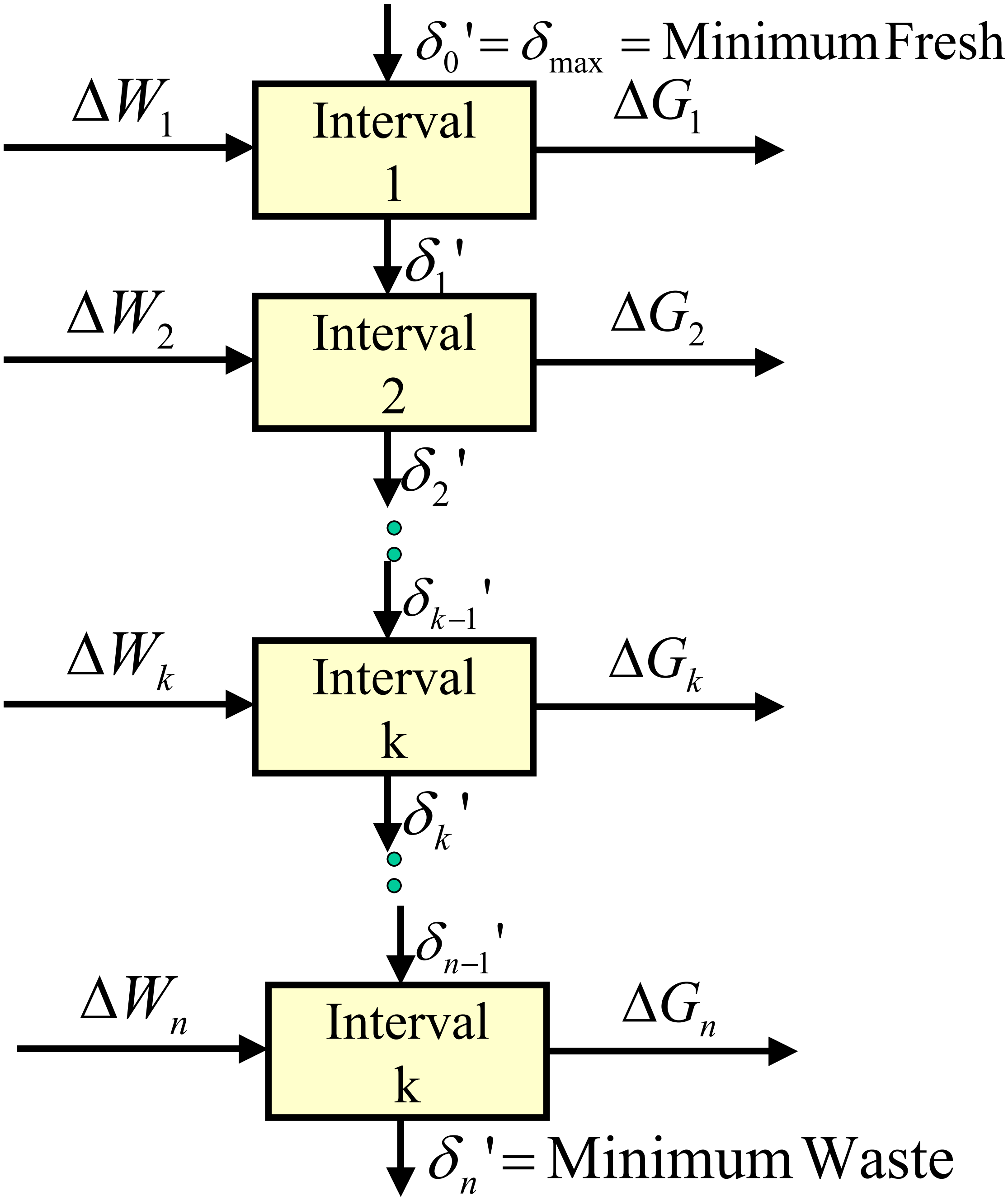

Fig. 6.7. Revised Cascade Diagram (Almutlaq and El-Halwagi, 2005)

6.3. ALGEBRAIC TARGETING PROCEDURE

Based on the foregoing analysis, the algebraic procedure can be summarized as follows:

1. Rank the sinks in ascending order of maximum admissible composition, $z_1^{\max} \le z_2^{\max} \le \ldots z_j^{\max} \ldots \le z_{N_{Sinks}}^{\max}$
2. Rank sources in ascending order of pollutant composition, i.e. $y_1 < y_2 < \ldots y_i \ldots\ldots < y_{N_{Sources}}$
3. Calculate the load of each sink ($M_j^{Sink,\max} = G_j z_j^{\max}$) and source ($M_i^{Source} = W_i y_i$).
4. Compute the cumulative loads for the sinks and for the sources (by summing up their individual loads).
5. Rank the cumulative loads in ascending order.
6. Develop the load-interval diagram (LID) shown in Fig. 6.8. First, the loads are represented in ascending order starting with zero load. The scale is irrelevant. Next, each source (and each sink) is represented as an arrow whose tail corresponds to its starting load and head corresponds to it ending load. Equations (6.3)-(6.5) are used to calculate the intervals load, source flowrate, and sink flowrate.
7. Based on the interval source- and sink flowrates, develop the cascade diagram and carry out flow balances around the intervals to calculate the values of the flow residuals (δ_k's). The most negative δ_k is the target for minimum fresh consumption, i.e.

   $\delta_{\max}$ = Target for minimum fresh usage (6.12)
8. Revise the cascade diagram by adding the maximum δ_k to the first interval and calculate the revised residuals. The interval with the first zero residual is the material recycle/reuse global pinch point. The residual flow leaving the last interval is the target for minimum waste discharge, i.e.

   $\delta_n^{'}$ = Target for minimum waste discharge (6.13)

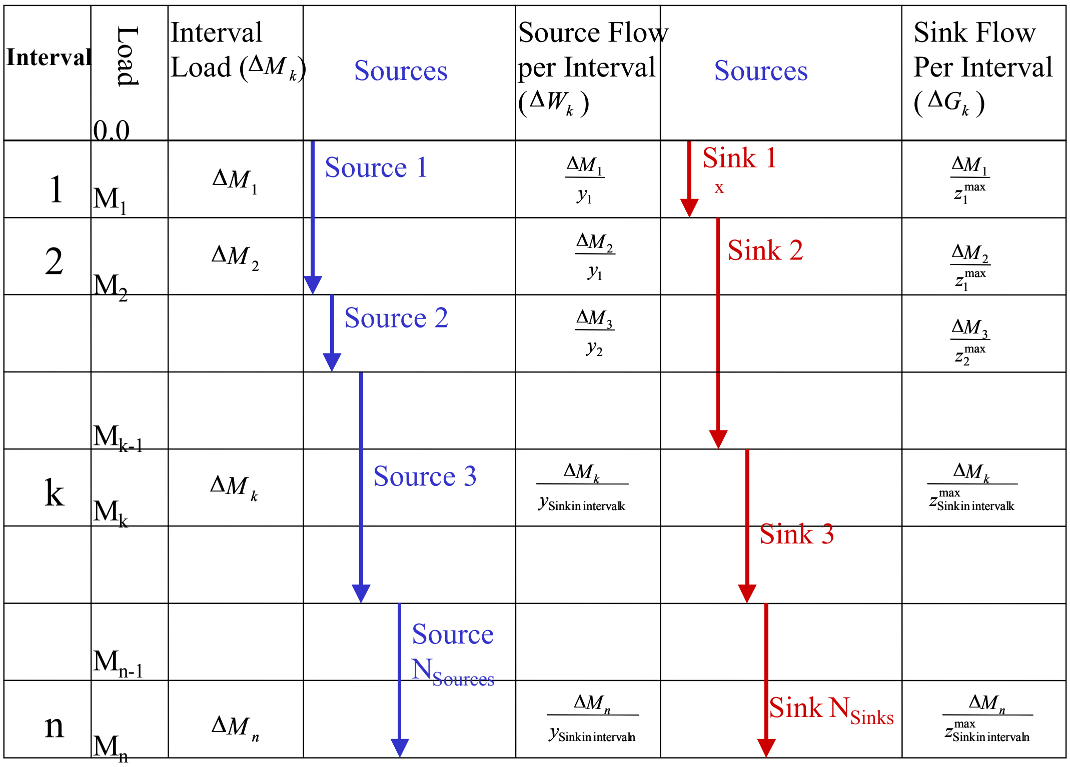

Fig. 6.8. Load-Interval Diagram (Almutlaq and El-Halwagi, 2005)

It is worth noting that when the fresh source in impure, the foregoing procedure can be modified to account for the concentration of contaminants. This procedure is described in details by Almutlaq et al. (2005).

6.4. CASE STUDY: TARGETING FOR ACETIC ACID USAGE IN A VINYAL ACETATE PLANT

Here, we revisit Example 3.4. on the recovery of AA from a VAM facility. The data for the problem are shown in Tables 6.1 and 6.2. The last column is calculated as the cumulative load.

Table 6.1. Source Data for the Vinyl Acetate Example

Source	Flowrate kg/hr	Inlet Mass Fraction	Inlet Load, kg/hr	Cumulative Load, kg/hr
Bottoms of Absorber II	1,400	0.14	196	196
Bottoms of Primary Tower	9,100	0.25	2,275	2,471

Table 6.2. Sink Data for the Vinyl Acetate Example

Sink	Flowrate Kg/hr	Maximum Inlet Mass Fraction	Maximum Inlet Load, kg/hr	Cumulative Maximum Load, kg/hr
Absorber I	5,100	0.05	255	255
Acid Tower	10,200	0.10	1,020	1,275

The LID is illustrated in Fig. 6.9. The cascade diagram is given by Fig. 6.10(a). As can be seen, the most negative residual is –9,584 kg/hr. Therefore, the target for minimum fresh AA is 9,584 kg/hr. When this value is added to the first interval, we can carry out the revised cascade calculations leading to a target of minimum waste discharge (residual leaving last interval) of 4,784 kg/hr. The zero residual designates the pinch location. Hence, the material recycle pinch point is located at the horizontal lines separating intervals 3 and 4. As can be seen from the LID, this location corresponds to a cumulative load of 1,275 kg/hr and a source mass fraction of water being 0.25 (between intervals 3 and 4 which corresponds to a mass fraction of 0.25 on the source side). These results are consistent with the ones determined graphically in Chapter Three.

Interval	Load, kg/hr	Interval Load (ΔM_k) kg/hr	Sources	Source Flow per Interval (ΔW_k),ton/hr	Sources	Sink Flow Per Interval (ΔG_k),ton/hr
	0					
1	196	196	Source 1 y = 0.14	1,400	Sink 1 z^{max}=0.05	3,920
2	255	59		236		1,180
3	1275	1,020	Source 2 y = 0.25	4,080	Sink 2 z^{max}=0.10	10,200
4	2471	1,196		4,784		0

Fig. 6.9. LID for the VAM Case Study

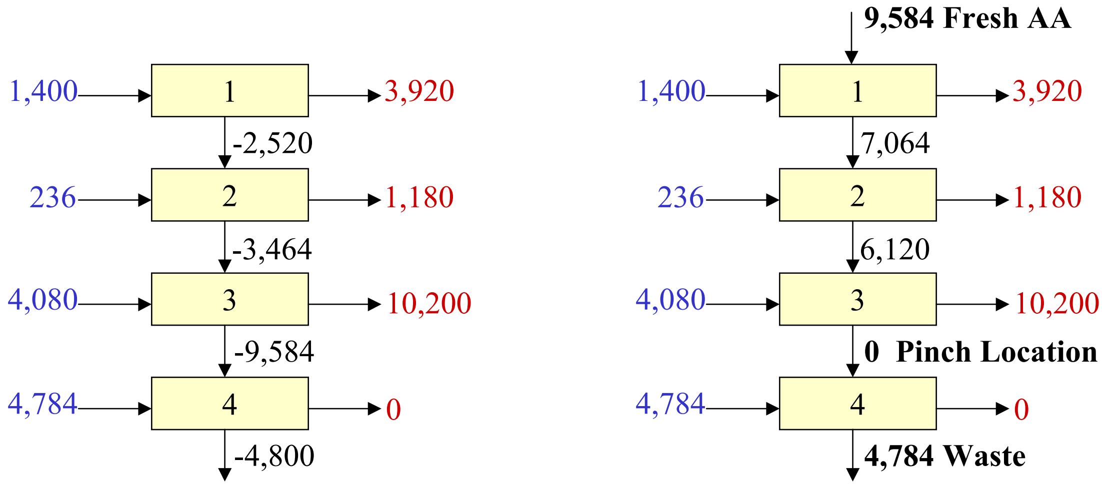

Fig. 6.10. Cascade Diagram for the VAM Case Study (a) With Infeasibilities (b) Revised

HOMEWORK

6.1. Solve problem 3.1 using the algebraic method.

6.2. Solve problem 3.2 using the algebraic method.

6.3. Solve problem 3.3 using the algebraic method.

6.4. Solve problem 3.4 using the algebraic method.

6.5. Solve the food processing case study (Example 3.6) using the algebraic method.

6.6. Describe the algebraic procedure for direct-recycle target when the fresh resource is impure.

NOMENCLATURE

G	Sink (unit) flowrate, mass/time
M	Load of contaminant, mass/time
$M^{\text{Sink, max}}$	Maximum admissible load to the sink, mass/time
$M^{\text{Source, max}}$	Contaminant load in source, mass/time
$N_{sources}$	Number of process streams (or sources)
$N_{\sin ks}$	Number of process units (sinks)
W	Sink (unit) flow, mass or volume/time
y	Contaminant composition of process streams (or sources)
z	Contaminant composition of process streams (or sources)
$\bar{k}$	Total number of intervals

Superscripts

min	Lower bound of allowable contaminant concentration to the sink
max	Upper bound of allowable contaminant concentration to the sink

Subscripts

i	Index for sources

j Index for sinks
k Index for load intervals

Greek Letters
δ Interval Residual
Δ Difference between two consecutive intervals

REFERENCES

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