DESIGN OF RECYCLE/REUSE NETWORKS WITH THERMAL EFFECTS AND VARIABLE SOURCES

A Thesis

by

JOSE GUADALUPE ZAVALA OSEGUERA

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

August 2009

Major Subject: Chemical Engineering

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Approved by:

Chair of Committee,	Mahmoud M. El-Halwagi
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ABSTRACT

Design of Recycle/Reuse Networks with Thermal Effects and Variable Sources.

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Recycle/reuse networks are commonly used in industrial facilities to conserve natural resources, reduce environmental impact, and improve process economics. The design of these networks is a challenging task because of the numerous possibilities of assigning stream (process sources) to units that may potentially employ them (process sinks). Additionally, several fresh streams with different qualities and costs may be used to supplement the recycle of process streams. The selection of the type and flow of these fresh resources is an important step in the design of the recycle/reuse networks. This work introduces systematic approaches to address two new categories in the design of recycle/reuse networks:

(a) The incorporation of thermal effects in the network. Two new aspects are introduced: heat of mixing of process sources and temperature constraints imposed on the feed to the process sinks

(b) Dealing with variation in process sources. Two types of source variability are addressed: flowrate and composition

For networks with thermal effects, an assignment optimization formulation is developed. Depending on the functional form of the heat of mixing, the formulation may be a linear or a nonlinear program. The solution of this program provides optimum flowrates of the fresh streams as well as the segregation, mixing, and allocation of the process sources to sinks. For networks with variable sources, a computer code is developed to solve the problem. It is based on discretizing the search space and using the concept of "floating pinch" to insure solution feasibility and optimal targets. Case studies are solved to illustrate the applicability of the new approaches.

DEDICATION

To my beloved son: Alex.

ACKNOWLEDGEMENTS

I want to acknowledge their support to all of those who where helping me in this marvelous stage of my life. In this way, first I would like to acknowledge my advisor because of his net style of lifelong leadership and dedication. Also, I want to say thanks to my family and friends for their support during the difficulties, and to my classmates for sharing this experience with me. At the same time, is not possible to found the correct phase to express all my gratitude to Texas A&M University for giving me the opportunity to continue my studies in such a great environment. In the same way, I wish to express my most sincere gratitude to the people of the great state of Texas and thanks to God for his forgiveness, for his help, and for his love.

NOMENCLATURE

C_{Fresh} = cost of the fresh resource (\$/kg)

G_j = flowrate demand for sink j (tons/hr)

N_{sinks} = number of sinks

$N_{sources}$ = number of sources

T_i = temperature of source i (K)

waste = total amount of flow going to waste (kg/hr)

W_i = flow rate of source i (kg/hr)

$w_{i,j}$ = amount of flow from source i to sink j (kg/hr)

$y_{i,k}^{in}$ = composition k^th^ component of source i (ppm)

$z_{j,k}^{\min}$ = lower bound for kth-component composition to sink j (ppm)

$z_{j,k}^{in}$ = inlet composition for kth-component composition to sink j (ppm)

$z_{j,k}^{\max}$ = upper bound for kth-component composition to sink j(ppm)

Indices

i = sources

j = sinks

k = component

u = interceptor

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER I

INTRODUCTION: DESIGN OF RECYCLE/REUSE NETWORKS WITH THERMAL EFFECTS AND VARIABLE SOURCES

Process Integration (PI) is an effective framework for continuous improvement in the performance of industrial processes. One category of improvements focuses on the structural configuration of the chemical processes in a comprehensive context. Several categories of structural improvements have already been addressed in literature and associated methodologies have been developed. Of particular interest in the structural modification geared towards recovering materials via recycle/reuse approaches. Material recycle/reuse is a primary industrial strategy for conserving natural resources, reducing operating costs, and mitigating the negative environmental impact. The direct recycle/reuse is one category of the general recycle/reuse network. The objective of this problem is to identify cost-effective allocation of process streams (sources) to process units (sinks) without adding new equipment to the process. Examples of sources in direct recycle/reuse systems are the waste or low value streams considered for recycling. Examples of sinks are those units to which such streams may be recycled.

This thesis follows the style of *Computers and Chemical Engineering*.

In addressing recycle/reuse, various objectives may be used. These include cost, flowrates of fresh resources, and flowrates and loads of discharge wastes. Other important metrics include operability, reliability, and safety. It is also possible to establish trade-offs among these objective functions. These objective functions are subject to a variety of constraints. Direct recycle/reuse will search for the appropriate stream allocation without violating the process specification and constraints.

One of the hallmarks of process integration is to use systematic procedures to find solutions. It is important here to identify properly the type of method which should be applied for each application. Sometimes, structural representation approaches are used to determine the exact configuration of the solutions. In other cases, approaches are used to determine performance targets which can be determined ahead of detailed design. In this regard, the "pinch" technology is quite effective. Performance targets in terms of minimum amount of fresh requirements and waste flow are necessary for direct recycle/reuse integration. These targets are very important in benchmarking the performance of the recycle/reuse network.

It is worth noting that several systematic procedures to design material recovery networks have been proposed. These procedures include the allocation or reuse of materials in process units through graphic, algebraic, and optimization methods as will be described in Chapter II of this work. In many cases, constraints on process sinks are not limited to purity (or concentration of certain components). Instead, there is typically a combination of composition and temperature constraints. Therefore, the design of recycle/reuse network must include the consideration of both composition and temperature. Chapter III describes the problem statement which addresses two new classes of recycle/reuse networks: thermal effects for source mixing and sink constraints and variation in flowrate and composition of the sources. Chapters IV and V present the proposed solution procedures, mathematical formulations, and case studies. Chapter VI discusses the conclusions of this thesis and recommendations for future work.

CHAPTER II

LITERATURE REVIEW

Material recycle/reuse has received much research attention. Recycle corresponds to the utilization of a process stream (e.g., a waste or a low-value stream) in a process unit (a sink). On the other hand, reuse refers to the reapplication of the stream for the original intent or in the original unit. Ensuring optimum recycle/reuse of process streams is among the key objectives of processing facilities. Therefore, it is important to develop systematic procedures to design the material recovery networks and to assign the recovered materials to proper process units. Several research efforts have endeavored to address the problem of designing recycle/reuse systems. These efforts include graphical, algebraic, and optimization approaches.

Several graphical approaches have been devised to minimize wastewater discharge by fostering recycle/reuse of process water streams. Wang and Smith (1994) developed a pinch-based visualization technique to minimize fresh water consumption and wastewater discharged while transferring contaminants from process streams to water streams in units that function as mass exchangers. This approach is an extension of the mass-exchange network problem introduced by El-Halwagi and Manousiouthakis (1989) and is based on modeling water-using units as mass exchangers. Dhole et al. (1996) and El-Halwagi and Spriggs (1996) noted that there are various water units that may not be treated as mass exchangers. They explain the problem of material usage and discharge as a source-sink mapping task. According to their study, each process has a number of sources (streams available for recycle/reuse) that may be allocated to sinks (units that demand certain feeds and may accept the recycled sources). Fresh resources (e.g., fresh water, solvents, material utilities) may be used to supplement the use of process sources so as to meet the sink demands at minimum cost. Dhole et al. (1996) developed a graphical representation of concentration versus flowrate. Composite curves for supply and demand are overlapped until a pinch point is created. El-Halwagi and Spriggs (1996) developed a source-sink mapping representation and used lever-arm rules to identify optimum allocation of sources to sinks. Polley and Polley (2000) outlined optimality conditions for sequencing recycles. El-Halwagi et al. (2003) developed a material recovery pinch analysis that rigorously identifies minimum fresh usage, maximum recycle, and minimum waste discharge.

Algebraic techniques have also been developed to address recycle/reuse problems. Sorin and Bedard (1999) introduced an evolutionary technique based on mixing source streams at concentrations bordering the demand location and moving on progressively to higher concentration. This approach may become tedious for systems involving many sources and sinks. Hallale (2002), Alves and Towler (2002), and Alves (1999) developed a surplus diagram for the recycle of species such as water and hydrogen. This approach involves extensive computations to reconcile flowrate and purity requirements. Manan et al. (2004) refined the surplus approach by developing a cascade approach to avoid the extensive calculations in identifying the targets.

Takama et al. (1980) developed an optimization-based approach to recycle water. This approach has been generalized later by several researchers (e.g., Alva-Argaez et al., 1999; Keckler and Allen, 1999; Benko et al., 2000; Savelski and Bagajewicz, 2000, 2001; and Dunn et al., 2001).

The aforementioned research efforts have been limited to ***direct*** recycle/reuse strategies in which sources are directly assigned to sinks. No new equipment is added. To overcome this limitation, Gabriel and El-Halwagi (2005) developed an optimization approach which includes interception devices in addition to sources and sinks. The interception devices are new equipment that are added to the process in order to adjust the purity of the various sources prior to recycle/reuse.

CHAPTER III

PROBLEM STATEMENT

Two new recycle/reuse problems will be addressed by this work: I Networks with thermal effects, II Variable-source problems. The following are the formal statement for the two problems.

III.1 Networks with Thermal Effects

Given a process with:

- A set of process sinks (units): SINKS = $\{j \mid j = 1,2, \ldots, N_{sinks}\}$. Each sinks requires a given flowrate, G_j. The constraints for the compositions and temperature entering the unit (referred to as $z_{j,k}^{in}$ and T_j^{in}, respectively) are expressed by:

$$z_{j,k}^{\min} \leq z_{j,k}^{in} \leq z_{j,k}^{\max} \qquad j \in \text{SINKS},\ k=1,2,\ldots,N_{Components} \tag{3.1}$$

$$T_j^{\min} \leq T_j^{in} \leq T_j^{\max} \qquad j \in \text{SINKS} \tag{3.2}$$

where $z_{j,k}^{\min}$ and $z_{j,k}^{\max}$ are given lower and upper bounds on acceptable compositions to unit j for component k. Also, $T_j^{\min}$ and $T_j^{\max}$ are given lower and upper bounds on acceptable temperatures to unit j.

- A set of process sources: SOURCES = $\{i \mid i = 1,2, \ldots, N_{sources}\}$ which can be recycled/reused in process sinks. Each sources has a given flowrate, F_i, and a given composition of component k, $y_{i,k}$, and a given temperature T_i.

- A set of fresh sources: FRESH = $\{i|i= N_{sources}+1, N_{sources}+2, \ldots, N_{sources} + N_{Fresh}\}$. Each fresh source has a given cost, C_i expressed as $/kg of the fresh , and a given composition, $y_{i,k}^{in}$ and temperature T_i. The flowrate of each rich stream, F_i, is unknown and is to be determined through optimization.

III.2 Networks with Variable Sources

Given a process with:

- A set of process sinks (units): SINKS = $\{j \mid j = 1,2, \ldots, N_{sinks}\}$. Each sinks requires a given flowrate, G_j. The constraints for the compositions are expressed by:

$$z_{j,k}^{\min} \le z_{j,k}^{in} \le z_{j,k}^{\max} \qquad j \in \text{SINKS}, k=1,2,\ldots,N_{Components} \tag{3.1}$$

where $z_{j,k}^{\min}$ and $z_{j,k}^{\max}$ are given lower and upper bounds on acceptable compositions to unit j for component k.

- A set of process sources: SOURCES = $\{i \mid i = 1,2, \ldots, N_{sources}\}$ which can be recycled/reused in process sinks. Each sources has *an unknown flowrate, F_i, and an unknown composition of component k,* $y_{i,k}$. The flowrate and composition for each source are bound by the following constraints which are tied to the process performance and the design and operating degrees of freedom:

$$F_i^{\min} \le F_i \le F_i^{\max} \qquad i \in \text{SOURCES} \tag{3.3}$$

$$y_{i,k}^{\min} \le y_{i,k} \le y_{i,k}^{\max} \qquad i \in \text{SOURCES}, k=1,2,\ldots,N_{Components} \tag{3.4}$$

- A set of fresh sources: FRESH = $\{i|i= N_{sources}+1, N_{sources}+2, \ldots, N_{sources} + N_{Fresh}\}$. Each fresh source has a given cost, C_i expressed as $/kg of the fresh and a given composition, $y_{i,k}^{in}$. The flowrate of each rich stream, F_i, is unknown and is to be determined through optimization.

The goal is to develop systematic and generally applicable procedures for the optimal synthesis of a cost-effective recycle/reuse networks for the two abovementioned classes of problems.

III.3. Design Challenges

The new procedure should provide answers to the following difficult design challenges:

- Should process sources be segregated or mixed? How? Should they be mixed with fresh resources? Which ones? To what extent?
- How should the sources be allocated to sinks?
- Which fresh sources should be used? What are their optimal flowrates?
- How much waste should be discharged?

Chapters IV and V provide answers to these questions.

CHAPTER IV

OPTIMIZATION APPROACH FOR DESIGN RECYCLE/REUSE NETWORKS WITH THERMAL EFFECTS

IV.1 Problem Representation

The first step in addressing the problem is to develop a structural representation which is rich enough to embed all potential configurations of interest. This representation is shown in Figure 4.1. It is composed of sources and sinks. Each source is split into a number of streams. Each split is assigned to a sink. The various split assigned to a sink are mixed prior to entering the sink. The flowrate of each split is unknown and is to be determined through optimization. Each fresh stream is also split into fractions that are assigned to the sinks. The flowrate of each split is to be determined so as to optimize the objective function. The unused portions of the process streams are discharged as waste streams.

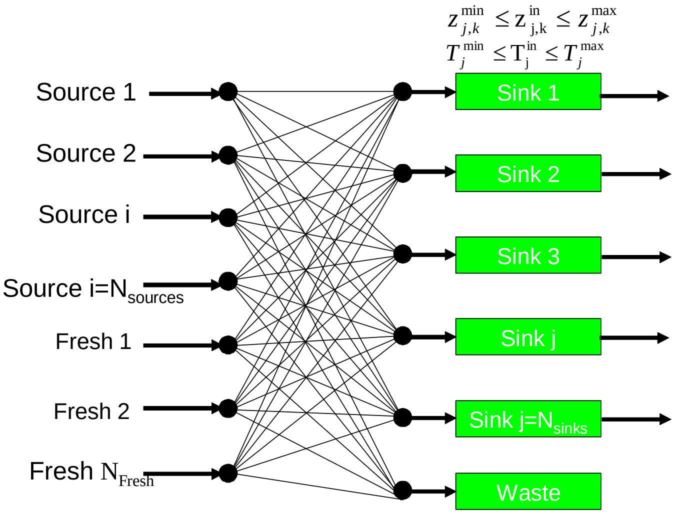

Figure 4.1 Direct recycle problem representation

IV.2 Mathematical Formulation

Two special cases are address: (1) direct recycle without heat of mixing consideration and (2) direct recycle with heat of mixing considerations. When no heat of mixing is considered, the problem may be formulated as the following optimization program:

The objective is to minimize the cost of the fresh resources and waste discharge, i.e.

$$\text{Minimize} \sum_{i=N_{Sources}+1}^{N_{Sources}+N_{Fresh}} C_i * W_i + Waste\_Cost(Waste, Z_{waste,k}) \qquad (4.1)$$

If it is desired to minimize the cost of the fresh, then the objective function can be expressed as:

$$\text{Minimize} \sum_{i=N_{Sources}+1}^{N_{Sources}+N_{Fresh}} C_i * W_i \qquad (4.2)$$

Subject to the following constraints:

Splitting of sources:

$$W_i = \sum_{j=1}^{N_{Sinks}} w_{i,j} + w_{i,waste} \qquad i=1,2,\ldots,N_{Sources} \qquad (4.3)$$

A similar constraint can be written for the splitting of the ith fresh resource but without assigning fresh to waste:

$$W_i = \sum_{j=1}^{N_{Sinks}} w_{i,j} \qquad i=N_{Sources}, N_{Sources}+1,\ldots, N_{Sources}+,N_{Fresh} \qquad (4.4)$$

Mixing for the jth sink:

Flow balance:

$$G_j = \sum_{i=1}^{N_{Sources}+N_{Fresh}} w_{i,j} \qquad \text{where } j = 1,2, \ldots, N_{Sinks} \qquad (4.5)$$

Component material balances:

$$G_j * z_{j,k}^{in} = \sum_{i=1}^{N_{Sources}+N_{Fresh}} w_{i,j} * y_{i,k} \qquad \text{where } j = 1,2, \ldots, N_{Sinks} \text{ and } k=1,2,\ldots,N_{Components} \qquad (4.6)$$

Assuming adiabatic mixing with no phase change, the following heat balance may be written:

$$G_j * C_{p,j} * T_j^{in} = \sum_{i=1}^{N_{Sources}+N_{Fresh}} w_{i,j} * c_{p,i} * T_i \qquad (4.7)$$

Sink Constraints:

$$z_{j,k}^{\min} \le z_{j,k}^{in} \le z_{j,k}^{\max} \qquad j \in \text{SINKS}, k=1,2,\ldots,N_{Components} \qquad (4.8)$$

$$T_j^{\min} \le T_j^{in} \le T_j^{\max} \qquad j \in \text{SINKS} \qquad (4.9)$$

Waste Balances:

The waste flowrate is given by:

$$Waste = \sum_{i=1}^{N_{Sources}} w_{i,waste} \tag{4.10}$$

The waste concentration may be calculated through:

$$Waste * Z_{waste,k} = \sum_{i=1}^{N_{Sources}} w_{i,waste} * y_{i,k} \tag{4.11}$$

Finally, non-negativity constraints are added for the unknown flowrate splits of all sources:

$$w_{i,j} \geq 0 \quad \text{where } i = 1,2, \ldots, N_{\text{Sources}} + N_{\text{Fresh}} \text{ and } j = 1,2, \ldots, N_{\text{sinks}} \tag{4.12}$$

When the objective function is linear, the program becomes a linear program which can be solved globally using commercial software LINGO to identify the minimum cost as well as optimum allocation of process sources to sinks, and the discharged waste.

Next, the effect of heat of mixing is included. In this case, the foregoing formulation is achieved by revising Eq. (4.7) to be expressed as:

$$G_j * C_{p,j} * T_j^{in} = \sum_{i=1}^{N_{Sources}+N_{Fresh}} w_{i,j} * c_{p,i} * T_i + \Delta H_{mixing}(w_{i,j} \forall i, j) \tag{4.13}$$

where $\Delta H_{mixing}(w_{i,j} \forall i, j)$ is the heat-of-mixing function which depends on the identity, conditions, and fractions of mixed streams. While the heat of mixing introduces additional accuracy for the heat balance, it introduces nonlinearity for the formulation. Therefore, it is suggested to first solve the problem globally without heat of mixing, then to use this solution for initializing the solution of the nonlinear program with heat-of-mixing effects.

IV.3 Case Study: Reduction of Acetic Acid Usage in a Vinyl Acetate Monomer Plant

This case study is an extension of an example reported by El-Halwagi (2006). The extension is to include thermal effects. The problem has two sources and two sinks. The fresh is pure Acetic Acid (AA) at 360 K. The data for the problem are shown in Tables 4.1 and 4.2. It is desired to solve three different versions of the problem:

a) When there are no temperature constraints for the sinks.

b) When there are temperature constraints for the sinks (as shown by Table 4.2)

c) When there are temperature constraints for the sinks and the heat of mixing for various streams is taken into consideration. For simplicity, it is assumed that the sources have similar heat capacities of 2.5 kJ/kgK and the average heat of mixing of 4 kJ/kg of mixture.

Table 4.1 Source data for the vinyl acetate example

Source	Flowrate Kg/hr	Mass Fraction	Temperature K
Bottoms of Absorber II	1,400	0.14	370
Bottoms of Primary Tower	9,100	0.25	470

Table 4.2 Sink data for the vinyl acetate example

Sink	Flowrate kg/hr	Minimum Inlet Mass Fraction	Maximum Inlet Mass Fraction	Minimum Inlet Temperature K	Maximum Inlet Temperature K
Absorber I	5,100	0.00	0.05	350	380
Acid Tower	10,200	0.00	0.10	340	380

As shown in Figure 4.2 (a, b, and c), after solving this linear optimization problem, as more constraints are added, the more fresh acetic acid is used. Indeed, the minimum consumption of fresh acetic acid increases from 9584 kg/hr (in the case of no thermal considerations) to 11,468 kg/hr (in the case of thermal constraints for the sinks) to 11,496 kg/hr (in the case of thermal constraints for the sinks with heat of mixing for the sources).

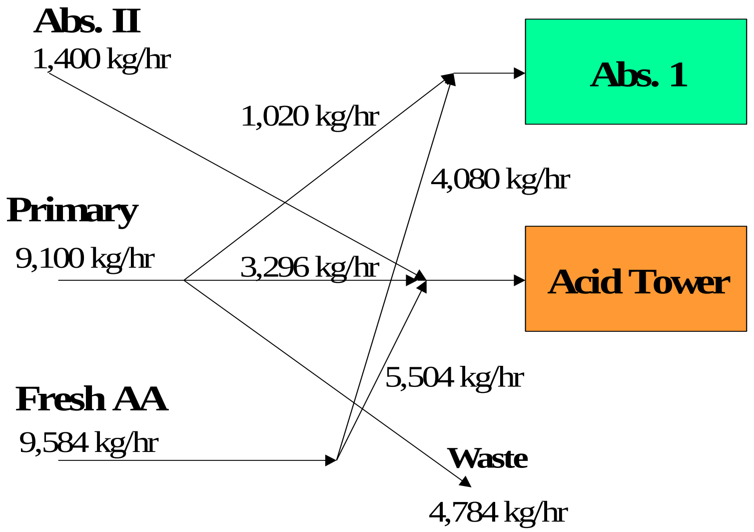

Figure 4.2a Direct recycle configurations: without thermal constraints

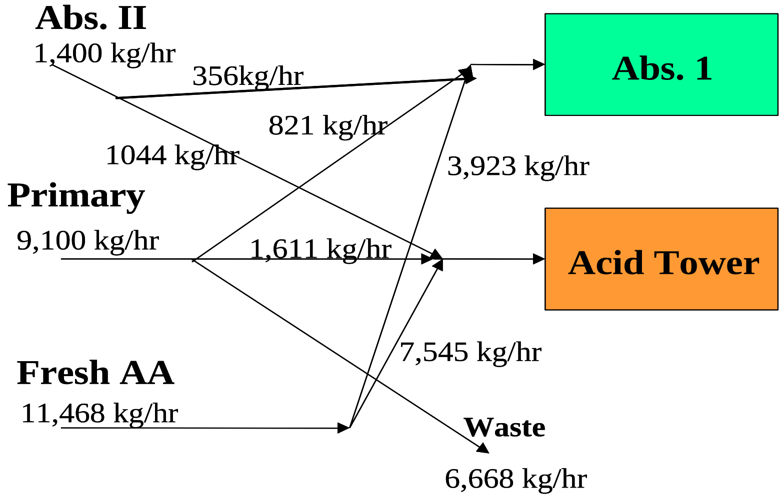

Figure 4.2b Direct recycle configurations: with temperature constraints for the sinks

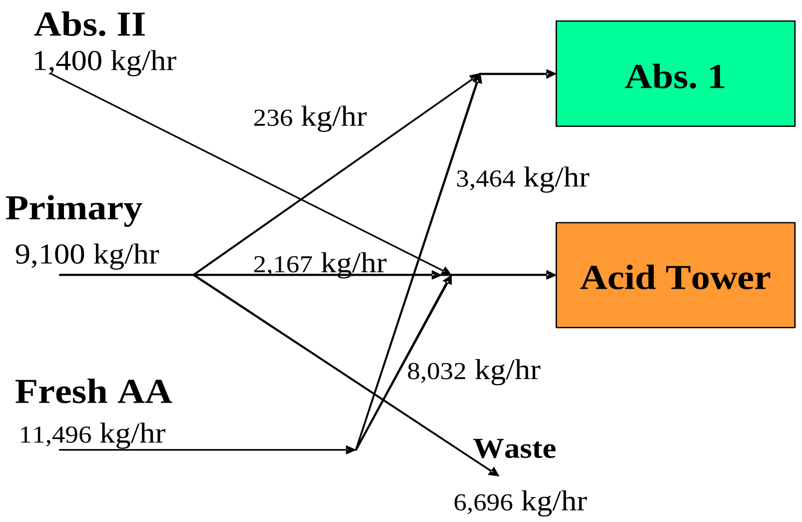

Figure 4.2c Direct recycle configurations: with temperature constraints with heat of mixing considerations

CHAPTER V

DIRECT RECYCLE WITH VARIABLE SOURCES

V.1 Problem Scope

A second class of direct recycle problems is addressed in this chapter. Here, the sources are allowed to vary in flowrate and composition. This problem is more difficult than the conventional direct recycle problem with fixed sources because of the variability in flowrate and composition. From an optimization perspective, this introduces bilinear terms which are nonconvex. As such, there is no guarantee for global solution. In order to address these challenges, an approach is developed based on extending the concept of *floating pinch* which was developed for other applications such as heat exchange networks (Duran and Grossman, 1986) and mass exchange networks (El-Halwagi and Manousiouthakis, 1990).

V.2 Basics of the Floating Pinch Concept

First, let us consider the analogy between the direct recycle problem and the heat integration problem. To this end, a simple schematic of the pinch diagrams is useful. In the direct recycle and heat systems, the construction of composite curves can lead to the realization of the objective function to maximize recycle and heat integration correspondingly. This appears in Figure 5.1 where both composite curve representations, direct recycle and heat integration, are shown. In direct recycle, the composite curves represent a set of streams conditions with given data. Notice that for direct recycle, one source or sink represents a segment in the composite, whereas a segment in a composite for heat integration might contain more than one hot or cold stream. The important point here is that the composite curve vertices come from specifications of process sources or sink and among these vertices the pinch has to be identified. The details in the identification of the pinch with a mathematical programming approach are shown on detail in the literature (Duran and Grossman, 1986; and El-Halwagi and Manousiouthakis, 1990). In this work, this concept will be extrapolated to the direct recycle problem and will be implemented into an optimization framework. In this way, the code for the implementation of the floating pinch algorithm for direct recycle should be developed.

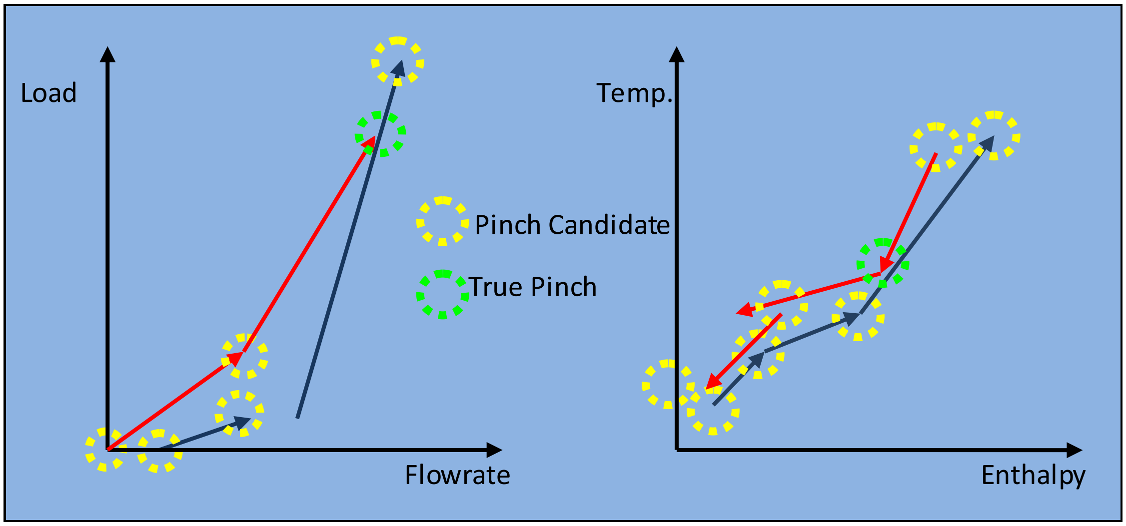

Figure 5.1 Direct recycle and heat integration pinch location

Another important observation is that the pinch separates the design problem in different regions: the region above the pinch, and the region below the pinch. For the load or heat balances a process source or sink can contribute within the region below the pinch or the region above the pinch or both. For the load or heat balances, take a single stream where the point A is the initial state and the final state is represented by point B as shown in the left of Figure 5.2. A stream keeps its initial and final conditions while identifying the location during one of the iterations. In the context of optimization, the stream flows could be changing and therefore those conditions in a specified stream could change in the next iteration, after the flows had change. In Figure 5.2, the left part makes the case of a pinch identification problem and the right applies for the identification of the pinch in an optimization environment.

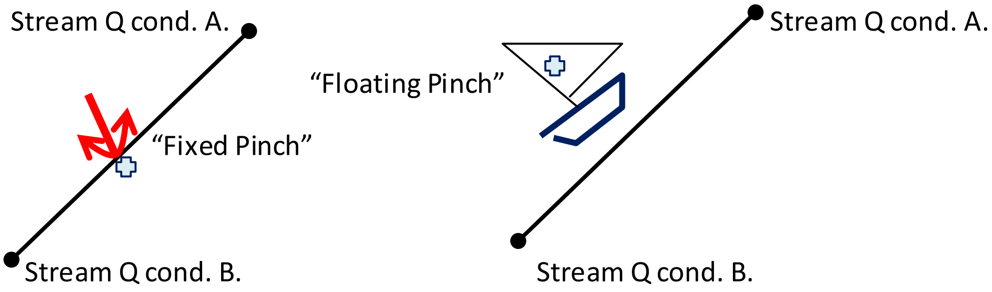

Figure 5.2 Schematic representation of the floating pinch concept

Before developing the approach for the variable sources, it is useful to consider the case of fixed sources. In this case, the objective is the replacement of valuable fresh loads with in-plant or terminal resources. This gives economic benefits for the process.

By virtue of savings in fresh usage and waste discharge, the economic impact is evident even without any further in the specification of the process configuration. The algebraic calculation of performance targets is explained in the literature (El-Halwagi, 2006). Some key points are discussed here. As shown in Figure 5.3, in recycle/reuse, the source composite represents all the process streams being considered for recycle, and a sink composite is the cumulative representation of the sink requirements. According to the constraint derived from the second law of thermodynamics or from process constraints, the location of the pinch has a sink composite always to the left of the source composite. The composites will touch each other just at the pinch. With the process data, and as the two axes are representing load and flow correspondingly, we can observe that the composites will be fixed in the load scale. The displacement of the source composite over the horizontal axis (flow) is necessary to locate the pinch. As shown in Figure 5.3, both composites are initially starting at the origin of the load and flow coordinate system. The pinch is located where the sink composite is entirely on the left of the source composite and they touch each other just at the pinch point.

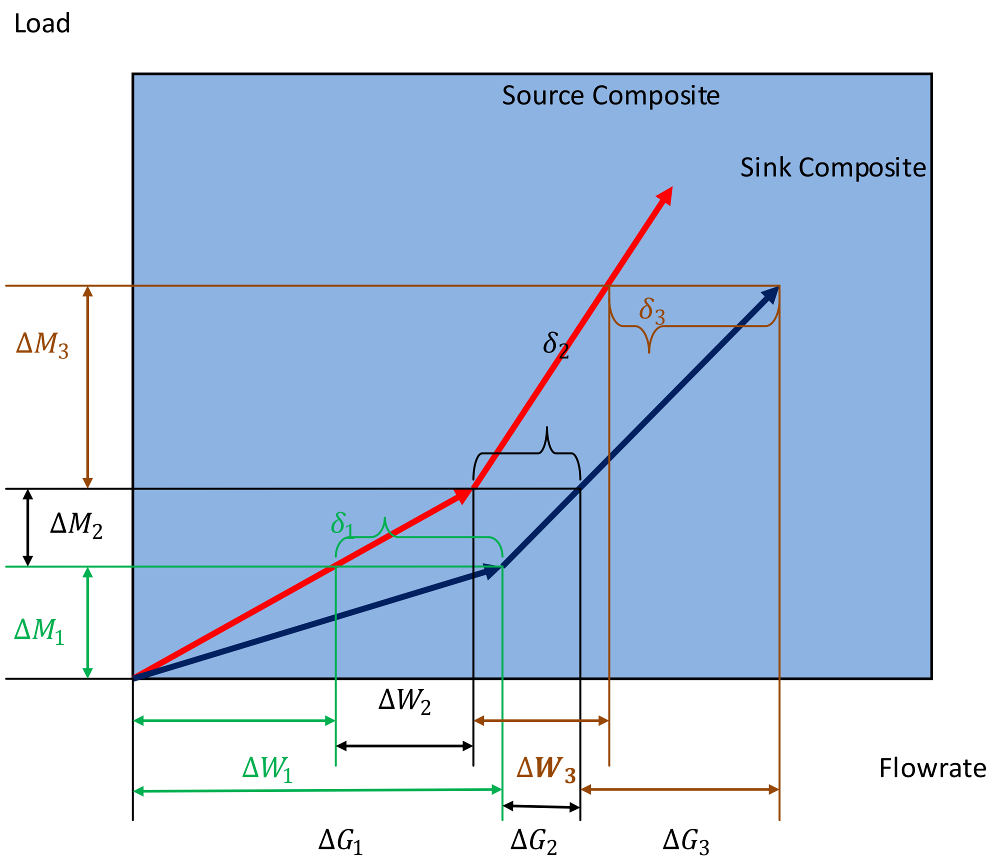

Figure 5.3 Source-sink composite diagram to define load intervals

Any point should be considered as a pinch candidate, and then the computations are done considering that both composites just touch each other at that point. Notice that all the projection of the vertices of the sink composite in the source composite should have a higher load value when the real pinch is located. As the balance of loads remains constant, and the composites are moving just horizontally, the performance targets are identified with a flow balance.

Then, taking advantage of the flexibility of LINGO to compile lower level programming code, with a set of algebraic expression both composites could be specified within the software. This can be done in a CALC section in LINGO. Also a data section is needed to identify and characterize the set of pinch point candidates, and a to finish the model the expressions for the flow balances are needed.

V.3 Computer-Aided Approach for the Floating Pinch Implementation in Recycle/Reuse Targeting

The application of the pinch strategies in more elaborate processes will require the management of a large amount of data. This management of large amount of data can be complicated. For this reason, we have to develop an appropriate and homogeneous nomenclature. Thus, we will continue the use of the nomenclature introduced in the problem statement. In this way, the problem statement for targeting in direct recycle/reuse is with the following terms:

Set of sinks: $DRUNITS = \{i = 1,2,\ldots,N_{Sinks}\}$

Sinks flowrate: G_i

Sinks input compositions: z_i^{in}

Sink constraints for compositions: $z_i^{min} \leq z_i^{in} \leq z_i^{max}$

Sinks input loads: $M_i = G_i z_i$

Sink constraints for input loads: $0 \leq M_i \leq M_i^{max}$

Set of sources: $PSTREAMS = \{j = 1,2,\ldots,N_{Sources}\}$

Source flowrates: W_j

Source compositions: y_j

Source loads: $M_j = W_j y_j$

Set of fresh resources: $PFRESH = \{r = 1,2, \dots, N_{Fresh}\}$

Set of fresh compositions: x_r

Set of fresh flowrates: F_r

Number of possible pinch points: $p = i + j + r + 1$

The pinch is identified in a similar way in direct recycle to that in heat integration. This is the idea behind the modular approach. With the use of modules, those modules will require the implicit use of interval diagrams. For the case of mass, the implicit use of composition interval diagrams is needed. For the case of heat, the use of a temperature interval diagram is required. For the case of direct recycle/reuse, which is the one addressed in this section, this will require the implicit use of load interval diagrams. With the pinch candidates being the set of vertices in the composite curves, the floating pinch concept is applied here for the performance targeting in recycle/reuse.

For the location of the pinch, once the stream conditions for direct recycle are specified, the following sets of binary variables are defined. These are the corresponding to those used in the MINLP expressions recommended by El-Halwagi and Manousiouthakis (1990). Nevertheless, in this case the implementation will be done as a lower level code section:

$$\lambda_{i,p}^{t} = \begin{cases} 1 \text{ if } G_i z_i^t < Gz^p & i \in DRUNITS \\ 0 \text{ if } G_i z_i^t \geq Gz^p \end{cases} \tag{5.1}$$

$$\lambda_{i,p}^{s} = \begin{cases} 1 \text{ if } G_i z_i^s < Gz^p & i \in DRUNITS \\ 0 \text{ if } G_i z_i^s \geq Gz^p \end{cases} \tag{5.2}$$

$$\eta_{j,p}^{t} = \begin{cases} 1 \text{ if } W_j y_j^t < W y_j^p & j \in PSTREAMS \\ 0 \text{ if } W_j y_j^t \geq W y_j^p \end{cases} \tag{5.3}$$

$$\eta_{j,p}^{s} = \begin{cases} 1 \text{ if } W_j y_j^s < W y_j^p & j \in PSTREAMS \\ 0 \text{ if } W_j y_j^s \geq W y_j^p \end{cases} \tag{5.4}$$

To locate the pinch with a series of programming commands, a series of sets are defined in LINGO. The sets will have the values used for the case of load versus flowrate diagram. For example, the sets have the values corresponding to those of the vertex coordinates in the graph of load versus flowrate. Therefore, the code is developed in a way such that the load and flow coordinates for sources and sinks are identified. With a set of equations, again implemented through code commands in the lower level section, the location of the pinch has to arrange the order of the sinks and sources to calculate the composites coordinates, or loads and flowrates values.

Values of stream data will be changing to account for the variability of the sources and will lead to displacements of the composite. It is intuited that the general model as implemented in LINGO will present different sections. Such sections, as implemented for the general structure of the LINGO model to develop the direct recycle/reuse case study, are shown in the Figure 5.4. Here, the correct coordinates in both composites are very significant. The values for the loads, according to the set of operations that should be performed, will not change at all during the model execution. These values, the load coordinates, allow the location of one specific process stream coordinates relative to the pinch candidate under consideration. Consequently, the contribution of that specific stream above and below the pinch can be accounted for.

Figure 5.4 Structure of the generic LINGO model for the direct recycle/reuse case study

Notice that the set of pinch point candidates (p) is the sum of all the point coordinates in both composites. Once a pinch candidate is selected, the composite stream contributions below or above the pinch must be calculated. This contribution accounting is done with the use of the binary variables defined above. The sequence of steps which is implemented in the lower level coding section of LINGO for this particular step is intricate. Once the case of a source contribution or a sink contribution is recognized, then the relative load contributions will be calculated according to the pinch candidate under consideration. Finally, the following equations will account for the flow balances:

Flow required in unit "i" (sink)

below a pinch point candidate $= -\lambda^{s}_{i,p}\left(G^{p} - G^{s}_{i}\right) + \lambda^{t}_{i,p}\left(G^{p} - G^{t}_{i}\right)$ (5.5)

"p" in the recycle/reuse network:"LSI_i"

With the corresponding for source contribution:

Flow recycled from stream "j" (source)

below a pinch point candidate "p" $= \eta^{t}_{j}\left(W^{p}_{j} - W^{t}_{j}\right) - \eta^{s}_{j}\left(W^{p}_{j} - W^{s}_{j}\right)$ (5.6)

in the recycle/reuse network: "LSO_j"

These equations work out the recycle/reuse balance of streams below the pinch point candidate. The next analysis shows the scenarios for set of equations, when a stream in the sink composite is going to be accounted. As observed, these equations provide an accurate performance target calculation:

1. When the load to be disposed in the sink unit i is located completely above the pinch point candidate p, then according to equations 5.1 and 5.2 the next values

apply: $\lambda_{i,p}^{t} = \lambda_{i,p}^{s} = 0$, and the flow to be accounted as flow recycled to that particular unit below the potential pinch point is zero.

2. When coordinates corresponding to the value of the load that should be recycled in the sink unit i is located completely below the potential pinch point, then with equations 5.1 and 5.2 the values for $\lambda_{i,p}^{t}$ and $\lambda_{i,p}^{s}$ is one ($\lambda_{i,p}^{t} = \lambda_{i,p}^{s} = 1$) and the flow to be accounted as flow recycled to that particulars unit below the potential pinch point is given by:

$$-\left(G_p - G_i^t\right) + \left(G_p - G_t^s\right) = -G_i^s + G_i^t$$

which is correct.

3. When the coordinates of the load that should be recycled to the sink unit i is partially across the pinch point candidate $(G_i z_i^s < Gz^p \ and \ G_i z_i^t > Gz^p)$, then with the use of equations (5.1) and (5.2) the values of the binary variables: $\lambda_{i,p}^{s} = 1, \lambda_{i,p}^{t} = 0$. And the net flow which should be accounted for the recycle balance below the pinch is:

$$[(G^p - G_i^t) - 0] = (G^p - G_i^s)$$

Some other considerations in order to apply correctly the algorithm are going to be necessary. As the pinch is thermodynamically constrained, the ultimate weighting regarding the stream overall impact in the process, should be provided after the real pinch is identified. This is going to be the assessment of the stream recycling strategy. After all, *the games behind an effective allocation of capital in process industries are subject to the rules of thermodynamics* and the pinch constraint should have to be helpful in the way in which such effectiveness is quantified. This applies when optimizing the material allocation in recycle/reuse studies. In recycle/reuse integration the design variables are material flowrates. The floating pinch algorithm locates the pinch under variable stream conditions. Those conditions are going to be having an outstanding role after the heat and mass integration tradeoff are considered. The splitting of streams for an appropriate heat exchange and/or an appropriate direct recycle/reuse requires also the simultaneous pinch location or the extension of the basic floating pinch calculation, as mentioned before.

For the direct recycle reuse, the pinch is located either at the supply or output conditions of a process stream. The next step is to complete the flow balance. In the direct recycle/reuse network the total load from the sources must be equal to the total load delivered to the sinks below and above the pinch.

Therefore, the flowrates is computed by selecting the section below the pinch. Correspondingly, the fresh flowrate has to be computed. The fresh flowrate below the pinch is the difference of total sink and source flowrates.

With equations 5.5 and 5.6 is possible to get the loads in the individual intervals. Then, a summation must be done through both composites in order to complete the balance in the below the pinch section. Hence, the amount of fresh for process is:

$$LFR = \sum_i LSI_i - \sum_j LSO_j \tag{5.7}$$

For direct recycle, the waste discharge calculation will completes the targeting stage. To get the amount of waste discharge we need a total mass balance. This total mass balance comes with the result of equation 5.7. Also, the waste flow rate is given by:

$$LWA = \sum_i G_i(z_i^t - z_i^s) - \sum_j W_j\left(x_j^s - x_j^t\right) - LFR \tag{5.8}$$

These are the stages for the complete mathematical formulation for the recycle/reuse performance targeting. This formulation is flexible and can be part of a more general and modular approach in a novel process integration methodology as already mentioned. The complete model with the modular approach as coded in LINGO 10 is presented in Appendix 1.

It is worth noting that the abovementioned MINLP involves bilinear terms which induce non-convexity; thereby creating difficulty for reaching a global solution (or sometimes even convergence to a local solution). Therefore, a new iterative procedure is introduced in the next section.

V.4 Iterative Procedure for Global Solution

In order to avoid the problems encountered in the solution of the non-convex MINLP, an iterative procedure is proposed. The implementation is developed according to the order described in the flow diagram of Figure 5.5. The basic concept is to discretize the domain for the variable flowrate(s) and composition(s). Once the flowrate and/or composition is discretized, the MINLP becomes a linear program which can be globally solved. The results of the various iterations are compared and the cheapest solution is selected as the global solution.

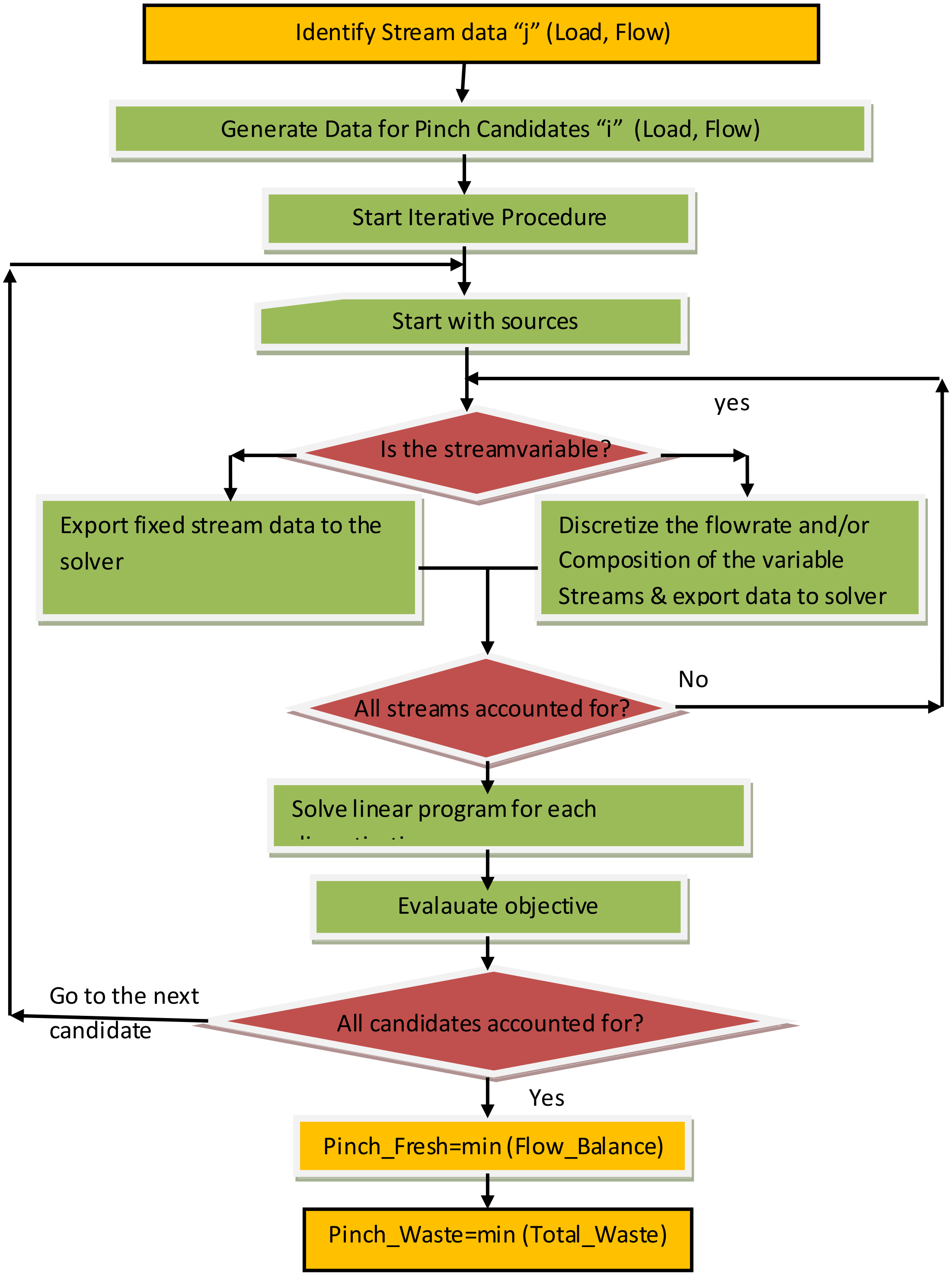

Figure 5.5 Flowchart for pinch candidate analysis and source-sink balances

V.5 Acetic Acid Case Study

The modular approach was implemented for the acetic acid example (described in Chapter IV and adapted from El-Halwagi, 2006). Here, the flowrates and compositions of the sources are kept constant. The intention is to test the variable source algorithm with known results of fixed sources. The lower level programming section will not have to be modified at all whenever the sources are varied or when a new case study has to be solved.

The module as presented in Appendix 1 gives the results as shown in Figure 5.6. These results coincide with those reported by El-Halwagi (2006) and confirm the validity of the developed algorithm in the special case of fixed sources.

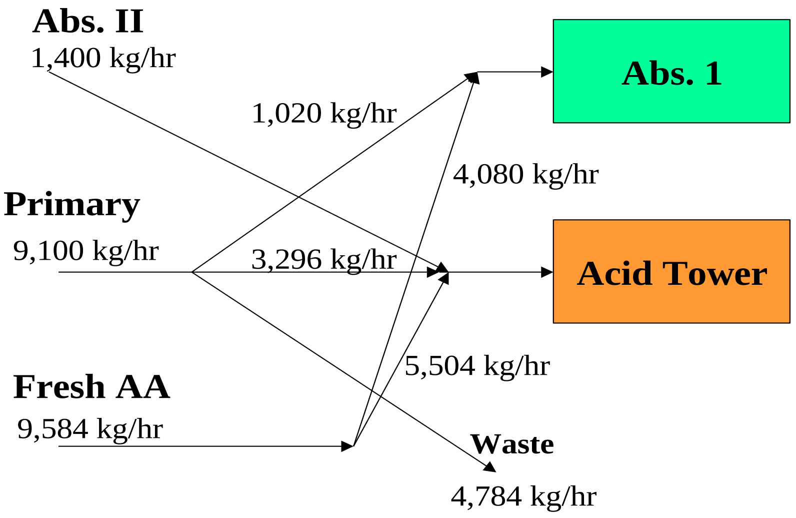

Figure 5.6 Direct recycle configuration results for the acetic acid case study

V.6 Water Recycle Example

Consider a process with six sinks and five sources (Sorin and Bedard, 1999). The process data are given in Tables 5.1 and 5.2. These data have been revised from the original case study of Sorin and Bedard (1999) to allow the source variability. Fresh water is used in the sinks and it is desired to replace as much fresh water as possible through the direct recycle of process sources. Determine the target for minimum amount of fresh water and waste discharge after direct recycle.

Table 5.1 Sink data for the water reuse example

Sink	**Flow (tonnes/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

Table 5.2 Source data for the water reuse example

Source	**Flow** **(tonnes/h)**	**Concentration** **(ppm)**
1	$95 \leq Flowrate \leq 120$	$100 \leq Composition \leq 150$
2	80	140
3	140	180
4	80	230
5	195	250

Results: The modular approach applied explicitly for this problem is shown in Appendix 1. As expected, the solver of LINGO reports that the model is non-linear and therefore no-global optimum solution can be obtained. In this way, if we specify explicitly the range for flow and concentration as a constraint into the model, according to the values stated in Table 5.2, then error message is got from LINGO. Therefore, we decide to implement a set of discrete changes in the flowrate and concentration values in the model. In this way, only the data section is going to change without affecting the lower level code section of the module. The results with the modular approach for direct recycle integration are shown in the Table 5.3. For the objective function, a requirement of 200 tonnes/hr of fresh is obtained. The corresponding value of the minimum flowrate of wastewater discharge is found to be 120 tonnes/hr.

Table 5.3 Results with the modular approach for direct recycle integration

Concentration ppm	**Flow rate**	**Global Optimum**		
		Total	**Waste**	**Fresh_Water**
100	95	295	195	200
	100	300	100	200
	105	305	105	200
	110	310	110	200
	115	315	115	200
	120	320	120	200
110	95	309.54	102.27	207.27
	100	314.54	107.27	207.27
	105	319.54	112.24	207.27
	110	324.54	117.27	207.27
	115	329.54	122.27	207.27
	120	334.54	127.27	207.27
120	95	321.66	108.33	213.33
	100	326.66	113.33	213.33
	105	331.66	118.33	213.33
	110	336.66	123.33	213.33
	115	341.66	128.33	213.33
	120	346.66	133.33	213.33
130	95	331.92	113.46	218.46
	100	336.92	118.46	218.46
	105	341.92	123.46	218.46
	110	346.92	128.46	218.46
	115	351.92	133.46	218.46
	120	356.92	138.46	218.46
140	95	340.71	117.86	222.85
	100	345.71	122.86	222.85
	105	350.71	127.86	222.85
	110	355.71	132.86	222.85
	115	360.71	137.86	222.85
	120	365.71	142.86	222.85
150	95	348.33	121.67	226.66
	100	353.33	126.67	226.66
	105	**358.33**	**131.67**	**226.66**
	110	**371.42**	**140.71**	**230.71**
	115	377.14	146.07	231.07
	120	382.85	151.43	231.42

The results show that an increase of 5 tonnes/hr in the source 1 flowrate will increase the performance targets by 5 tonnes/hr until the concentration moves to 150 ppm and the flowrate goes to 110 tonnes/hr. This can be understood easily with the composite curve diagram (figure 5.7). The pinch changes its location once this source conditions are implemented. In this way, the new location of the pinch is detected with our generic module.

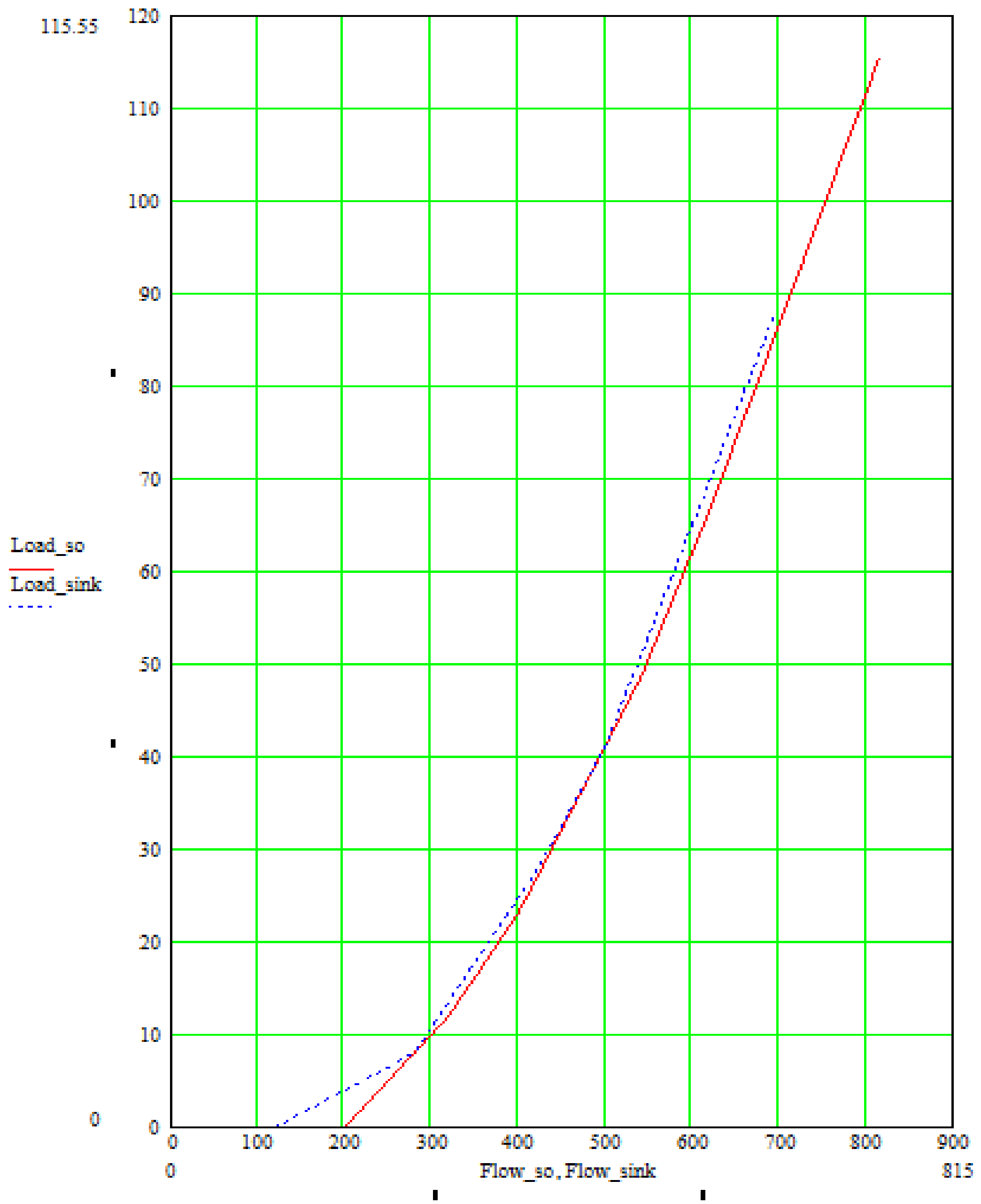

Figure 5.7 Pinch location for the variable flow case study with a flowrate of 120 tonnes/hr and concentration of 100 ppm for source 1

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

VI.1 Conclusions

This work has introduced systematic approaches to solving two new classes of the problem of designing recycle/reuse networks:

a. Thermal effects. Two new aspects have been introduced: heat of mixing of process sources and temperature constraints imposed on the feed to the process sinks

b. Source variability. Two types of source variability are addressed: flowrate and composition

A source-sink assignment problem formulation has been developed for the thermal effects problem. This formulation is based on a structural representation which is rich enough to embed potential configurations of interest and to allow for tracking of mass and heat. Depending on the characteristics of the heat of mixing, the problem can be linear or nonlinear. The solution of this program provides optimum flowrates of the fresh streams as well as the segregation, mixing, and allocation of the process sources to sinks. For the problem of variable sources, the concept of floating pinch has been extended from heat integration and mass exchange networks. Next, a computer code has been developed to solve the problem. It included a combination of computer coding and linkage with an optimization solver. To overcome nonconvexity and convergence problems of the MINLP, an iterative procedure was proposed. Case studies have been solved to illustrate the applicability of the new approaches.

VI.2 Recommendations for Future Work

The work developed in this thesis can constitute the basis for more complex design problems. Of particular interest is the problem of simultaneous synthesis for direct recycle/reuse (DRR), heat exchange networks (HEN) and mass exchange networks (MEN). A schematic representation of this general problem is shown by Fig. 6.1.

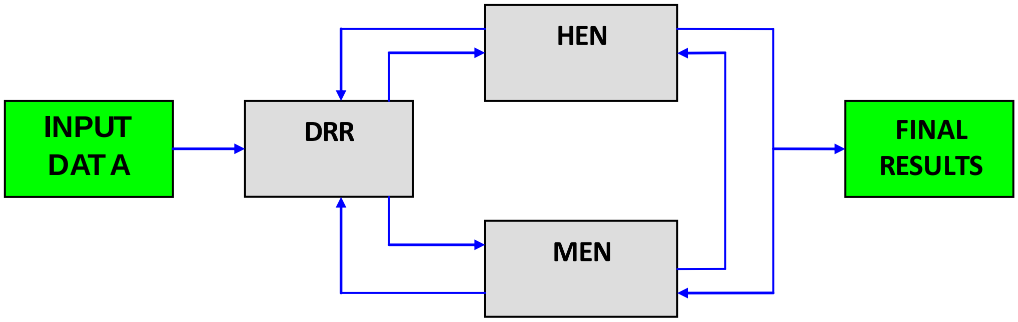

Figure 6.1 Simultaneous synthesis for direct recycle/reuse (DRR), heat exchange networks (HEN) and mass exchange networks (MEN).

To get a complete comprehensive approach, the next research stages are suggested:

- **To develop and validate the module for evaluation of performance targets in heat integration.** Once this module has been developed, some simultaneous direct recycle and heat integration case studies should be explored. A direct recycle/reuse-heat exchange modular approach should be validated.

- **To develop and validate the module for evaluation of performance targets in mass exchange.** This is similar to the case of heat integration. Once this module had been validated for mass transfer, the mathematical programming platform of LINGO makes possible to trade off simultaneous performance targets for direct recycle, heat and mass integration. A new interface for the data section could be convenient to facilitate this point with which concludes our original objectives in PI.
- **Exploration for particular applications:** Reactive systems could be part of a total process modeling approach. In addition to physical separation, reactive separation models could be implemented and the attainable region for reactive systems could be explored from an even more generic PI perspective. Then, a property-based framework for process integration could be explored as well.

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APPENDIX A

OPTIMIZATION CODING FOR THE VARIABLE SOURCE FORMULATION

```
MIN = TOTAL_COST;


!*** CONSIDER THE ADITION OF A FINAL FEASIBILITY-PINCH-
PROVE-SCAN!!!
!   INTRODUCTION
MODIFIED FILE FOR PROBLEM 3.1
THE GOAL IS TO DEAL WITH SIMULATANEOUS DIRECT RECYCLE,
MASS, HEAT,
OR WHATEVER PROPERTY WHICH CAN BE CHARACTERIZED THROUGH
SOURCES AND
SINKS. THE OBJECTIVE FUNCTION WILL REFLECT SEQUENTIALLY THE
CONSIDE-
RATION OF THESE PROCESS INTEGRATION ATTRIBUTES.
THE BASIC UNIT FOR PROCESS DELIVERING OF PROPERTIES IS THE
"STREAM"
WHICH CAN BE SOURCE,SINK, HOT, COLD, RICH, OR POOR.
DEPENDING ON
WHAT STATE OR INTEGRATION PROPERTY ARE WE DEALING WITH.
```

```
THE ATTRIBUTES OF THE STREAMS DEFINED THROUGH SET
ATTRIBUTES, AND
SERIES OF SETS ARE DEFINED FOR THE SOLUTION PROCESS.
ATTRIBUTES FOR
THE STREAMS ARE FOR EXAMPLE: INITIAL CONDITIONS, FINAL
CONDIONS, FLOW, CONCENTRATION, ETC.
THE OBJECTIVE FUNCTION WILL BE WEIGHTING ULTIMATELLY IN
TERMS OF
COSTS THE STREAMS COMING FROM THE INPUT DATA.  A
SENSITIVITY ANALY-
SIS MUST BE DEVELOPED IF REQUIRED.
DIRECT RECYCLE:;

SETS:
     L_CANDIDATE;
     L_SINK_COMP;
     E_CANDIDATE;
     E_SOURCE_COMP;
     STREAMS:       FEED,STREAM_NO,DRECYCLE, MASS_EXC,
HEAT_EXC,
                    SOURCE_SINK, RICH_POOR, HOT_COLD,
FLOWRATE,
                    LOAD, CONCENTRATION;
```

```
     DR_SOURCE_COMP:     DR_FLOWRATE_SO, DR_LOAD_SO;

     DR_SINK_COMP:  DR_FLOWRATE_SI, DR_LOAD_SI;

     DR_CANDIDATES:      DR_CAND_LOAD, DR_CAND_FLOW,

                    TOTAL_FLOW_BALANCE,

TOTAL_WASTE_BALANCE,

                    M_VERTEX, DIST_SO, DIST_FLOW_CAND,

                    PINCH_FRESHA;

     LAMBDA_T_SI(L_CANDIDATE,L_SINK_COMP):

                    L_T,L_S,SI_FLOW_CAND_INT;

     ETA_T_SO(E_CANDIDATE,E_SOURCE_COMP):

               E_T,E_S,SO_FLOW_CAND_INT,DR_FLOW_CONT_SO;

     MOD(E_CANDIDATE, DR_SINK_COMP): SI_FLOW;


ENDSETS


DATA:


FEED, STREAM_NO     ,DRECYCLE,     MASS_EXC, HEAT_EXC,

     SOURCE_SINK,

1    1         1         0         0         1

1    2         1         0         0         1

1    3         1         0         0         1

1    4         1         0         0         1
```

```
1    5         1         0         0         1
1    6         1         0         0         0
1    7         1         0         0         0
1    8         1         0         0         0
1    9         1         0         0         0
1    10        1         0         0         0
1    11        1         0         0         0
0    1         1         0         0         1
0    2         1         0         0         1

0    3         1         0         0         1
0    4         1         0         0         1
0    5         1         0         0         1
0    6         1         0         0         0
0    7         1         0         0         0
0    8         1         0         0         0
0    9         1         0         0         0
0    10        1         0         0         0
0    11        1         0         0         0

 RICH_POOR, HOT_COLD, FLOWRATE, CONCENTRATION =
0         0         120       0.10
0         0         80        0.14
```

```
0         0         140       0.18

0         0         80        0.23

0         0         195       0.25

0         0         120       0.0

0         0         80        0.05

0         0         80        0.05

0         0         140       0.140

0         0         80        0.170

0         0         195       0.240

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00

0         0         0         0.00;


DR_SOURCE_COMP = 1..6;  !POINTS IN THE SOURCE COMPOSITE;

DR_SINK_COMP   = 1..7;  !POINTS IN THE SINK COMPOSITE;
```

```
DR_CANDIDATES  = 1..13; !TOTAL CANDIDATES;


L_CANDIDATE       =1..13;  !SET FOR BINARY FOR THE
CANDIDATES;
L_SINK_COMP    =1..7;    !SET FOR BINARY FOR THE SOURCE
COMPOSITE;


E_CANDIDATE    =1..13;   !SET FOR BINARY FOR THE CANDIDATES
SINK;
E_SOURCE_COMP  =1..6;    !SET FOR BINARY FOR THE SOURCE
COMPOSITE;



ENDDATA


!This line gives the loads for the set of streams;


!VIRTUAL CALC SECTION
START*************************************;
@FOR(STREAMS(j):LOAD(j)=FLOWRATE(j)*CONCENTRATION(j));
```

```
@FOR(DR_SOURCE_COMP(J):
DR_FLOWRATE_SO(J)=@IF(J #GT# 1, @SUM(STREAMS(K)|((K#LE#(J-
1))
               #AND# (SOURCE_SINK #EQ#
1)):FLOWRATE(K)),0.0););
      !FLOWRATE COORDINATE VALUE SOURCE COMPOSITE OK -
1207-07;

@FOR (DR_SOURCE_COMP(J):
DR_LOAD_SO(J)=@IF(J #GT# 1, @SUM(STREAMS(K)| ((K#LE#(J-1))
            #AND# (SOURCE_SINK #EQ# 1)):LOAD(K)),0.0););
     !LOAD COORDINATE VALUE SOURCE COMPOSITE CURVE ;

@FOR (DR_SINK_COMP(J):
DR_FLOWRATE_SI(J)=@IF(J #GT# 1, @SUM(STREAMS(K)|(K #LE#
               (J-1+@SUM(STREAMS(L):SOURCE_SINK(L))/2))
#AND#
               (SOURCE_SINK(K) #EQ# 0):FLOWRATE(K)),0.0););
     !FLOWRATE COORDINATE VALUE SINK COMPOSITE CURVE;

@FOR (DR_SINK_COMP(J):
DR_LOAD_SI(J) = @IF(J #GT#1, @SUM(STREAMS(K)|(K #LE# (J-
1+@SUM
```

```
     (STREAMS(L):SOURCE_SINK(L))/2)) #AND# (SOURCE_SINK(K)
     #EQ# 0):LOAD(K)),!@IF(J #EQ#3,3, ;0.0!););););
     !LOAD COORDINATE VALUE SOURCE COMPOSITE CURVE;

!   ASSIGNING VALUES TO THE PINCH CANDIDATES;
@FOR (DR_CANDIDATES(J):
     DR_CAND_LOAD(J) = @IF(J #LE#
(1+@SUM(STREAMS(L):SOURCE_SINK(L))/2)
     ,DR_LOAD_SO(J),DR_LOAD_SI(J-
(1+(@SUM(STREAMS(L):SOURCE_SINK(L))/2)
     )));););

!CASE FOR THE VERTEX IS A POINT FROM THE SINK;
@FOR (DR_CANDIDATES(M)|M #GE# (2+ @SUM(STREAMS(L):
SOURCE_SINK(L))/2):
DR_CAND_FLOW(M) = DR_FLOWRATE_SI(M-
(2+@SUM(STREAMS(Z):SOURCE_SINK(Z))
)/2) );



!CASE FOR THE VERTEX IS A POINT FROM THE SOURCE;
@FOR (DR_CANDIDATES(R)|R #LE# (1 +
@SUM(STREAMS(L):SOURCE_SINK(L))/2):
```

```
@FOR (DR_SINK_COMP(S):
SI_FLOW(R,S) = @IF((DR_CAND_LOAD(R) #EQ# 0) #OR# (S #EQ#
1),0.0,
               @IF((DR_CAND_LOAD(R) #GT# DR_LOAD_SI(S-1))
#AND#
               (DR_CAND_LOAD(R) #LT# DR_LOAD_SI(S)),
               (DR_CAND_LOAD(R)-DR_LOAD_SI(S-1))/
               ((DR_LOAD_SI(S)-DR_LOAD_SI(S-
1))/(DR_FLOWRATE_SI(S)
               -DR_FLOWRATE_SI(S-1))),
                @IF(DR_CAND_LOAD(R) #LT# DR_LOAD_SI(S-
1),0.0,
                @IF(DR_CAND_LOAD(R) #GT# DR_LOAD_SI(S),
                =DR_FLOWRATE_SI(S)-DR_FLOWRATE_SI(S-
1),0!*****;);););
               );););
          DR_CAND_FLOW(R) = @SUM(MOD(R,k):SI_FLOW(R,k););
     );



!MODIFIERS:  I.P.H.E.S.;
```

```
@FOR (DR_CANDIDATES(i)|i #GE# (2+
@SUM(STREAMS(L):SOURCE_SINK(L))/2)
:
     @FOR (DR_SOURCE_COMP(j):
     DR_FLOW_CONT_SO(i,j)= @IF((DR_CAND_LOAD(i) #EQ# 0)
#OR#
                         (j #EQ# 1),0.0,
                         @IF(DR_CAND_LOAD(i) #EQ#
                         DR_LOAD_SO(j-1),0.0,
                           @IF(DR_CAND_LOAD(i) #EQ#
DR_LOAD_SO(j),
                           DR_FLOWRATE_SO(j),
       @IF( (DR_CAND_LOAD(i) #LT# DR_LOAD_SO(j)) #AND#
     (DR_CAND_LOAD(i) #GT# DR_LOAD_SO(j-1)),
     (DR_CAND_LOAD(i)-DR_LOAD_SO(j-1))/((DR_LOAD_SO(j)-
DR_LOAD_SO(j-1))
      /(DR_FLOWRATE_SO(j)-DR_FLOWRATE_SO(j-1))),
     !***Few;  @IF(DR_CAND_LOAD(i) #LT# DR_LOAD_SO(j-
1),0.0,
     @IF(DR_CAND_LOAD(i) #GT#
DR_LOAD_SO(j),DR_FLOWRATE_SO(j),0!******;
     ););););););
     DIST_SO(i)= @SUM(ETA_T_SO(i,k):DR_FLOW_CONT_SO(i,k));
```

```
     DIST_FLOW_CAND(i)= DR_CAND_FLOW(i)-DIST_SO(i);
     );

!6666 stands for silly error in the calculation;
!BINARY VARIABLES FOR DIRECT RECYCLE PLUS...;
!LOOPING FOR LOAD CALCULATION EVERY SPECIFIC PINCH
CANDIDATES;
!FLOW REQ. FOR EVERY INTERVAL IN ALL THE CANDIDATES -
SOURCES-?;

@FOR (DR_CANDIDATES(i):
     @FOR (DR_SOURCE_COMP(j):
     E_S(i,j)= @IF(j #LE# (@SUM(STREAMS(L):SOURCE_SINK))/2,
     @IF(DR_LOAD_SO(j+1) #GE#
DR_CAND_LOAD(i),0,1),0!*******;);
     E_T(i,j)= @IF(j #LE# (@SUM(STREAMS(L):SOURCE_SINK))/2,
     @IF(DR_LOAD_SO(j) #GE#
DR_CAND_LOAD(i),0,1),0!******;);
     SO_FLOW_CAND_INT(i,j) = @IF(j #LE# (@SUM(STREAMS(L):
     SOURCE_SINK))/2,E_T(i,j)*(DR_CAND_FLOW(i)-
DR_FLOWRATE_SO(j)
     -DIST_FLOW_CAND(i))
     -E_S(i,j)*(DR_CAND_FLOW(i)-DR_FLOWRATE_SO(j+1)
```

```
    -DIST_FLOW_CAND(i)),0.0);
        );
    );

!FLOWS REQ. FOR EVERY INTERVAL IN ALL THE CANDIDATES -
SINKS-?;
@FOR (DR_CANDIDATES(i):
    @FOR (DR_SINK_COMP(j):
    L_S(i,j)= @IF(j #LE# (@SUM(STREAMS(L):DRECYCLE(L))/2-
    @SUM(STREAMS(L):SOURCE_SINK(L))/2),
    @IF(DR_LOAD_SI(j) #GE# DR_CAND_LOAD(i),0,1),0!*****;);

    L_T(i,j)= @IF(j #LE# (@SUM(STREAMS(L):DRECYCLE(L))/2-
    @SUM(STREAMS(L):SOURCE_SINK(L))/2),
    @IF(DR_LOAD_SI(j+1) #GE#
DR_CAND_LOAD(i),0,1),0!******;);
    SI_FLOW_CAND_INT(i,j) = @IF(j #LE# (@SUM(STREAMS(L):
    DRECYCLE(L))/2-@SUM(STREAMS(L):SOURCE_SINK(L))/2),
    L_S(i,j)*(DR_CAND_FLOW(i)-DR_FLOWRATE_SI(j))-L_T(i,j)*
    (DR_CAND_FLOW(i)-DR_FLOWRATE_SI(j+1)),0.0);
        );
    );
```

```
!BALANCE OF FLOWS: (EQ. 22) TOTAL FLOW FOR THE SET OF
CANDIDATES note %%% ;!BELOW THE PINCH... FRESH STREAM;

@FOR (DR_CANDIDATES(i):
     TOTAL_FLOW_BALANCE(i) = @SUM (LAMBDA_T_SI(i,k):
     SI_FLOW_CAND_INT(i,k)) -
     @SUM (ETA_T_SO(i,k):SO_FLOW_CAND_INT(i,k));
     );

@FOR (DR_CANDIDATES(i):
     TOTAL_WASTE_BALANCE(i) = @SUM(DR_SINK_COMP(J)|J #LE#
     (@SUM(STREAMS(L):DRECYCLE(L))/2 -
     @SUM(STREAMS(L):SOURCE_SINK(L))/2):
     (DR_FLOWRATE_SI(J+1)-DR_FLOWRATE_SI(J)))-@SUM
     (DR_SOURCE_COMP(J)|J#LE#5 :(DR_FLOWRATE_SO(J+1)
     -DR_FLOWRATE_SO(J)))-TOTAL_FLOW_BALANCE(i)
     );

@FOR (DR_CANDIDATES(J):
     PINCH_FRESHA(J) = @IF(TOTAL_WASTE_BALANCE #EQ#
     @MIN(DR_CANDIDATES(R):TOTAL_WASTE_BALANCE(R)),
     @ABS(TOTAL_FLOW_BALANCE(J)),0.0);
     );
```

```
PINCH_FRESH = @MAX(DR_CANDIDATES(J):PINCH_FRESHA);

!***THE ONLY ONE WITH A VALUE DIFFERENT THAN 0.0;

!VIRTUAL CALC SECTION

END****************************************;


PINCH_WASTE =-1*@MIN(DR_CANDIDATES:TOTAL_WASTE_BALANCE);

TOTAL_COST = PINCH_FRESH + PINCH_WASTE;


!RESTRICTIONS... solver fails!!!;

!FLOWRATE(1) >0;          !CONCENTRATION(1)>0.0;

!FLOWRATE(2) >0;          !CONCENTRATION(2)>0.0;

!FLOWRATE(3) >0;          !CONCENTRATION(3)>0.0;

!FLOWRATE(4) >0;          !CONCENTRATION(4)>0.0;

!FLOWRATE(5) >0;          !CONCENTRATION(5)>0.0;

!FLOWRATE(6) >=0;         !CONCENTRATION(6)>=0.0;

!FLOWRATE(7) >0;          !CONCENTRATION(7)>0.0;

!FLOWRATE(8) >0;          !CONCENTRATION(8)>0.0;

!FLOWRATE(9) >0;          !CONCENTRATION(9)>0.0;

!FLOWRATE(10)>0;          !CONCENTRATION(10)>0.0;

!FLOWRATE(11)>0;          !CONCENTRATION(11)>0.0;

!FLOWRATE(12)=0;

!FLOWRATE(13)=0;
```

```
!FLOWRATE(14)=0;
!FLOWRATE(15)=0;
!FLOWRATE(16)=0;
!FLOWRATE(17)=0;
!FLOWRATE(18)=0;
!FLOWRATE(19)=0;
!FLOWRATE(20)=0;
!FLOWRATE(21)=0;
!FLOWRATE(22)=0;

!FLOWRATE(1) =120;       !CONCENTRATION(1)<0.1;
!FLOWRATE(2) =80;        !CONCENTRATION(2)<0.14;
!FLOWRATE(3) =140;  !CONCENTRATION(3)<0.18;
!FLOWRATE(4) =80;        !CONCENTRATION(4)<0.23;
!FLOWRATE(5) =195;  !CONCENTRATION(5)<0.25;
!FLOWRATE(6) =120;  !CONCENTRATION(6)<0.0;
!FLOWRATE(7) =80;        !CONCENTRATION(7)<0.05;
!FLOWRATE(8) =80;        !CONCENTRATION(8)<0.05;
!FLOWRATE(9) =140;  !CONCENTRATION(9)<0.140;
!FLOWRATE(10)=80;        !CONCENTRATION(10)<0.170;
!FLOWRATE(11)>193;
!FLOWRATE(11)<195;  !CONCENTRATION(11)<0.240;
```

```
!PINCH_WASTE>0;

!PINCH_FRESH>0;

END
```

VITA

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