Property-Based Optimization of Direct-Recycle Networks and Wastewater Treatment Processes

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Abstract

This paper presents a mathematical programming model to simultaneously optimize a recycle-reuse mass exchange network together with a wastewater treatment process. The model is based on disjunctive programming, and considers the technologies that are commonly used to treat wastewater streams so that they meet environmental regulations. In addition to standard mass balance and composition constraints, the model incorporates environmental constraint properties such as toxicity, theoretical oxygen demand, pH, color, and odor. The problem results in an MINLP model, and is used to minimize the total annual cost of the system, which includes the cost for the fresh sources, the piping cost for the mass integration and the wastewater treatment cost. The model is formulated with linear relationships in the disjunctions to avoid numerical complications. The solution of the proposed model shows that the simultaneous consideration of the mass integration and wastewater treatment sections yields important economic savings with respect to the solution that considers the mass integration first and then takes into account the wastewater treatment facilities. Also, the simultaneous optimization can yield solutions that require more consumption of the cleaner fresh sources than the one provided with the optimization of the mass exchange network alone, and the overall integration results in a lower total annual cost. The model did not show any numerical problems, and the CPU time required for the solution of the numerical examples was relatively small.

Introduction

Mass integration strategies have been the subject of study of much research efforts because of the economical and environmental benefits they provide. In the area of sustainable design, mass integration can be used to lower the consumption of fresh sources and to reduce the waste materials discharged to the environment. Recent surveys on mass integration can be found in literature.[1,2] A particular application of the mass integration is in the area of minimizing fresh water usage and wastewater discharge through recycle/reuse strategies. Bagajewicz[3] has published a paper review on the procedures reported to design water networks. Previous works have provided major contributions to the synthesis of water recycle/reuse networks. However, they have a couple of limitations. First, their focus has been given to in-plant recycle strategies with constraints limited to process units and without considering the effects of the resulting terminal wastewater streams and the environmental regulations. To satisfy the environmental constraints, the wastewater stream needs to be treated prior to be discharged to the environment; this situation may increase the total cost associated to the recycle-reuse mass integration process. For example, when the solution that minimizes fresh sources consumption yields a high wastewater treatment cost, then such a solution may not correspond to the overall optimal solution. In this case, it may be preferable to use more fresh sources and lower the wastewater treatment cost. Therefore, it is important to consider simultaneously the optimization of the process integration together with the wastewater treatment process to take into account the trade offs between both factors. Second, process characterization and recycle constraints have been based on compositions. It is worth noting that there are many industrial cases when such constraints should be based on properties. Examples include applications when the performance of the process units is affected by the properties of its feed and the cases when environmental regulations impose limits for specific properties of waste streams such as toxicity, theoretical oxygen demand (*ThOD*), *pH*, temperature, color, odor, viscosity and density. These properties are difficult to quantify as a function of composition because of the many components of the process streams. It is also difficult to track properties throughout the process because they are not conserved. To overcome this limitation, Shelley and El-Halwagi[4] introduced the concept of property-based componentless design by defining surrogate properties (called clusters) that enable the conserved tracking of properties.

This paper presents a mathematical programming model to simultaneously optimize the direct recycle networks together with the wastewater treatment process in order to satisfy a set of process and environmental constraints. An optimization formulation is developed based on disjunctive programming. The model is formulated to consider environmental-constrained properties such as toxicity, *ThOD*, *pH*, color, odor, and any other property that may cause pollution to the environment, in addition to the mass and composition constraints for hazardous compounds in the waste stream. The problem is formulated with proper constraints as an MINLP problem that minimizes the total annual cost of the system, which includes the cost for the fresh sources, the piping cost for the process integration and the wastewater treatment cost.

Model formulation

The problem addressed is defined as follows. Given is a set of process and fresh sources with known flowrates, compositions and properties. Also given is a set of sinks (process units) with constraints for the inlet flowrates and allowed compositions and properties. In addition, there is a set of constraints given by the environmental regulations for the waste streams discharged to the environment. The problem then consists of finding the optimal mass and property integration network that includes a direct recycle strategy that meets the environmental regulations for the waste streams and minimizes the total annual cost of the overall process (see Figure 1).

Splitting of process source streams.

$$W_i = \sum_{j \in NSINKS} w_{i,j} + waste_i, \qquad i \in NSOURCES \tag{1}$$

Splitting of fresh source streams.

$$F_r = \sum_{j \in NSINKS} f_{r,j}, \qquad r \in NFRESH \tag{2}$$

Total waste.

$$WASTE = \sum_{i \in NSOURCES} waste_i \tag{3}$$

Mass balances at the mixing point before each sink.

$$G_j = \sum_{i \in NSOURCES} w_{i,j} + \sum_{r \in NFRESH} f_{r,j}, \qquad j \in NSINKS \tag{4}$$

Component balances at the mixing point before each sink.

$$z_{j,c}^{in} G_j = \sum_{i \in NSOURCES} \left[z_{i,c}\, w_{i,j} \right] + \sum_{r \in NFRESH} \left[z_{r,c}\, f_{r,j} \right], \qquad j \in NSINKS, c \in NCOMP \tag{5}$$

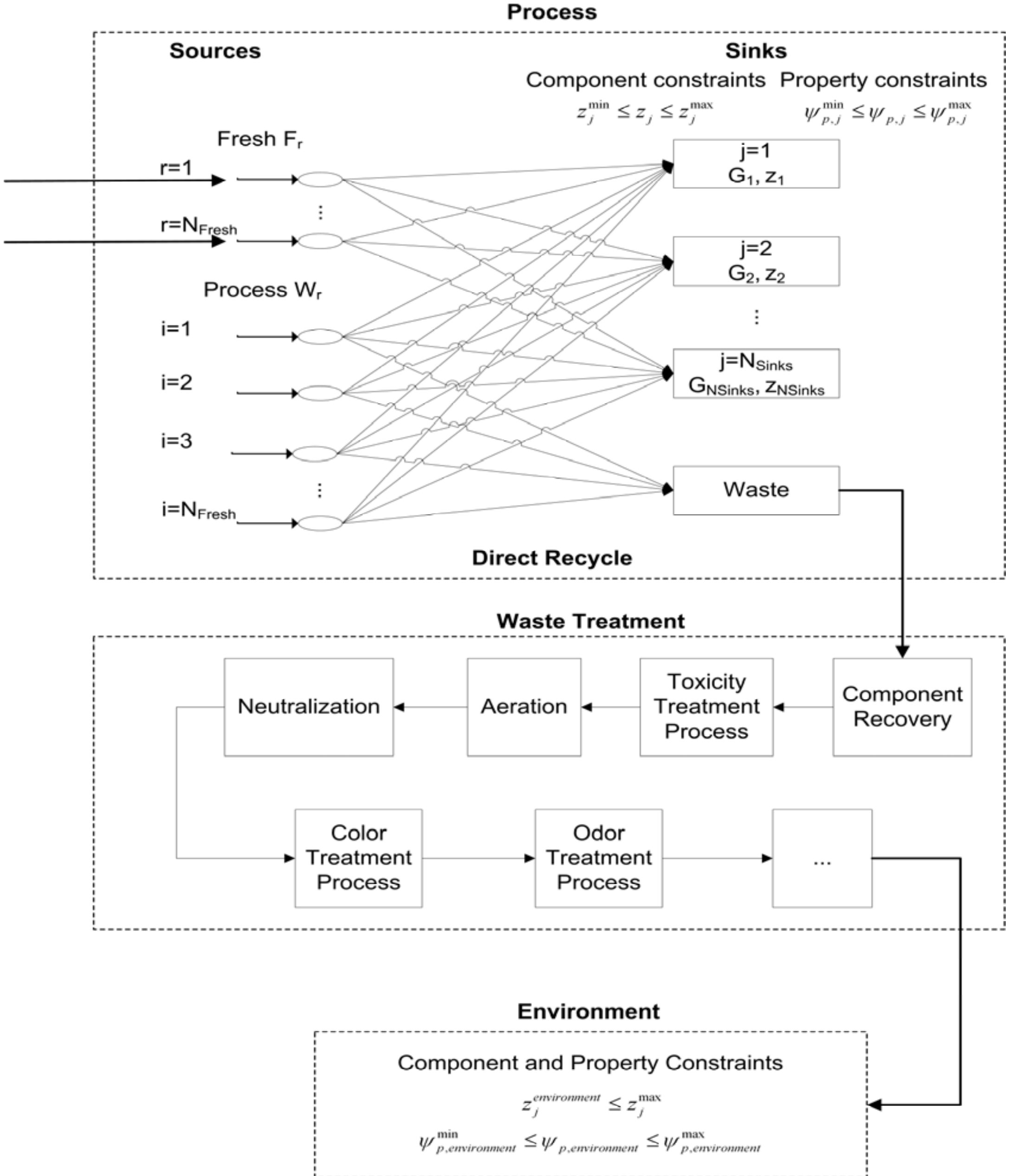

Figure 1. Source-sink representation for mass and property integration including waste treatment

Property balance at the mixing point before each sink.

$$\psi_p\left(p_{j,p}^{in}\right) G_j = \sum_{i \in NSOURCES} \left[\psi_p\left(p_{i,p}\right) w_{i,j} \right] + \sum_{r \in NFRESH} \left[\psi_p\left(p_{r,p}\right) f_{r,j} \right], \qquad j \in NSINKS, p \in NPROP \tag{6}$$

Sinks properties constraints.

$$p_{p,j}^{\min} \le p_{p.j}^{in} \le p_{p.j}^{\max}, \quad j \in NSINKS, p \in NPROP \tag{7}$$

Waste stream treatment constraints

A waste stream needs to satisfy the environmental regulations before it is discharged to the environment. Constraints are formulated from the environmental regulations for hazardous materials. Whenever possible, they are based on component constraints, but for properties that are difficult to characterize because of the large number of components in some waste streams, they are formulated as property constraints.

Ratio waste stream.

$$Ratio_i = \frac{waste_i}{\sum_{i \in SOURCES} waste_i} \tag{8}$$

Density for the waste stream.

$$\frac{1}{\rho_{waste}} = \sum_{i \in SOURCES} \left[\frac{Ratio_i}{\rho_i} \right] \tag{9}$$

General property treatment. For any property, the property integration principle yields,

$$f_{\mathrm{Pr}operty}\left(\mathrm{Pr}operty_{mean}\right) = \sum_{i \in NSOURCES} f_{\mathrm{Pr}operty}\left(Ratio_i \ \mathrm{Pr}operty_i\right) \tag{10}$$

$$Wn^{\mathrm{Pr}operty} = Wn \ \mathrm{Pr}operty_{mean} \tag{11}$$

$$Wn^{\mathrm{Pr}operty\,\mathrm{Reg}} = Wn \ \mathrm{Pr}operty_{\mathrm{Reg}} \tag{12}$$

Accordingly, the following disjunction can be formulated,

$$\begin{bmatrix} Y^{\mathrm{Pr}operty} \\ Wn^{\mathrm{Pr}operty} \geq Wn^{\mathrm{Pr}operty\,\mathrm{Reg}} \\ Cost^{\mathrm{Pr}operty} = \left(Wn^{\mathrm{Pr}operty} - Wn^{\mathrm{Pr}operty\,\mathrm{Reg}}\right) Costu^{\mathrm{Pr}operty} H_Y \end{bmatrix} \vee \begin{bmatrix} \neg Y^{\mathrm{Pr}operty} \\ Wn^{\mathrm{Pr}operty} \leq Wn^{\mathrm{Pr}operty\,\mathrm{Reg}} \\ Cost^{\mathrm{Pr}operty} = 0 \end{bmatrix}$$

which can be modeled as follows,

$$Wn^{\mathrm{Pr}operty} = Wn^{\mathrm{Pr}operty^1} + Wn^{\mathrm{Pr}operty^2} \tag{13}$$

$$Wn^{\mathrm{Pr}operty\,\mathrm{Reg}} = Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^1} + Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^2} \tag{14}$$

$$Wn^{\mathrm{Pr}operty^1} \geq Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^1} \tag{15}$$

$$Cost^{\mathrm{Pr}operty} = \left(Wn^{\mathrm{Pr}operty^1} - Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^1}\right) Costu^{\mathrm{Pr}operty} H_Y \tag{16}$$

$$Wn^{\mathrm{Pr}operty^2} \leq Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^2} \tag{17}$$

$$Wn^{\mathrm{Pr}operty^1} \leq M^{Wn^{\mathrm{Pr}operty}} \ y^{\mathrm{Pr}operty} \tag{18}$$

$$Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^1} \leq M^{Wn^{\mathrm{Pr}operty}} \ y^{\mathrm{Pr}operty} \tag{19}$$

$$Wn^{\mathrm{Pr}operty^2} \leq M^{Wn^{\mathrm{Pr}operty}} \left(1 - y^{\mathrm{Pr}operty}\right) \tag{20}$$

$$Wn^{\mathrm{Pr}operty\,\mathrm{Reg}^2} \leq M^{Wn^{\mathrm{Pr}operty}} \left(1 - y^{\mathrm{Pr}operty}\right) \tag{21}$$

Objective function. The objective function consists of the minimization of the total annual cost associated with both the mass integration and the waste treatment processes. The costs of the mass integration process include the cost due to the fresh sources and the piping costs to build the mass integration network. Piping costs are important to be accounted for, and they are a function of the layout (which is known prior to the mass integration) and the flowrate of the streams. To meet the environmental regulations, it may be necessary to treat the waste streams. The costs associated with the waste treatment process include the cost for the recovery of specific compounds in the waste streams, the cost to remove the toxic compounds, the cost of aeration to satisfy the theoretical oxygen demand regulation, the cost for the neutralization process, the cost to decrease color, odor, and any other property that may cause contamination. The objective function can be formulated as follows,

$$
\begin{aligned}
TAC = & \sum_{r \in FRESH} Cost_r^{Fresh} F_r \; H_Y \\
& + \sum_{\substack{i \in SOURCES \\ j \in SINKS}} pip_{i,j} \; w_{i,j} + \sum_{\substack{r \in FRESH \\ j \in SINKS}} pip_{r,j} \; f_{r,j} \\
& + \sum_{u \in RECOV} Cost_u^{\mathrm{Recov}eryu} + \sum_{t \in TOX} Cost_t^{Toxicity} \\
& + Cost^{ThoD} + Cost^{Neu} + Cost^{Color} + Cost^{Odor} + \cdots + Cost^{\mathrm{Pr}operty}
\end{aligned}
\tag{22}
$$

Results

This section presents the application of the proposed algorithm. For the mass integration process, two fresh sources are available with a phenol impurity of 0 and 0.012 mass fraction, and with unit costs of \$0.0006/lb and \$0.0004/lb, respectively. In addition there are three process sources; the stream data for these sources are given in Table 1. The data for the sinks are given in Table 2.

Table 1. Sources data for the Example

Source, *i*	W_i [lb/hr]	$z_{i,\ phenol}$	$z_{i,\ acetone}$	*ThOD* [gO_2/l]	*pH*	ρ [lb/l]
1	8,083	0.016	0.000	0.187	5.4	2.205
2	3,900	0.024	0.010	48.850	5.1	2.205
3	3,279	0.22	0.028	92.100	4.8	2.205

Table 2. Sinks data for the Example

Sink, *j*	G_j [lb/hr]	$z_j^{\max}$
1	6,000	0.013
2	4,400	0.013
3	2,490	0.1

The environmental regulations applied to this specific process are as follows. The maximum concentration allowed to be discharged to the environment for acetone and phenol is 0.005. The toxicity must be zero, and the maximum concentration and discharge load of phenol, the toxic material, are 0.0000011 (mass fraction) and 0.00541 lb/hr respectively. The theoretical oxygen demand of the waste stream must be lower than 75 mg O_2/l, and finally the *pH* must be between 5.5 and 9.0.

The unit costs for the recovery processes are 0.065 \$/lb and \$0.033 \$/lb for phenol and acetone, respectively. The unit cost for aeration is 0.006\$/lb air diffused, and the unit costs for the H_2SO_4 and NaOH used for the neutralization process are \$46/l and \$31/l, respectively.

Table 3 gives the unit piping cost for the mass integration process.

Table 3. Piping costs for the Example*

Sink, *j*	Sources				
	Process, *i*			Fresh, *r*	
	1	2	3	1	2
1	5	2	3	4.5	2.5
2	3.5	1	5	3	1
3	2	4	2	3.5	1.5

* Units in $/year

Figure 2 shows the results for the case when only process constraints are considered, without including the waste treatment process. We refer to this structure as Solution A. Notice that the waste stream does not satisfy the environmental constraints; therefore, it will be necessary to include a waste treatment process to the solution obtained here.

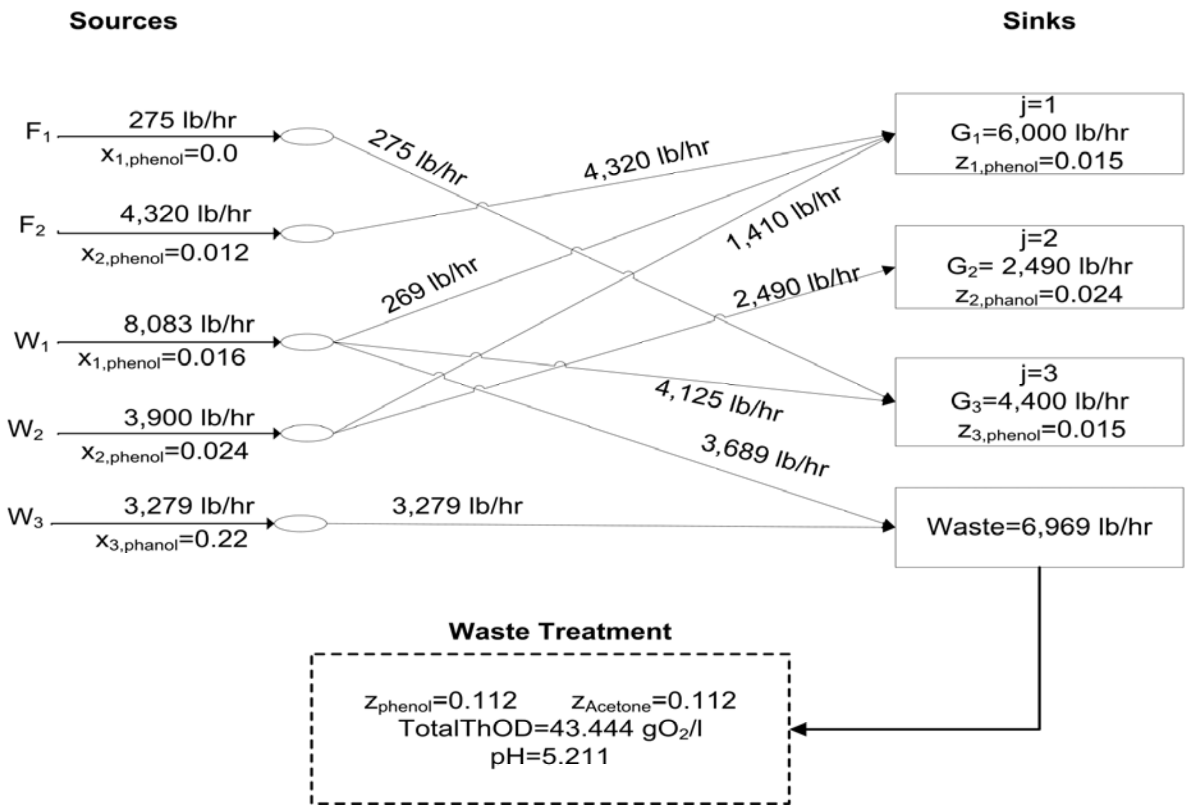

Figure 2. Mass integration without environmental constraints (solution A)

Figure 3 shows the solution of the example problem including all the environmental constraints for this example (Solution B). Notice that the total waste is reduced in the solution that incorporates the waste treatment process by 11.1% with respect to the solution that considered only the process constraints. In addition, in the optimal solution shown in Figure 3, the total consumption of fresh source 1 (with an impurity concentration of phenol of 0) is increased by 76.1% with respect to Solution A of Figure 2; this yields a decrease in the concentration of phenol and acetone in the waste stream by 22.2% and 30%, respectively. The theoretical oxygen demand in the waste stream for the optimal solution that considers the waste treatment process is reduced by 27.4% with respect to the simplified solution of Figure 2. The *pH* in the optimal solution B is increased by 0.93% with respect to the simplified Solution A.

Table 4 shows a summary of the costs associated with both solutions. For comparison purposes, the costs of the waste treatment processes that would be needed for Solution A were calculated after the optimization procedure. Notice in Table 4 that the sum of the costs associated with the process (fresh sources and piping costs) in solution B is 8% higher than those required for solution A. In addition, the total costs associated with the waste treatment process for the optimal solution B is 41.3% lower than those required by the simplified solution

A. Therefore, the solution that simultaneously optimize the process and the waste treatment process yields a total annual cost with savings of 25.4% with respect to the solution that only optimizes the process. This result confirms the advantage to simultaneously consider mass and property integration and to trade off direct recycle, usage of fresh resource, and treatment of waste streams while satisfying process constraints and environmental regulations.

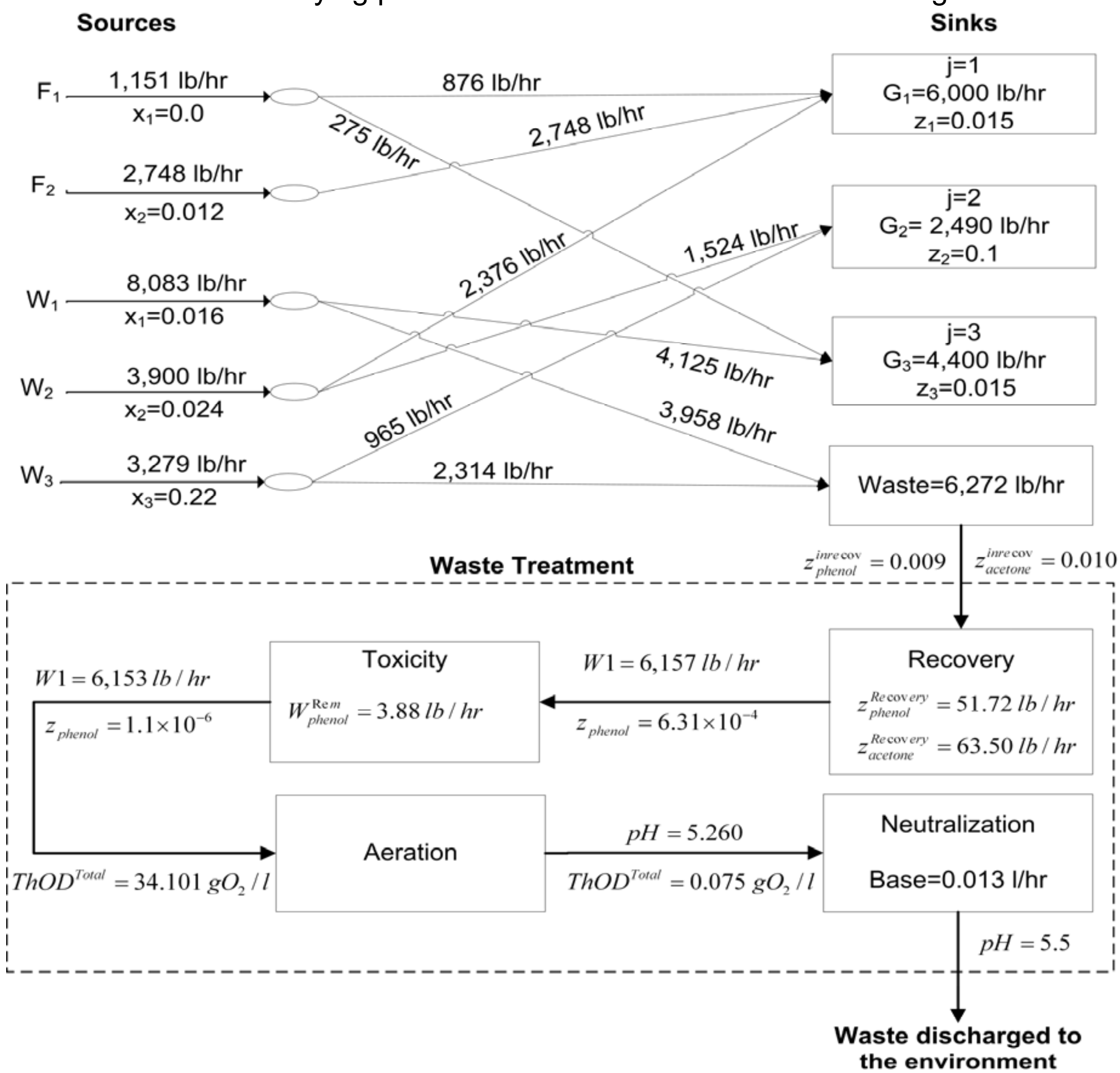

Figure 3. Mass integration including waste treatment process (solution B)

This example has shown that if one does not consider the waste treatment cost to satisfy the environmental regulations as part of the mass integration problem, the model can lead to sub-optimum solutions. We have shown in this paper how a simultaneous model can be formulated, which provides a better basis for the optimization of these types of systems.

Conclusions

A new framework has been introduced to (1) integrate the design of in-plant recycle/reuse networks with the end-of-pipe waste treatment facilities, (2) consider composition- and property-based constraints and process models. An optimization formulation has been developed to implement the devised framework. The model is based on disjunctive programming, and considers the technologies that are commonly used to treat wastewater streams so that they meet environmental regulations. The model is formulated with linear relationships within each one of the disjunctions, which aids its numerical solution. In addition to standard mass balance and composition constraints, the model incorporates property-based models, property mixing rules, and environmental constraints based on properties such as toxicity, theoretical oxygen demand, *pH*, color, and odor, and it is generalized to any other property that may cause pollution. The methodology has also shown how property integration can be used for cases in which a given property is difficult to estimate when there are many compounds in a waste stream. The formulation results in an MINLP model, which has been used to minimize the total annual cost of the system. The solution of the proposed model shows that the simultaneous consideration of mass and property integration and the tradeoff between in-plant recycle/reuse with wastewater treatment sections can yield important economic savings. The model did not show any numerical problems, and the CPU times required for the solution of the solutions of the example problem were relatively small.

Table 4. Comparison of results

Concept	With process constraints (Solution A)	With process and environmental constraints (Solution B)
Waste [lb/hr]	6,969	6,273
Fresh sources cost [$/yr]	15,146	14,318
Piping cost [$/yr]	26,669	31,128
Recovery cost [$/yr]	*61,859*	43,661
Toxicity cost [$/yr]	*7,226*	5,098
Aeration cost [$/yr]	*161,083*	43,363
Neutralization cost [$/yr]	*4,567*	3,237
Total process costs [$/yr]	41,816	45,446
Total waste treatment costs [$/yr]	*134,734*	95,360
TAC [$/yr]	*176,550*	140,807

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