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A Property-Based Approach to the Synthesis of Material Conservation Networks with Economic and Environmental Objectives

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This article presents a multiobjective optimization model for the recycle and reuse networks based on properties while accounting for the environmental implications of the discharged wastes using life-cycle assessment. The economic objective function considers fresh sources and treatment costs, whereas the environmental objective function is measured through the eco-indicator 99. The model considers constraints in the process sinks as well as in the environment based on stream properties such as pH, chemical oxygen demand, toxicity, density, and color, in addition to the composition of the waste streams. A global optimization procedure is developed by indirectly tackling properties through property operators and by segregating the process streams before treatment. Three examples are included, and the results show that it is possible to consider simultaneously the trade-offs between the total annual costs and the overall environmental impact using the proposed methodology. © 2010 American Institute of Chemical Engineers *AIChE J,* 57: 2369–2387, 2011
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Introduction

The proper use of resources is one of the major concerns of the chemical industry. Resources in the form of mass and energy constitute the main raw materials for the industry that impact the processes both economically and environmentally. A good number of methodologies have been reported to address the problem of the efficient use of energy as a response to the energy crisis of the last decades of the 20th century, such as those related to the synthesis of heat exchanger networks.[1] Based on reported principles for energy integration, mass integration strategies for the reuse of wastewater streams have been proposed aiming to minimize the use of fresh streams and the amount of wastewater discharged to the environment.[2] Particularly, the synthesis of recycle and reuse mass integration networks constitutes a powerful tool that enables the simultaneous minimization of fresh water usage and wastewater discharge. As an example of the mass integration advantages, Figure 1a shows a flow sheet for a process without integration, and Figure 1b shows

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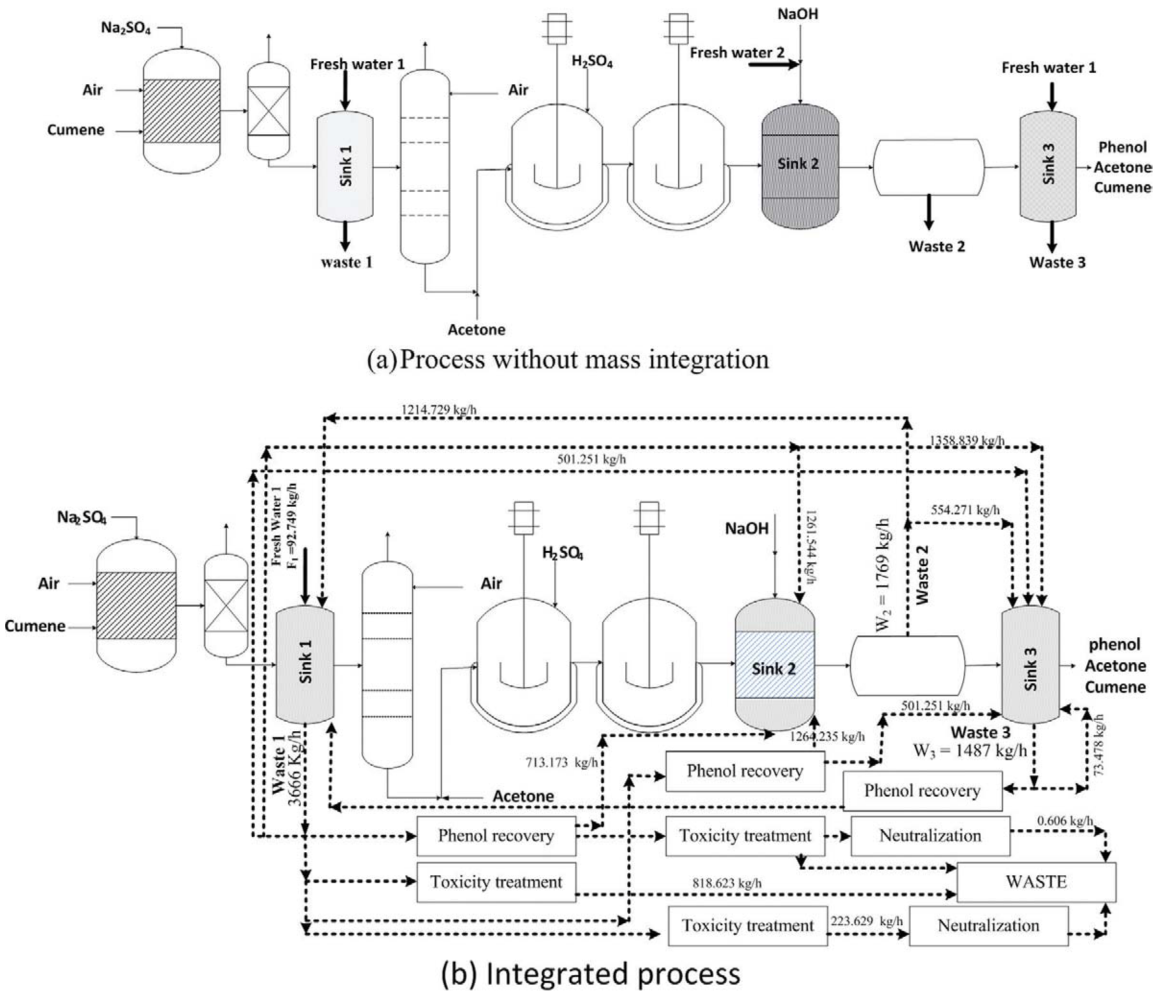

Figure 1. Some effects of mass integration within a process.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

the same process integrated to reduce the consumption of fresh sources while also reducing the wastewater discharged to the environment.

Several techniques have been reported for the synthesis of mass integration networks. The articles by Foo,[3] Bagajewicz and Faria,[4] and Dunn and El-Halwagi[5] present reviews on the methodologies for the synthesis of recycle and reuse mass integration networks. These methodologies can be classified as techniques that make use of graphical approaches,[6–12] algorithmic or algebraic techniques,[13–19] and formulations based on mathematical programing models.[20–28] Another set of articles based on mathematical programing approaches to address the problem of wastewater treatment system have also been proposed.[29–35]

Early mass integration methodologies were based on stream compositions. Nonetheless, there are many wastewater streams that are characterized by properties in addition to concentrations. These problems can be effectively addressed by the property-integration framework defined by El-Halwagi et al.[36] as "a functionality-based holistic approach for the allocation and manipulation of streams and processing units, which is based on functionality tracking, adjustment, and assignment throughout the process." Using the property balance approach of Shelley and El-Halwagi[37] and El-Halwagi et al.,[36] Qin et al.[38] and Ng et al.[39] developed algebraic techniques for property-based recycle networks. Kazantzi and El-Halwagi[40] introduced a graphical property-based pinch analysis for material recovery. Ponce-Ortega et al.[41,42] developed property-based formulations for the optimization of direct recycle–reuse networks together with wastewater treatment processes to satisfy given sets of process constraints and environmental regulations. In those works, several properties such as pH, toxicity, chemical oxygen demand (COD), color, and odor were considered in addition to composition constraints. Recently, Nápoles-Rivera et al.[43] have developed a model for the optimal design of mass and property integration networks including property interceptors within the structure of the networks and used a global optimization approach to handle the bilinear terms of the model as part of a global optimization approach.

Many of the solutions provided by existing mass integration methodologies give important contributions, such as solutions that minimize the consumption of fresh sources and the wastewater discharged to the environment. If one considers a broader view, however, one may find that such solutions may pose additional environmental burdens somewhere else in the life cycle. For example, the treatment units required for the process sources may increase the pollution to the environment, or the use of one type of fresh source may reduce the pollution in the plant, but the pollution to treat that fresh source may be higher than the one avoided in the plant. In this context, an overall approach that combines economic and environmental impacts (EIs) is particularly useful. Life-cycle assessment (LCA) provides a useful tool to evaluate the overall environmental loads associated with a process, product, or activity that identifies and quantifies the materials and energy used as well as the wastes released to the environment.[44] The articles by Azapagic and Clift,[45] Alexander et al.,[46] Hoffmann et al.,[47] Chen and Shonnard,[48] Hugo and Pistikopoulos,[49] Guillén-Gosalbez et al.,[50] and Gebreslassie et al.[51] present some applications of the LCA methodology for some chemical process design problems to improve their environmental performance. Recently, some articles have been reported to address the problem of the design of supply chain considering economic and environment concerns.[52,53] In the context of water integration, Ku-Pineda and Tan[54] presented a case of study to integrate the water pinch technique and the sustainable process index using the LCA technique to analyze different scenarios for the fresh water consumption. Tan et al.[55] proposed a mixed-integer linear programing model to minimize the total resource consumption impact (based on the idea of emergy) of a water recycle/reuse network. Lim and Park[56] presented a study to illustrate the necessity of the cooperation of industrial plants to reduce the total carbon footprint of their water supply systems. Another set of articles have been reported that include environmental aspects for the synthesis of water networks systems.[57–62]

This article presents a multiobjective optimization model for the design of property-based recycle and reuse networks considering simultaneously economic and EIs. The economic objective function considers the fresh sources costs, the treatment costs, and the piping costs, whereas the environmental objective function is measured through the eco-indicator 99, which is based on the LCA methodology. The problem consists then in a multiobjective mixed-integer nonlinear programing model (moMINLP).

Problem Statement

The problem addressed in this article is defined as follows. Given are (a) A set of waste streams, with known flow rates and properties such as pH, toxicity, color, density, COD, viscosity, and composition of specific components that can be measured directly; (b) a set of process equipments that require a specific amount of raw material with limits on the property levels that they can process; (c) a set of environmental regulations for waste streams; such constraints are given as limits on the properties of the waste stream discharged to the environment; and (d) a set of fresh sources with different purities and costs that can be used to satisfy the process and environmental constraints. The problem consists in finding the recycle and reuse network that optimizes a combined objective of the total annual cost (TAC) and the EI as accounted for by an LCA, while satisfying the given sets of process requirements and environmental constraints.

Outline of the Model

The following sets are used in the model formulation. NSINKS, NSOURCES, and NFRESH are sets for process sinks, process sources, and the fresh sources, respectively. INT^p is a set for the interceptors used for property p, whereas NPROP is a set for properties. Indices i, j, r, and p are used to denote the process sources, the process sinks, fresh sources, and properties, respectively. All the symbols used are defined in the nomenclature section.

As an example of the model formulation, Figure 2 shows the proposed superstructure for the recycle and reuse mass integration for two process sources, two sinks, and two properties to be intercepted. It is noted that each process source is segregated and sent without mixing to an available set of interceptors INT^1 that treat property 1. The optimization process must select the flow rate of each process source that is sent to each type of interceptor to treat such property. To model the case when property 1 does not require any treatment, an interceptor with a conversion factor of zero is used (which is modeled as the last one to treat the property). Then, each flow rate that exits the set of interceptors for property 1 is segregated and sent to the set of interceptors that treat property 2, without mixing with other streams. A similar approach is used for the remaining properties that may be treated. This configuration avoids mixing balances that yield bilinear nonconvex terms. In the last set of treatment units, the exit flow rate is segregated and sent to the process sinks or to the waste stream discharged to the environment. To satisfy the constraints for the process sinks, treated or nontreated process sources or fresh sources can be used. Therefore, the flow rates within the interception network as well as the flow rates for the fresh sources are optimization variables.

To model the property interceptors for the process sources, a conversion factor is used. This conversion factor depends on the design and operating variables for each interceptor, and it should be known before the optimization task. As a consequence, the properties at the exit of each interceptor for each process source can be directly determined, with the optimization variables being the flow rates for each interceptor. The following equation is used to determine the properties at the exit of each interceptor for each process source as a function of the extent of change in each property:

$$P_{i,p}^{\mathrm{OutPIN}} = f\left(P_{i,p}^{\mathrm{InSource}}, \text{design variables, operating variables}\right), \quad i \in N\mathrm{SOURCES},\ p \in N\mathrm{PROP}. \quad (1)$$

Model Formulation

The equations are given as follows.

Splitting of the fresh sources

Fresh sources can be segregated and directed to the process sinks but not to the waste stream.

$$F_r = \sum_{j \in N\mathrm{SINKS}} f_{r,j}, \quad r \in \mathrm{FRESH}. \quad (2)$$

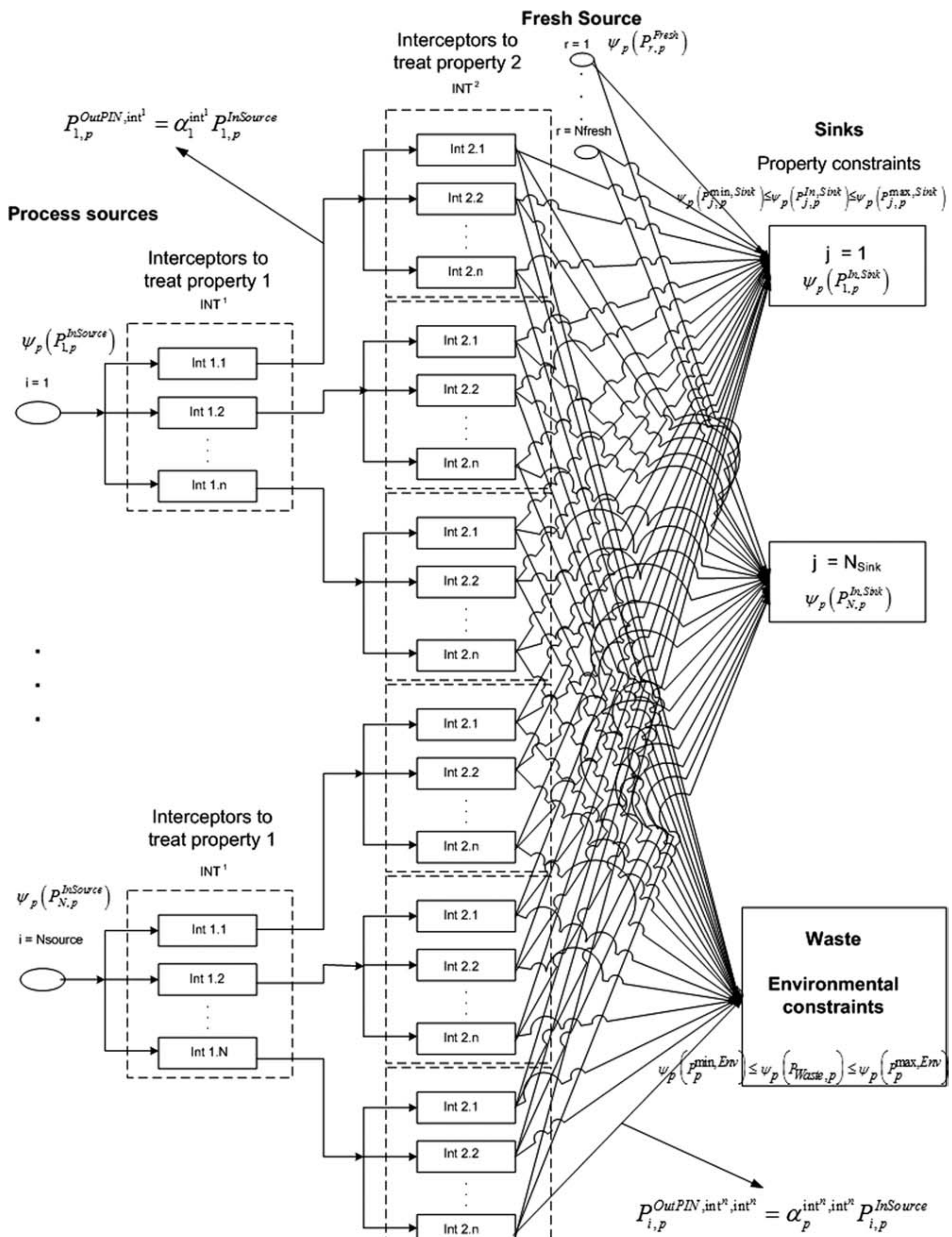

Figure 2. Superstructure for the recycle and reuse network for two process sources, two sinks, and two intercepted properties.

Splitting of the process sources sent to the property interceptors

For each process source, the flow rate can be segregated and sent to any interceptor to treat property 1 as follows:

$$W_i = \sum_{\mathrm{int}^1 \in \mathrm{INT}^1} w_i^{\mathrm{int}^1}, \quad i \in N\mathrm{SOURCES}. \tag{3}$$

For each process source at the exit of each interceptor that treats property 1, the flow rate is segregated and directed to the set of interceptors to treat property 2:

$$w_i^{\mathrm{int}^1} = \sum_{\mathrm{int}^2 \in \mathrm{INT}^2} w_i^{\mathrm{int}^1,\,\mathrm{int}^2}, \quad i \in N\mathrm{SOURCES},\ \mathrm{int}^1 \in \mathrm{INT}^1. \tag{4}$$

Similar balances are required for each process source at the exit of any interceptor to treat any property; the balance for the last set of interceptors is as follows:

$$w_i^{int^1,\mathrm{int}^2,\ldots,\mathrm{int}^{N-1}} = \sum_{\mathrm{int}^N \in \mathrm{INT}^N} w_i^{\mathrm{int}^1,\,\mathrm{int}^2,\ldots,\mathrm{int}^N},$$
$$i \in N\mathrm{SOURCES},\ \mathrm{int}^1 \in \mathrm{INT}^1, \ldots, \mathrm{int}^{N-1} \in \mathrm{INT}^{N-1}. \tag{5}$$

Splitting of the sources at the exit of the property interception network

Each process source from the last property interceptor can be segregated and sent to the process sinks and to the waste stream as follows:

$$w_i^{\mathrm{int}^1,\ldots,\mathrm{int}^N} = \sum_{j\in \mathrm{SINKS}} g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} + g_{i,\mathrm{waste}}^{int^1,\ldots,\mathrm{int}^N},$$
$$i \in N\mathrm{SOURCES},\ \mathrm{int}^1 \in \mathrm{INT}^1,\ldots,\mathrm{int}^N \in \mathrm{INT}^N. \quad (6)$$

Overall mass balance at the mixing point before any sink

The inlet mass flow rate to each process sink is equal to the sum of the flow rate from any interceptor plus the fresh sources:

$$G_j = \sum_{i\in N\mathrm{SOURCES}} \sum_{\mathrm{int}^1} \cdots \sum_{\mathrm{int}^N} g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} + \sum_{r\in \mathrm{FRESH}} f_{r,j}, \quad j \in N\mathrm{SINKS}. \quad (7)$$

Property balances at the mixing point before any sink

In the context of property integration, property balances in the mixing point before the process sinks are required to determine the properties of the streams in the sinks. Such property balances are based on the mixing rules proposed by Shelley and El-Halwagi[37] and El-Halwagi et al.,[36] which make use of property operators ψ_p related to property values as shown in Table 1 for several properties. To have linear relationships, the property operators are treated as optimization variables (instead of the property values which can still be nonlinear functions) as follows:

$$\psi_p\left(P_{j,p}^{\mathrm{InSink}}\right)G_j = \sum_{i\in N\mathrm{SOURCES}} \sum_{\mathrm{int}^1} \cdots \sum_{\mathrm{int}^N} \left[\psi_p\left(P_{i,p}^{\mathrm{OutPIN},\mathrm{int}^1,\ldots,\mathrm{int}^N}\right) g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}\right] + \sum_{r\in \mathrm{FRESH}} \left[\psi_p\left(P_{r,p}^{\mathrm{InFresh}}\right) f_{r,j}\right], \quad j \in N\mathrm{SINKS}, p \in N\mathrm{PROP}. \quad (8)$$

Mass balance for waste streams

The waste stream is calculated as follows:

$$\mathrm{waste} = \sum_{i\in N\mathrm{SOURCES}} \sum_{\mathrm{int}^1} \cdots \sum_{\mathrm{int}^N} g_{i,\mathrm{waste}}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}. \quad (9)$$

Property balances for waste streams

To determine the property operators (related to the stream properties) of the waste stream discharged to the environment, the following equation is used:

$$\psi_p\left(P_{\mathrm{waste},p}\right)\mathrm{waste} = \sum_{i\in N\mathrm{SOURCES}} \sum_{\mathrm{int}^1} \cdots \sum_{\mathrm{int}^N} \left(\psi_p\left(P_{i,p}^{\mathrm{OutPIN},\mathrm{int}^1,\ldots,\mathrm{int}^N}\right) g_{i,\mathrm{waste}}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}\right), \quad p \in N\mathrm{PROP}. \quad (10)$$

Table 1. Some Mixing Property Operators

Property	Operator
Composition or concentration	$\psi_z(z) = z$
Toxicity	$\psi_{\mathrm{Tox}}(\mathrm{Tox}) = \mathrm{Tox}$
Chemical oxygen demand	$\psi_{\mathrm{COD}}(\mathrm{COD}) = \mathrm{COD}$
pH	$\psi_{\mathrm{pH}}(\mathrm{pH}) = 10^{\mathrm{pH}}$
Density	$\psi_\rho(\rho) = \frac{1}{\rho}$
Viscosity	$\psi_\mu(\mu) = \log(\mu)$
Reid vapor pressure	$\psi_{\mathrm{RVP}}(\mathrm{RVP}) = \mathrm{RVP}^{1.44}$
Electric resistivity	$\psi_R(R) = \frac{1}{R}$
Paper reflectivity	$\psi_{R_\infty}(R_\infty) = R_\infty^{1/5.92}$
Color	$\psi_{\mathrm{Color}}(\mathrm{Color}) = \mathrm{Color}^{0.606}$
Odor	$\psi_{\mathrm{Odor}}(\mathrm{Odor}) = \mathrm{Odor}$
Absorption coefficient	$\psi_{\mathrm{Odor}}(k) = k$

Process sink constraints

Process sinks have limits on the properties, which are modeled in terms of the property operators as follows:

$$\psi_p\left(P_{j,p}^{\mathrm{min,Sink}}\right) \le \psi_p\left(P_{j,p}^{\mathrm{InSink}}\right) \le \psi_p\left(P_{j,p}^{\mathrm{max,Sink}}\right),$$
$$j \in N\mathrm{SINK},\ P \in N\mathrm{PROP}. \quad (11)$$

Environmental constraints

The environmental constraints for the waste discharged to the environment are given in terms of limits for the property operators as follows:

$$\psi_p\left(P_{j,p}^{\mathrm{min,Env}}\right) \le \psi_p\left(P_{\mathrm{waste},p}\right) \le \psi_p\left(P_{j,p}^{\mathrm{max,Env}}\right), \quad P \in N\mathrm{PROP}. \quad (12)$$

Objective function

The objective function consists in the minimization of the TAC of the recycle and reuse network and the whole EI that the implementation of the network produces:

$$\min\ Z = (\mathrm{TAC}; \mathrm{EI}) \quad (13)$$

It is noteworthy that the minimization of the TAC does not correspond to the minimum EI; therefore, the solution to this problem consists of a set of Pareto optimal solutions, as illustrated in Figure 3.

Economic objective function

The economic objective function considers the minimization of the TAC, which consists of the cost for the fresh sources and treatment units for waste streams

$$\mathrm{TAC} = H_Y \sum_{r\in \mathrm{FRESH}} \mathrm{Cost}_r^{\mathrm{Fresh}} F_r + H_Y \sum_{i\in N\mathrm{SOURCES}} \times \left(\sum_{\mathrm{int}^1\in \mathrm{INT}^1} \left(\mathrm{Cost}_p^{\mathrm{int}^1} w_i^{\mathrm{int}^1} + \cdots \sum_{\mathrm{int}^N\in \mathrm{INT}^N} \left(\mathrm{Cost}_p^{\mathrm{int}^N} w_i^{\mathrm{int}^1,\ldots,\mathrm{int}^N}\right)\right)\right). \quad (14)$$

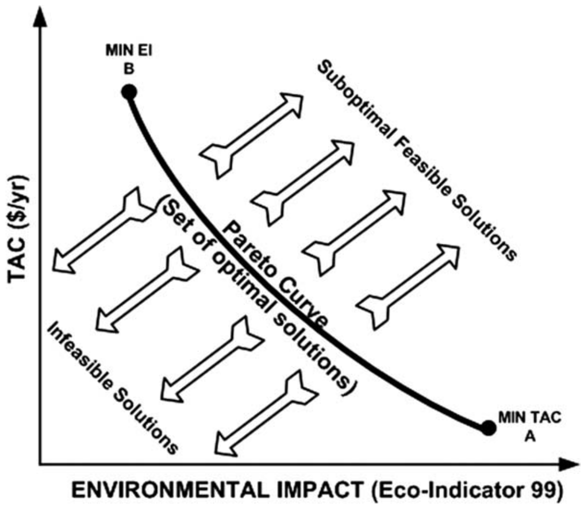

Figure 3. Schematic representation of the Pareto curve solutions.

Notice that this relationship is linear, and that the cost for the treatment units is calculated based on the property to be treated and an associated conversion factor.

Environmental objective function

The EI is measured through the eco-indicator 99, which is based on the methodology of the life cycle analysis[63] and is stated as follows:

$$\text{Eco Indicator} = \sum_{b}\sum_{d}\sum_{k\in K(d)} \delta_d \omega_d \beta_b \alpha_{b,k},$$

where β_b represents the total amount of chemical b released per unit of reference flow due to direct emissions, $\alpha_{b,k}$ is the damage caused in category k per unit of chemical b released to the environment, ω_d is a weighting factor for damage in category d, and δ_d is the normalization factor for damage of category d.

In the eco-indicator 99 methodology, 11 impact categories are considered:[63]

1. Carcinogenic effects on humans
2. Respiratory effects on humans that are caused by organic substances
3. Respiratory effects on humans caused by inorganic substances
4. Damage to human health that is caused by climate change
5. Human health effects that are caused by ionizing radiations
6. Human health effects that are caused by ozone layer depletion
7. Damage to ecosystem quality that is caused by ecosystem toxic emissions
8. Damage to ecosystem quality that is caused by the combined effect of acidification and eutrophication
9. Damage to ecosystem quality that is caused by land occupation and land conversion
10. Damage to resources caused by the extraction of minerals
11. Damage to resources caused by extraction of fossil fuels.

These 11 categories are aggregated into three major damages categories: (1) human health, (2) ecosystem quality, and (3) resources depletion. The human health damage is measured in terms of disability adjustment life years (DALYs); a damage of 1 DALY means that 1 life year of one individual is lost. The ecosystem quality damage measures the potential disappear fraction of species (PDF); a damage of 1 PDF means that all species disappear from 1 m^2 in 1 year. Finally, the damage to resources is measured in megajoules of surplus energy (MJ); a damage of 1 MJ means that 1 additional MJ will be required to accomplish further extraction of the same resource.

The damage factors for specific chemicals released to the environment have been reported in several databases, and these data are used in this article.[63] In addition, there are three normalization models called Egalitarian (for long-time perspective), Individualist (for short-time perspective), and Hierarchical perspective (balance time perspective). Four versions for the weighting methods are available, one that averages all penalties, and three versions for subgroups.

In this work, the EI objective function considers the categories affected by the release of pollutants to the ecosystem for the burdens obtained by the use of fresh sources, the burdens for the treatment units, and the burdens caused by the wastewater discharged directly to the environment. The production of fresh sources has several burdens (e.g., use of energy for transportation, extraction, etc.) that need to be quantified to determine the eco-indicator 99 per unit of mass for each fresh source. To operate each treatment unit, a set of burdens are required for the use of energy, solvents, etc., and one needs to quantify all of the burdens associated with the treatment unit per unit of mass to determine the unitary eco-indicator. For the wastewater discharged to the environment, the eco-indicator 99 per unit of mass is calculated according to the hazardous components present in the wastewater stream discharged to the environment. The life-cycle analysis methodology reported by Geodkoop and Spriensma[63] is used to determine the eco-indicators for each part of the mass integration networks, which depend on the quality of the wastewater streams. The following EI objective function is then formulated

$$\begin{aligned}
\text{EI} = {} & H_{\text{Y}} \sum_{b\in N\text{COMP}} \left(\text{waste } z_b \text{ Eco Indicator}_b^{\text{waste}}\right) \\
& + H_{\text{Y}} \sum_{r\in N\text{FRESH}} \left(F_r \text{ Eco Indicator}_r^{\text{fresh}}\right) \\
& + H_{\text{Y}} \sum_{i\in N\text{SOURCES}} \sum_{\text{int}^1\in \text{INT}^1} \left(w_i^{\text{int}^1} \text{Eco Indicator}_{\text{int}^1}^{\text{treatment}}\right) \\
& + H_{\text{Y}} \sum_{i\in N\text{SOURCES}} \sum_{\text{int}^1\in \text{INT}^1} \sum_{\text{int}^2\in \text{INT}^2} \left(w_i^{\text{int}^1,\text{int}^2} \text{Eco Indicator}_{\text{int}^2}^{\text{treatment}}\right) \\
& \vdots \\
& + H_{\text{Y}} \sum_{i\in N\text{SOURCES}} \sum_{\text{int}^1\in \text{INT}^1} \sum_{\cdots} \cdots \sum_{\text{int}^N\in \text{INT}^N} \\
& \qquad \times \left(w_i^{\text{int}^1,\cdots,\text{int}^N} \text{Eco Indicator}_{\text{int}^N}^{\text{treatment}}\right), \qquad (15)
\end{aligned}$$

where Eco-Indicator$^{\text{waste}}$, Eco-Indicator$^{\text{fresh}}$, and Eco-Indicator$^{\text{treatment}}$ are the eco-indicators 99 calculated for the waste

Table 2. Stream Data for Example 1

Sources i	F (kg/h)	Z_{phenol} (ppm)	$Z_{acetone}$ (ppm)	Z_{cumene} (ppm)	Tox (%)	pH	COD (mg O_2/l)	Color	ρ (kg/m^3)	μ (cP)
Process Sources										
1	3666	0.016	$1.071E - -9$	$1.6281E - 4$	0.3	5.4	0.187	0.0003	907.19	1.256
2	1769	0.024	0.01676	0.0367	0.5	5.1	48.85	0.0009	1001.53	1.220
3	1487	0.220	0.0009916	$6.4599E - 5$	1.5	4.8	92.100	0.0002	1065.94	1.201
Fresh Sources										
1	–	0	0	0	0	7.0	0	0	999.72	1.002
2	–	0.010	0	0	0.1	7.1	0.010	0.0001	1001.99	0.992

released to the environment, production of fresh sources, and operation for the treatment units calculated following the life-cycle analysis methodology.

Solution Strategy

The multiobjective optimization problem addressed in this article has two objective functions (TAC and EI) that are in conflict with each other. In the Pareto curve (see Figure 3), the set of optimal solutions that compromises both objective functions can be identified. To determine the Pareto curve, the constraint method is used in this article,[64] in which the multiobjective problem is transformed into a series of single-objective optimization problems. In this case, the problem is solved without considering the EI objective function, i.e., minimizing only the TAC (Solution A). Then, the problem is solved minimizing the EI without considering the TAC (solution B). Solutions A and B correspond to two extreme solutions, Solution A yields the solution with the maximum EI and Solution B yields the solution with the minimum EI. Therefore, the interval for feasible values for EI has been determined, and the multiobjective problems can be solved for several single-objective constrained problems as follows:

$$\min\ \mathrm{TAC} \tag{16}$$

Subject to:

$$\mathrm{EI} \le \varepsilon \tag{17}$$

plus all the constraints given by Eqs. 2–15.

The single-objective problem is solved for several values of the parameter ε for values of EI between the maximum obtained from Solution A and the minimum obtained from Solution B to yield the Pareto frontier as shown in Figure 3; one can identify two regions, one above the Pareto curve that corresponds to feasible suboptimal solutions, and the other below the Pareto curve that corresponds to infeasible solutions. It is worth of notice that the Pareto curve corresponds to a set of optimal solutions from which the designer is able to select the one that he or she feels that provides a proper compromise between both objectives.

An alternative method can be used to determine a single solution in a straightforward way, which consists in the application of the Goal multiobjective optimization approach.[64] Here, the target for the TAC is identified from Solution A ($\mathrm{TAC}^{\min}$), and the target for the EI is obtained from Solution B ($\mathrm{EI}^{\min}$). The multiobjective problem is then transformed into the single-objective problem described as follows:

$$\min\ Z = \delta^{+}_{\mathrm{TAC}} + \delta^{+}_{\mathrm{EI}} + \delta^{-}_{\mathrm{TAC}} + \delta^{-}_{\mathrm{EI}} \tag{18}$$

Subject to:

$$\mathrm{TAC} - \mathrm{TAC}^{\min} = \delta^{+}_{\mathrm{TAC}} - \delta^{-}_{\mathrm{TAC}} \tag{19}$$

$$\mathrm{EI} - \mathrm{EI}^{\min} = \delta^{+}_{\mathrm{EI}} - \delta^{-}_{\mathrm{EI}} \tag{20}$$

plus all the constraints given by Eqs. 2–15.

In this problem, variables δ are deviations from the minimum values for the TAC and the EI. Notice that δ is restricted to have positive values, and that the objective problem is to determine the solution that minimizes the deviation from the minimum values for TAC and EI simultaneously.

Remarks

- The proposed model is quasi-linear; the only nonlinear term is given by the product of the property operator times the mass flow rate of the waste stream discharged to the environment in the left-hand side of Eq. 10. To address this bilinear term, the McCormick[65] relaxation and the spatial branch and bound approach proposed by Karuppiah and Grossmann[34] can be used.
- It is necessary to calculate the unitary eco-indicators for each specific case of study using the strategy of the eco-indicator 99 through the life-cycle analysis technique.

Table 3. Environmental Constraints for the Properties of Example 1

Property	Minimum	Maximum
z (ppm)	0	0.005
Tox (%)	0	0
pH	5.5	9
COD (mg O_2/l)	0	75
Color	0	300

Table 4. Conversion Factors and Costs for Interceptors

Property	Interceptor	Conversion Factor	Unitary Cost ($/kg)
z	REC^1	0.02	0.0143
	REC^2	0.15	0.0073
Toxicity	TOX^1	0.00	0.0216
	TOX^2	0.10	0.0165
COD	AER^1	0.20	0.0143
	AER^2	0.45	0.0071
pH	NEU^1	0.50	0.1389
	NEU^2	0.70	0.0397
	NEU^3	1.50	0.1433
	NEU^4	1.30	0.0419
Color	$COLOR^1$	0.10	0.1609
	$COLOR^2$	0.20	0.1345

Table 5. Process Sinks Constraints for Example 1

Sink j	G (kg/h)	$Z_{\text{phenol}}^{\min}$	$\text{pH}^{\min}$	$\text{pH}^{\max}$	$\rho^{\min}$ (kg/m^3)	$\rho^{\max}$ (kg/m^3)	$\mu^{\min}$ (cP)	$\mu^{\max}$ (cP)
1	2721	0.013	5.3	8.0	816	1270	0.900	1.202
2	1995	0.011	5.4	7.8	771	1113	0.905	2.230
3	1129	0.100	5.2	8.2	839	1315	0.903	1.260

• The superstructure formulation considers different options for the treatment of the process sources and the direct recycle of the process sources. To include the option of direct recycle, a set of interceptors with conversion factors and costs equal to zero are included. Such treatment units are fictitious, used to model the bypassing of streams as one way to implement the direct recycle structure.

Results

Three examples are used to show the applicability of the proposed methodology. These problems were implemented within the GAMS[66] software environment, with the CONOPT solver used to solve the NLP problems. For all examples, the operation time for (H_Y) was taken as 8000 h/year. The problems were solved in a computer with an i7 processor at 3.00 GHz with 9 MB of RAM.

For the three examples presented in this article, the performance for the treatment units is modeled as follows:

$$P_{i,p}^{\text{OutPIN},\text{int}^1,\ldots,\text{int}^N} = \left(\alpha_p^{\text{int}^1,\ldots,\text{int}^N}\right) P_{i,p}^{\text{InSource}},$$
$$i \in N\text{SOURCES}, p \in N\text{PROP}, \text{int}^1 \in \text{INT}^1, \ldots, \text{int}^N \in \text{INT}^N,$$

where α_p is a conversion factor used to treat property p. This conversion factor is known before the optimization process and it depends on the type of interceptor used.

Example 1

The data for this example are based on the process to produce phenol from cumene as reported by Hortua.[67] The process, shown in Figure 1a, has three waste streams, three equipments that require fresh sources, and two different types of fresh water. This process was selected because it has several toxic and hazardous compounds whose emissions impact directly human health, the ecosystem, and the extraction of natural resources. The waste streams contain several compounds (some of which are very toxic even at low concentration) making the mass integration based on properties a suitable method to address this problem. Table 2 shows the stream data for this example, including the flow rates and properties for the process and fresh sources, whereas Table 3 shows the environmental constraints for the properties of the waste stream discharged to the environment. The unit cost of fresh sources 1 and 2 is \$0.0198/kg and \$0.0162/kg, respectively. Table 4 shows the conversion factors and unit costs for each available treatment unit. It is worth noting that for each property there is a fictitious interceptor with conversion factor and cost equal to zero used to model bypassing streams. The process sinks requirements for this example are shown in Table 5.

The EI for this example depends on the waste stream discharged to the environment, which is constituted by several components (including acetone, cumene, and phenol, among others). It should be noticed that the direct discharge to the environment of these components impacts the human health even when limits given by the environmental regulation are satisfied. Another EI is the one caused by the use of fresh sources, which corresponds to CO_2 emissions produced from transportation as well as any treatment requirements (to calculate the eco-indicator for the use of fresh water, the entire life cycle is considered including piping, pumping, treatment, etc). Finally, four treatment options are considered for the treatment of the process sources. Solvent extraction facilities are available for the recovery of the hazardous compounds, aeration processes to fix the COD, neutralization process through additions of acid/base to fix the pH, and a secondary treatment unit for toxicity. The entire life-cycle process was analyzed to determine the eco-indicator for each treatment equipment.[63] Table 6 shows a summary of the normalized eco-indicator values for the waste discharged to the environment, fresh sources used, and treatment processes for the process sources (all given per 1 kg of stream). The eco-indicators for the fictitious treatment units were set equal to zero.

Figure 4 shows the network obtained for this example minimizing the TAC without considering the EI (i.e., solution corresponding to the maximum EI inside the optimal Pareto curve for this case of study). To minimize the annual cost, the impure, cheaper, fresh source is used; one can notice how the properties for the waste stream discharged to the environment are within allowable limits. Figure 5 shows the solution for the minimization of the EI without considering the TAC. This solution presents a reduction by 2.1% on the total waste discharged to the environment with respect to the solution of Figure 4, and, accordingly with the established objective function, the cleanest fresh source is selected in this case (with a reduction in total consumption of 21%). In both extreme cases, the properties of the waste stream discharged to the environment are at their upper limits. Three toxicity interceptors and one neutralization unit

Table 6. Eco-Indicators for the Burdens of Example 1

Concept	Eco-Indicator 99/kg	
Direct discharge	Phenol	0.10370
	Acetone	0.00530
	Cumene	0.02880
Fresh sources	Fresh 1	2.144E−5
	Fresh 2	9.02E−6
Recovery treatment	REC^1	0.05702
	REC^2	0.06578
Toxicity treatment	TOX^1	2.5E−1
	TOX^2	3.5E−1
Aeration treatment	AER^1	1.95E−5
	AER^2	2.5E−6
Neutralization treatment	NEU^1	6.11E−11
	NEU^2	7.436E−3
	NEU^3	1.27E−4
	NEU^4	8.92E−6

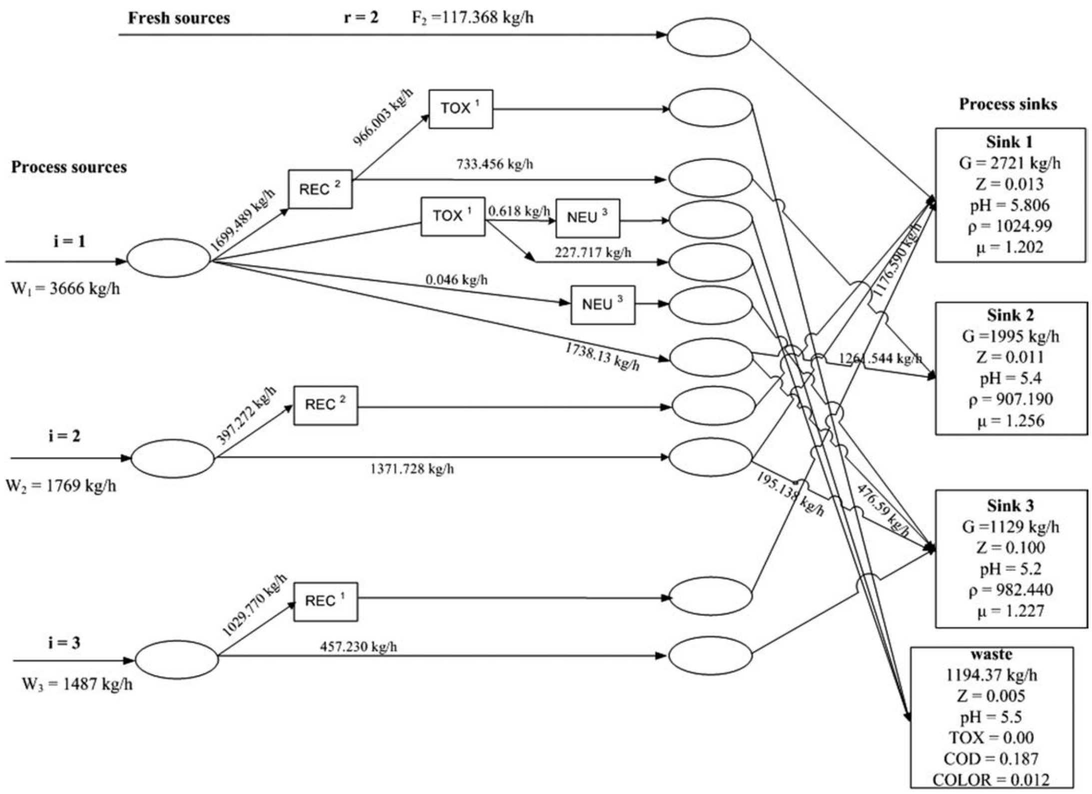

Figure 4. Solution for Example 1 minimizing only the total annual cost.

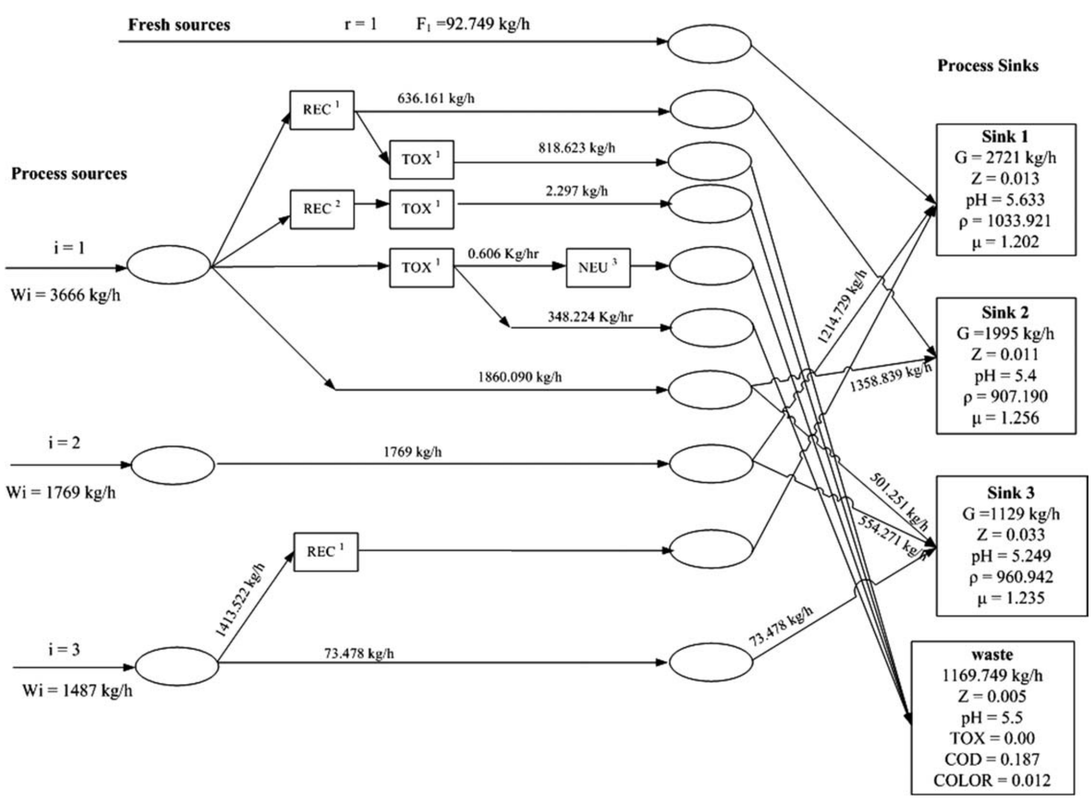

Figure 5. Solution for Example 1 minimizing only the environmental impact.

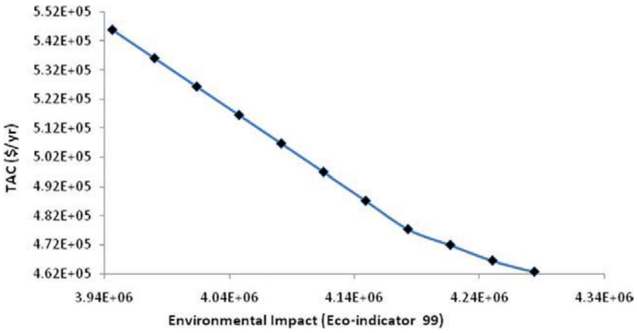

Figure 6. Pareto solutions for Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 7. Summary of Results for Example 1

Concept	Minimizing TAC	Minimizing EI	Goal Solution
F_1 (kg/h)	0	92.749	92.749
F_2 (kg/h)	117.368	0	0
Waste (kg/h)	1194.368	1169.749	1169.749
Fresh sources cost ($/year)	15210.869	14691.458	14691.458
Recovery cost ($/year)	240256.546	328268.215	260622.171
Toxicity treatment cost ($/year)	206386.758	202132.645	202132.645
Aeration cost ($/year)	0	0	0
Neutralization cost ($/year)	761.656	694.178	694.178
Eco-indicator 99	$4.2842E + 6$	$3.9463E + 6$	$4.1800E + 6$
Total annual cost ($/year)	462615.829	545786.496	478140.452

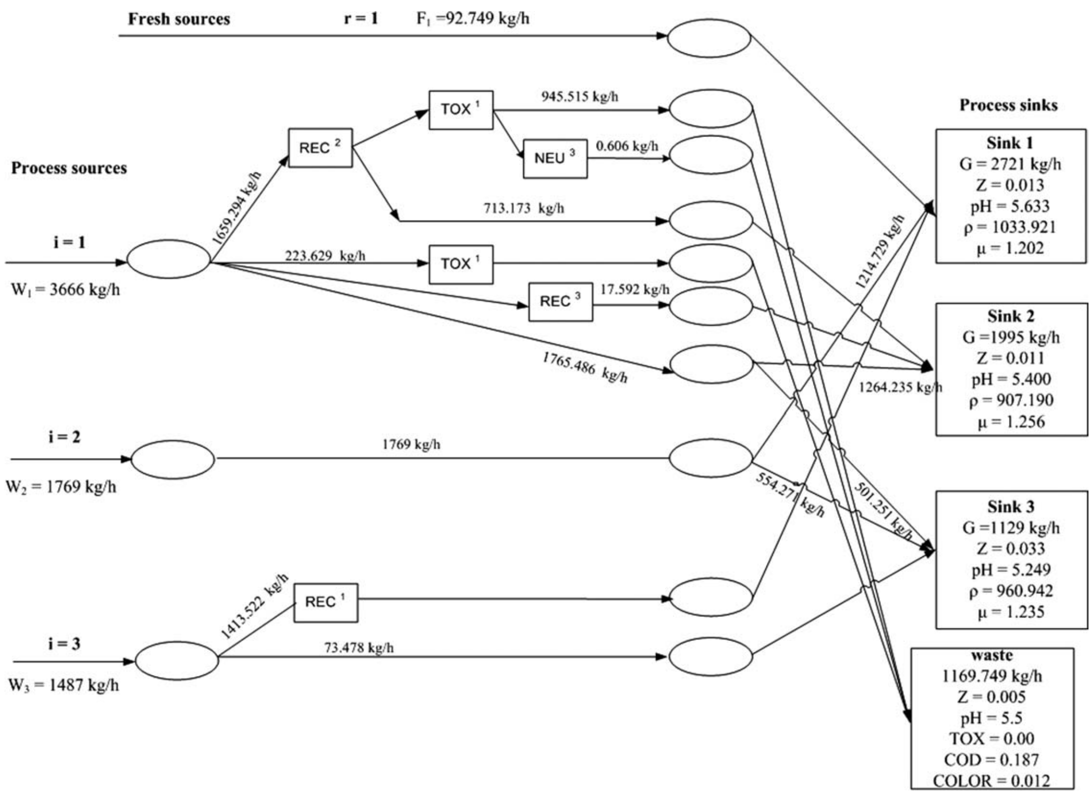

Figure 7. Optimal solution for Example 1 for the multiobjective problem obtained with the Goal method.

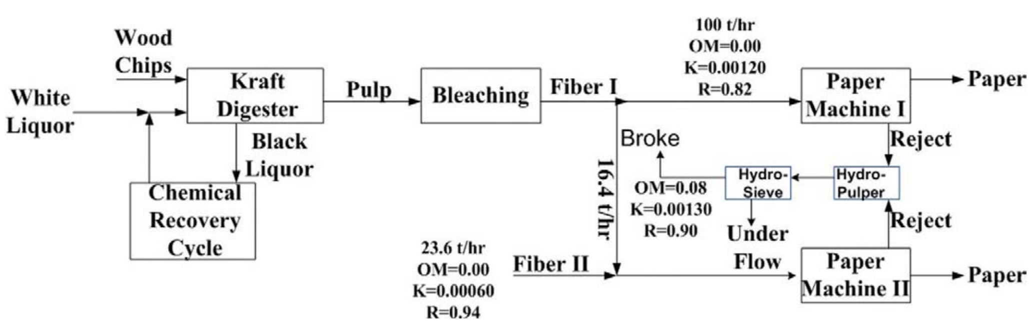

Figure 8. Process flow sheet for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 8. Constraints for the Sinks for Example 2

Property	Sink 1		Sink 2	
	Lower Limit	Upper Limit	Lower Limit	Upper Limit
Mass fraction	0.00	0.02	0.00	0
Absorption coefficient	0.0015	0.00125	0.00070	0.00125
Reflectivity	0.80	0.90	0.85	0.90
Flow rate (ton/h)	100	105	40	40

Table 9. Sources Data for Example 2

Source	Mass Fraction	k (m^2/g)	R_∞	Flow Rate (ton/h)	Cost ($/ton)
Waste	0.08	0.00130	0.90	30	0
Fiber 1	0.0	0.00120	0.82	–	21
Fiber 2	0.0	0.00060	0.94	–	40

Table 10. Eco-Indicators for the Burdens of Example 2

Concept	Eco-Indicator/kg	
Direct discharge waste	MO	1.31*E*6
Fresh sources	Fiber 1	0.37
	Fiber 2	0.1150
Recovery treatment	REC^1	1.37*E*−4
	REC^2	1.37*E*−3
Absorption treatment	ABS^1	2.5*E*−1
	ABS^2	3.5*E*−1
Reflectivity treatment	REF^1	1.95*E*−5
	REF^2	2.5*E*−6

Table 11. Conversion Factors and Costs for Interceptors for Example 2

Property	Interceptor	Conversion Factor	Unitary Cost ($/ton)
Material objectionable	REC^1	0.98	65
	REC^2	0.85	33
Absorption coefficient	$COEF^1$	0.93	98
	$COEF^2$	0.85	75
Reflectivity	REF^1	0.92	65
	REF^2	0.83	32

are required in the solution that minimizes EIs, as opposed to two of each suggested by the solution with minimum TAC. By applying the constraint multiobjective method, we obtained the optimal Pareto curve shown in Figure 6. It is worth noting that for the economic scenario considered in this case of study, the solutions with higher cost correspond to the solutions with lowest EI, and that the solutions with the lowest cost correspond to the highest EI. In addition, one can identify a set of solutions that compensate both objective functions, in which there is a relatively minor deviation on

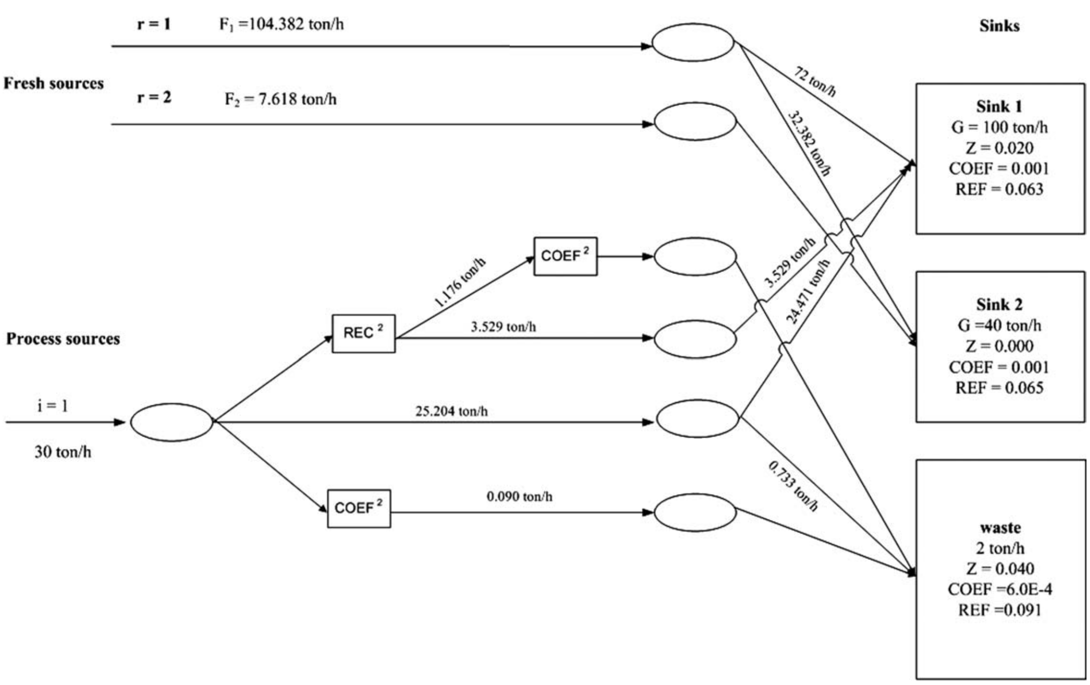

Figure 9. Solution for Example 2 minimizing only the total annual cost.

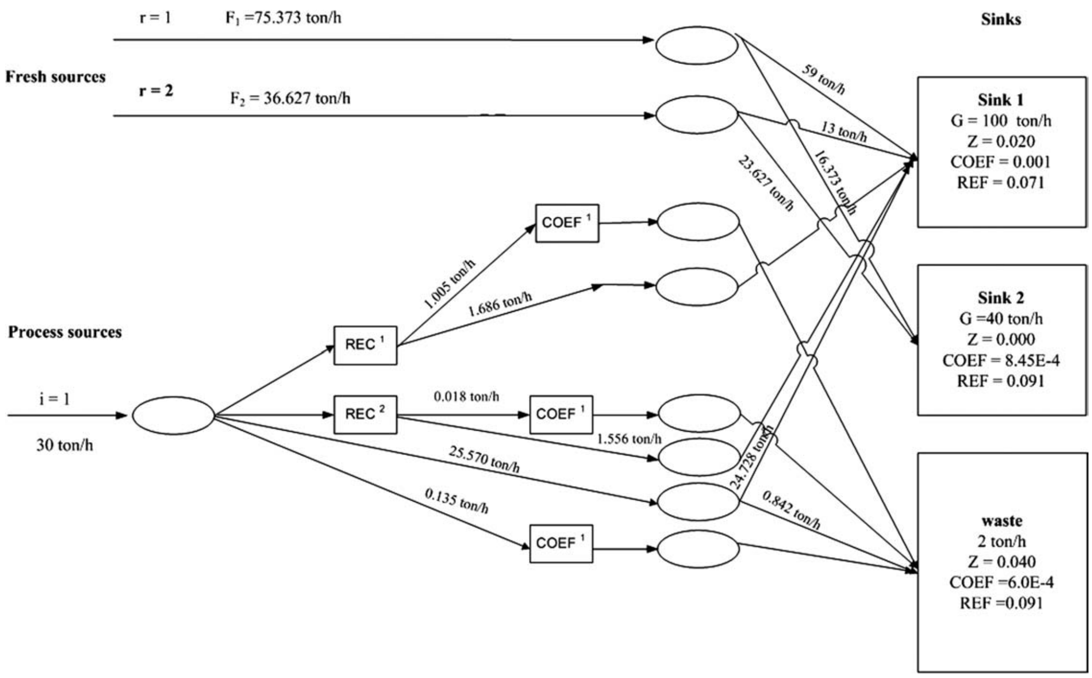

Figure 10. Solution for Example 2 minimizing only the environmental impact.

both objective functions with respect to their individual optimization. Finally, Figure 7 shows the solution for the multi-objective problem minimizing both the economic and environmental objective functions using the Goal method, and the resulting integrated process is shown in Figure 1b. It can be noticed that the fresh sources consumption (along with the selection of the cleanest type of fresh source available) and the amount of waste generated are the same as those in the solution with minimum EI, although the integration network is different. Six equipments for interception operations are used as opposed to seven of the minimum EI structure, with toxicity treatment carried out using one less unit. Table 7 shows a summary of results for the solutions identified for this problem; notice that the solution with the minimum cost has an EI 8.6% higher than the solution with the minimum EI, whereas the solution with the minimum EI has a cost increase by 18% with respect to the solution with the minimum TAC. The solution obtained with the Goal method, in which both objectives are considered simultaneously, represents an increase of 3.3 and 6.1% with respect to the minimum cost and minimum EI solutions, respectively. This set of Pareto optimal solutions could be a useful tool for the decision makers to select the best solution considering simultaneously both objectives. Finally, one may notice in the different solutions the existence of direct recycle streams (i.e., streams that are recycled to the process sinks without any treatment). Such streams were modeled using the fictitious treatment units in the superstructure of the interception network.

Example 2

This example is based on the pulp and paper process reported by El-Halwagi et al.[36] Figure 8 shows the flow sheet for the process where wood chips are chemically cooked in a Kraft digester using white liquor. The black liquor exit stream is converted back to white liquor, and the digested pulp is passed to a bleaching system to produce Fiber I. An external pulp called Fiber II is also available. Two different machines are used to produce two types of paper in Sinks I and II. The properties considered in this example are the following: (1) material objectionable (MO) that corresponds to the elements that need to be eliminated from the fiber, and it is expressed in terms of their total mass fraction, (2) reflectivity (R), and (3) absorption coefficient (k). Table 8 gives the requirements for the process sinks given in terms of property limits, and Table 9 lists the data for the process sources.

The life-cycle analysis methodology was applied to determine the eco-indicator 99 for the fresh sources, treatment facilities, and the waste components discharged to the environment. For the fresh sources (fibers), we need to consider from the initial stage corresponding to the tree cutting until the manufacturing of the fibers. The eco-indicator of the waste stream discharged to the environment was based on the stream components. Table 10 gives a summary of the eco-indicators used, and Table 11 shows the interceptor data for this example. It can be noticed that the three properties

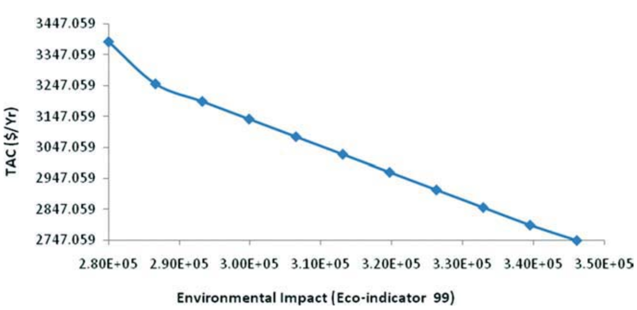

Figure 11. Pareto frontier for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

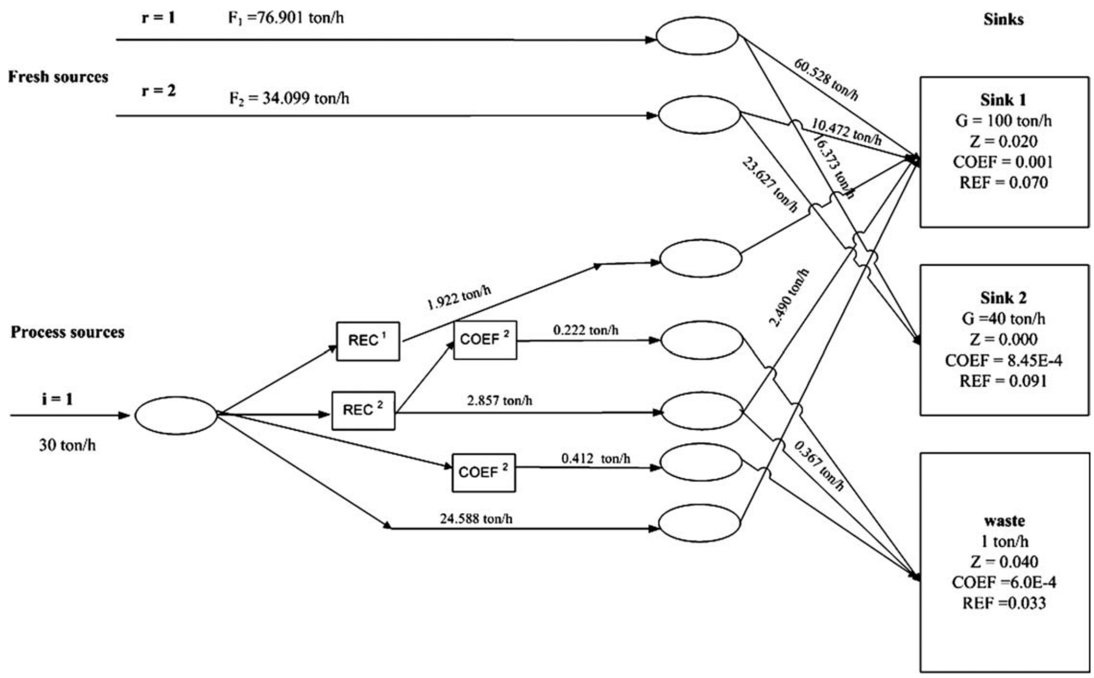

Figure 12. Optimal solution for Example 2 using the Goal method.

restricted by the sinks can be intercepted. A fictitious interceptor is again included for each property to model the bypass streams.

After the application of the proposed methodology, the solutions for the minimization of the total cost (Figure 9) and EI (Figure 10) were obtained. In this case, both extreme solutions use the same total quantity of fresh sources to yield a total waste of 2 ton/year; however, the solution for the minimum cost selects a higher quantity of the fresh source 1, along with the cheaper treatment units that have lower conversion factors. The Pareto frontier is shown in Figure 11, and Figure 12 shows the optimal solution obtained with the Goal methodology considering both objectives simultaneously. The solution for the Goal method consumes essentially the same amount and type of fresh sources as the solution for the minimum EI, and it requires one less interceptor unit. In addition, the solution for the Goal method yields a waste stream discharged to the environment with lower reflectivity than the other two extreme solutions.

Table 12 summarizes the results obtained for the cases of the minimization of the cost, the minimization of the EI, and the Goal solution. The solution with the minimum cost represents an increase in the EI by 23.6%, and the solution with the minimum EI represents an increase by 23.3% in the TAC. The solution obtained with the Goal approach represents increments by 18.4 and 2.37% for the TAC and EI, respectively. In this case, fresh sources yield the highest contribution to the TAC, and because the three solutions use the same overall amount of fresh sources, the main economic difference is due to type of fresh source selected in each of the three solutions.

Example 3

This example is a theoretical case study with six process sources and three fresh sources, as given in Table 13. This example is presented to show the applicability of the proposed methodology to a bigger problem. The unit costs for the three fresh sources are \$0.03/kg, \$0.02/kg, and \$0.01/kg. There are six process sinks with the characteristics and property requirements shown in Table 14. The properties intercepted in this example are the composition of hazardous chemicals, COD, pH, and toxicity. The available interceptors for this example are the same as the ones in Example 1 (see Table 4). For the EI, the eco-indicators 99 are shown in Table 15. Figure 13 shows the Pareto curve that was obtained with the application of the proposed methodology; this type of information (i.e., a set of optimal solutions that simultaneously compensate both objectives) should be of special value to decision makers.

Figures 14 and 15 show the solutions for the extremes of the Pareto curve that correspond to the minimum TAC and the minimum EI, respectively, while Table 16 reports a summary of results. Both extreme solutions use fresh source 1, but the solution for the minimum cost consumes 20% more. The waste generated by both solutions differs in only

Table 12. Results for Example 2

Concept	Minimum TAC	Minimum EI	Goal Solution
F_1 (ton/h)	104.364	75.373	76.901
F_2 (ton/h)	7.636	36.627	34.099
Waste (ton/h)	2.000	2.000	1.000
Fresh sources cost (\$/year)	2497.088	3047.912	2978.883
Recovery cost (\$/year)	155.294	227.808	226.505
Absorption treatment cost (\$/year)	95.023	113.482	47.511
Reflectivity treatment cost (\$/year)	0.00	0.00	0.00
Environmental impact (Eco-indicator 99/year)	346,010	$2.7989E+5$	$2.8651E+5$
Total annual cost	2747.405	3389.202	3252.899

Table 13. Stream Data for Example 3

Source i	F (Flow (kg/h))	Z (ppm)	Tox (%)	pH	COD (mg O_2/l)	ρ (kg/m^3)	μ (cP)
Process Sources							
1	2400	0.560	0.5	4.8	78.850	999.7	1.034
2	3800	0.970	0.9	4.7	89.210	1158	0.875
3	3500	0.590	0.7	5.2	105.408	563	1.241
4	1540	0.001	1.8	7.9	50.470	885	1.520
5	3950	0.045	5.4	8.2	20.587	932	0.987
6	2980	0.154	1.4	7.5	110.547	1062	1.201
Fresh Sources							
1	–	0.000	0.0	7.0	0.000	1000	1.002
2	–	0.010	0.1	6.8	0.010	1002	0.992
3	–	0.050	0.8	7.5	0.500	998	1.005

Table 14. Sinks Data for Example 3

Sink j	G (kg/h)	Z_i^{max}	pH^{min}	pH^{max}	ρ^{min} (kg/m^3)	ρ^{max} (kg/m^3)	μ^{min} (cP)	μ^{max} (cP)
1	1200	0.050	4.3	9.5	792	1338	0.840	1.204
2	2540	0.150	5.8	8.4	860	1304	0.740	1.340
3	985	0.015	6.8	7.9	914	1290	0.990	1.300
4	1570	0.001	4.5	7.5	728	1385	0.740	1.100
5	1150	0.010	5.6	8.4	850	1429	0.860	1.250
6	870	0.005	5.7	9.4	864	1304	0.820	1.350

1.4%. In this problem, the treatment costs are more important than the fresh sources cost, and one of the key properties to treat is the recovery of the hazardous materials. The results indicate that the solution with the minimum cost presents an increase in EI by 45.6%, whereas the solution for the minimum EI presents an increment in the TAC by 5.6%; this result shows that the major discrepancy between these two extreme solutions is in their EI. Figure 16 shows the solution obtained with the Goal method. The Goal solution presents a consumption of fresh source (Type 1) and treatment costs that are in between the values observed for the solutions with minimum cost and minimum EI, thus compensating both objectives. This aspect can be further noticed in Table 16; although the Goal solution uses the highest number of interceptor units (18), the increases in TAC and EI are only 1.15 and 0.5% with respect to networks with minimum TAC and minimum EI, respectively. Also, it can be noticed that the amount of waste generated by the Goal solution is practically the same as the one obtained in the solution with minimum EI.

Finally, Table 17 shows the problem size and the CPU time for the solution of each of the examples. It should be noticed that the number of variables and equations grow exponentially with the number of sources, sinks, and properties.

Conclusions

This work has introduced a property-based approach to the optimization of recycle/reuse networks while accounting for the EI of the discharged streams. A MINLP formulation has been proposed for the optimal design of the network, considering simultaneously the minimization of the TAC and an overall EI. The TAC included the costs of fresh sources and treatment units; for the EI, the burdens for the entire life cycle for the production of fresh sources, the waste released to the environment, and the effect of the treatment units were considered. The model formulation is based on stream properties in addition to compositions because many constraints for equipment operation and environmental

Table 15. Eco-Indicators for Example 3

Concept	Eco-Indicator/kg	
Direct discharge waste	Component 1	0.1037
Fresh sources	Fresh 1	2.1445E−5
	Fresh 2	9.02E−6
	Fresh 3	5.21E−5
Recovery treatment	REC^1	1.34E−4
	REC^2	1.37E−3
Toxicity treatment	TOX^1	2.5E−1
	TOX^2	3.5E−1
Neutralization treatment	NEU^1	6.11E−11
	NEU^2	8.7E−4
	NEU^3	1.27E−4
	NEU^4	8.92E−6
Aeration process	AER^1	1.95E−5
	AER^2	2.5E−6

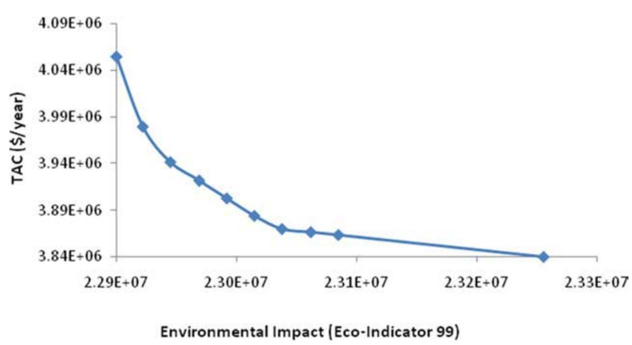

Figure 13. Pareto frontier for Example 3.

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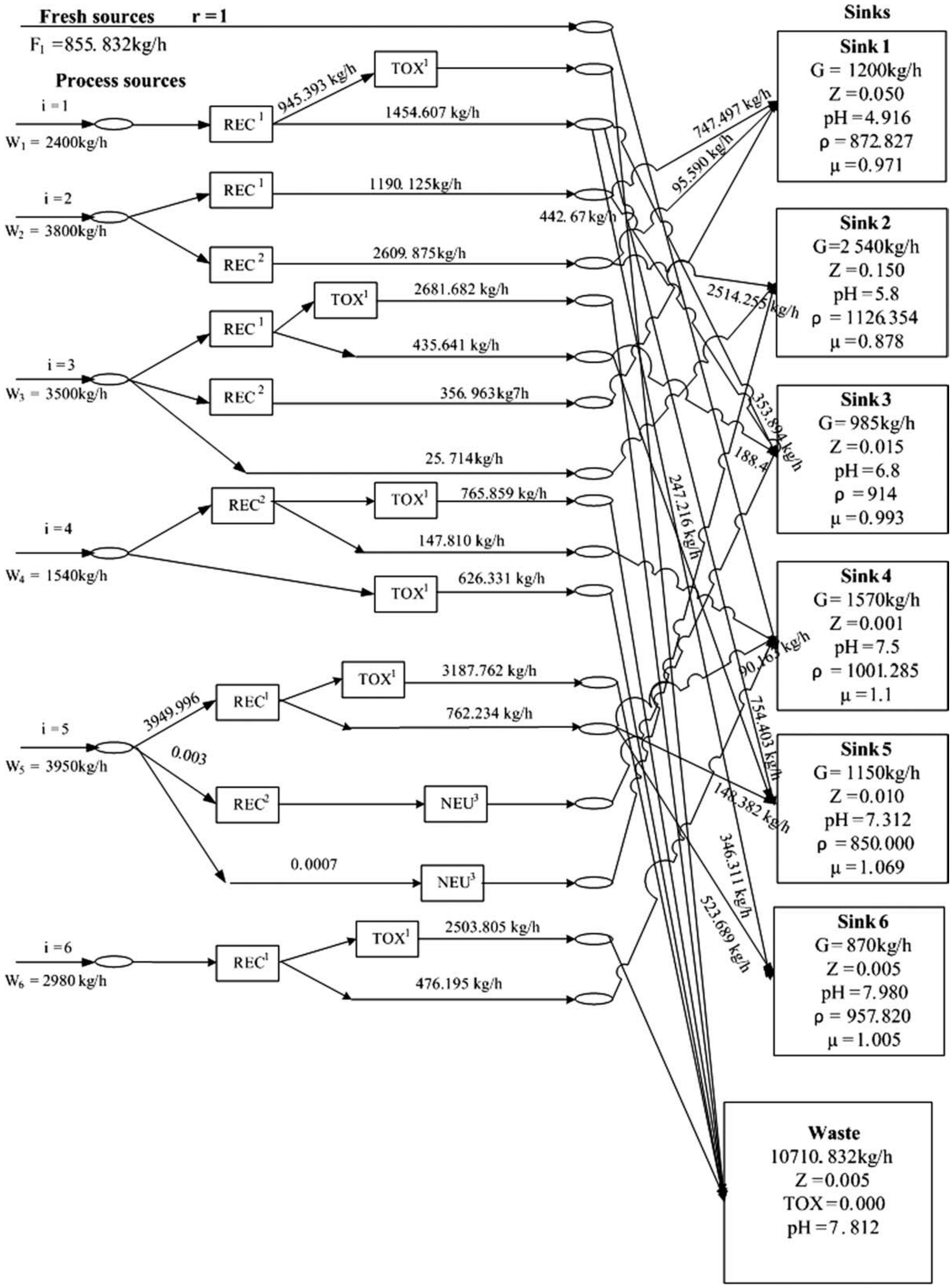

Figure 14. Solution for the minimum cost for Example 3.

regulations are given in terms of properties; also, tracking properties from composition data is a difficult task because of the large number of components typically present in waste streams. A superstructure is used as a basis for the optimization problem, and its formulation yields a quasi-linear model as a result of segregating the different process sources in the property interceptor network and using property operators as optimization variables. The solutions of the case studies

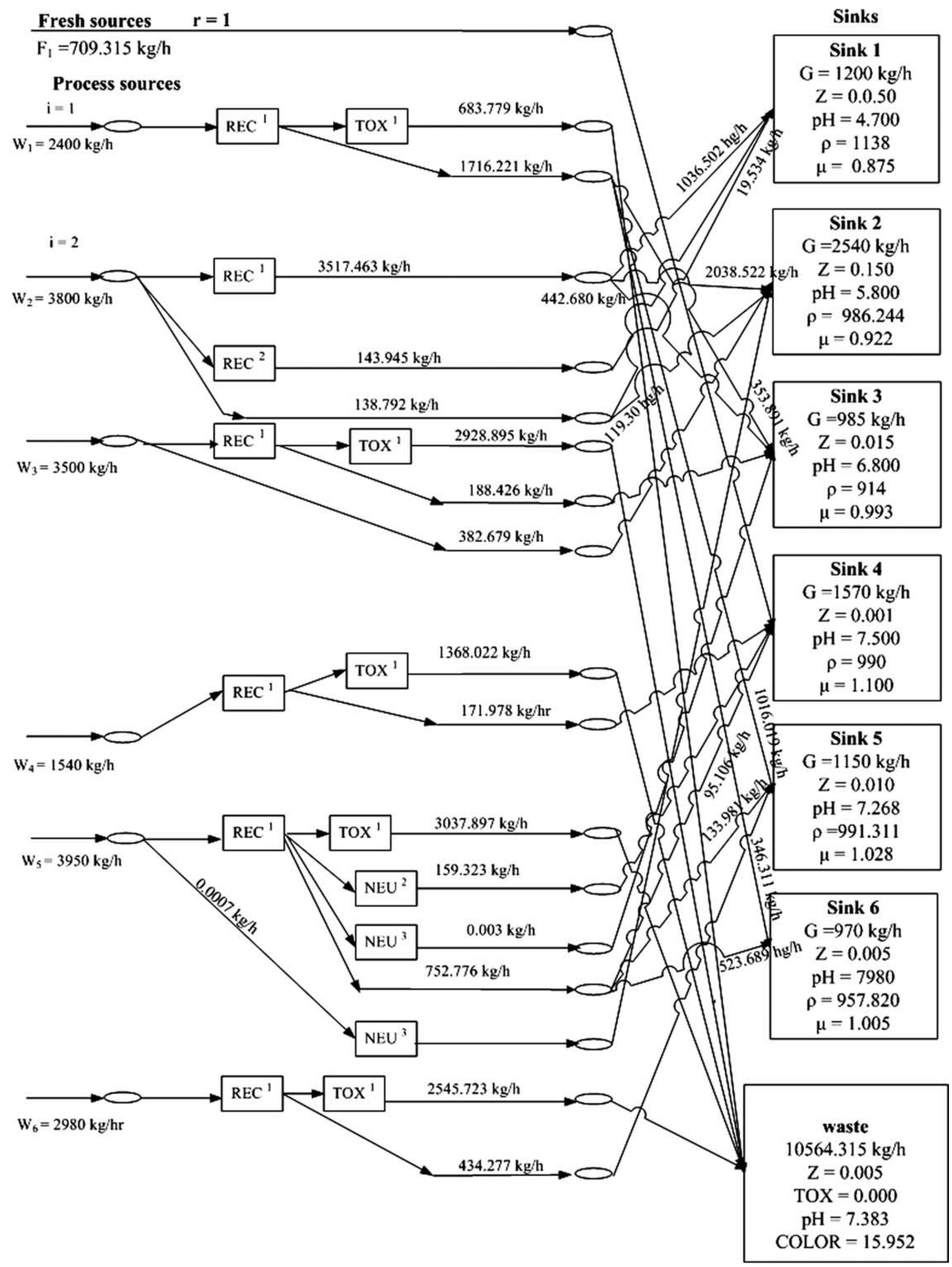

Figure 15. Solution for minimum EI for Example 3.

support the computational efficiency of the proposed methodology. It is also worth noting that in the set of Pareto optimal solutions for the cases presented here, the solutions that minimize the TAC corresponded to those with the highest overall EI; therefore, the proposed methodology can be used to identify solutions that show a proper compromise between economic and EIs in the form of a set of Pareto solutions. It should, however, be recognized that costs are local specific, so that there could be cases in which the cost of fresh resources could be high enough to make the economic and environmental objectives coincide. In any event, the proposed methodology could be applied to provide the corresponding solution or set of solutions.

Table 16. Summary of Results for Example 3

Concept	Minimum TAC	Minimum EI	Goal Solution
F_1 (kg/h)	855.832	709.315	742.184
F_2 (kg/h)	0.000	0.000	0.000
F_3 (kg/h)	0.000	0.000	0.000
Waste (kg/h)	10710.832	10564.315	10597.184
Fresh sources cost ($/year)	205399.638	170235.651	178124.071
Recovery cost ($/year)	1786745.391	2010930.695	1838769.818
Toxicity treatment cost ($/year)	1850831.739	1825513.669	1831193.331
Aeration cost ($/year)	0.000	0.000	0.0000
Neutralization cost ($/year)	4.374	50605.365	38948.408
Eco-indicator 99	3.33246E7	2.2889E7	2.3005$E + 7$
Total annual cost ($/year)	3842981.142	4057285.379	3887035.628

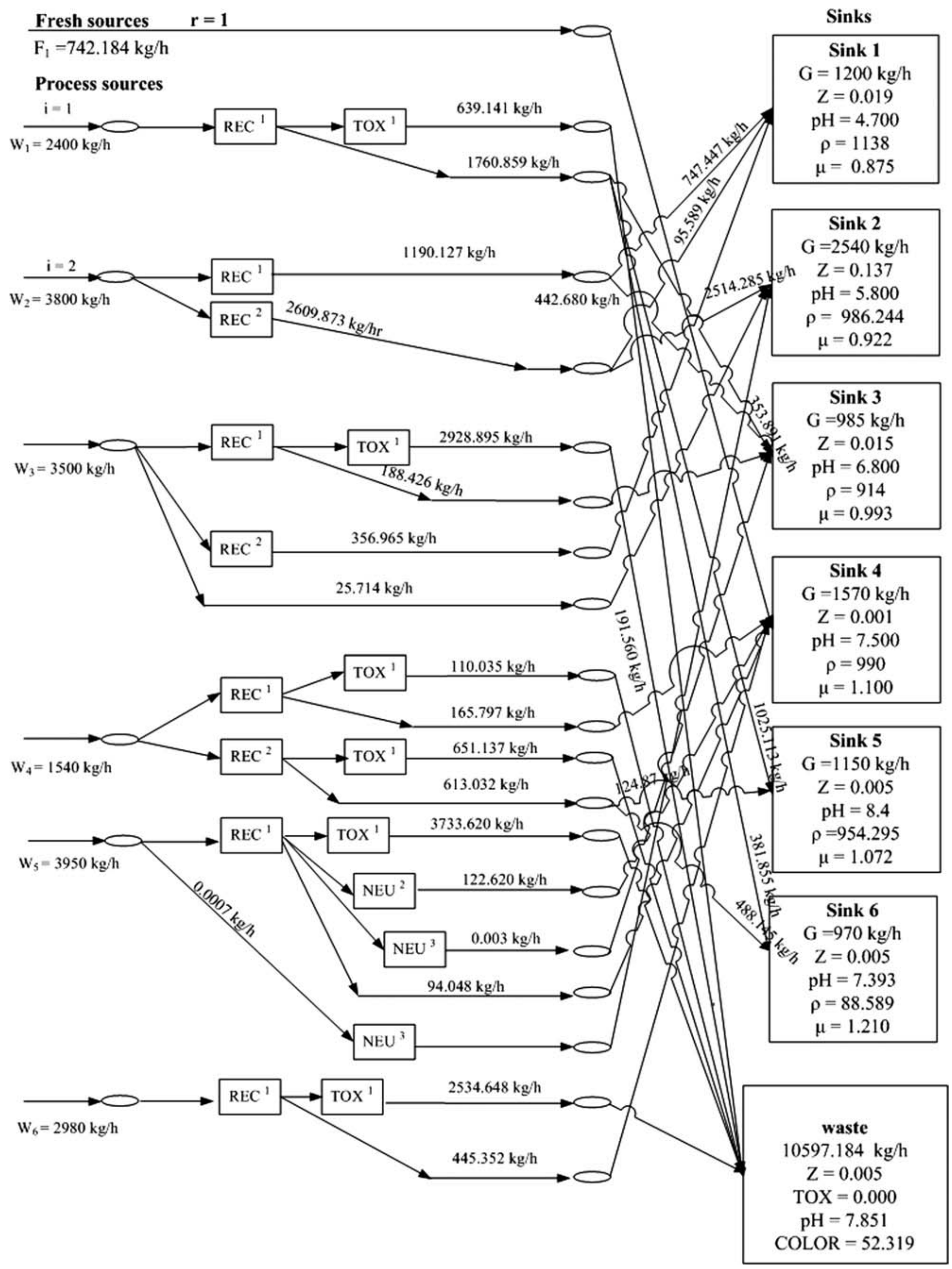

Figure 16. Optimal solution with the Goal method for Example 3.

Table 17. Problem Size and Computer Effort for Each Example

Problem	Variables	Constraints	CPU Time (s)
Example 1	6632	1797	0.156
Example 2	143	75	0.010
Example 3	20,537	3570	0.453

Notation

AER = aeration process
C = concentration (ppm)
COD = chemical oxygen demand
Color = property color
$\mathrm{Cost}^{\mathrm{Fresh}}$ = unit cost for fresh utility
$\mathrm{Cost}^{\mathrm{int}^N}$ = unit cost for interceptor N
EI = environmental impact
$\mathrm{Eco\ Indicator}_b^{\mathrm{waste}}$ = eco-indicator 99 for the chemical b in the waste stream discharged to the environment
$\mathrm{Eco\ Indicator}_r^{\mathrm{fresh}}$ = eco-indicator 99 for the whole life cycle for the production of fresh source r
$\mathrm{Eco\ Indicator}_{\mathrm{int1}}^{\mathrm{treatment}}$ = eco-indicator 99 for the operation of the treatment unit int^1
H_{Y} = operating time of the plant, h/year
int^n = interceptor for property n
INT^n = set for the property interceptor n
F_r = total flow rate for fresh source r
$f_{r,j}$ = segregated flow rate from fresh source r to sink j
G_j = total flow rate for process sink j
$g_{i,j}^{\mathrm{int1},\ldots,\mathrm{int}N}$ = segregated flow rate from interceptors, $\mathrm{int}^1,\ldots,\mathrm{int}^N$ to process sink j for process source i
$g_{i,\mathrm{waste}}^{\mathrm{int1},\ldots,\mathrm{int}N}$ = segregated flow rate from interceptors, $\mathrm{int}^1,\ldots,\mathrm{int}^N$ to waste for process source i
N_{Fresh} = total number of fresh sources
N_{Sinks} = total number of sinks
N_{Sources} = total number of process sources
NEU = neutralization process
NFRESH = set for the fresh sources, $\{r|r = 1,\ldots,N_{\mathrm{Fresh}}\}$
NPROP = set for the properties intercepted, $\{p|p = 1,\ldots, N_{\mathrm{Prop}}\}$
NSINKS = set for the sinks, $\{j \mid j = 1,\ldots,N_{\mathrm{Sinks}}\}$
NSOURCES = set for the process sources, $\{i \mid i = 1,\ldots,N_{\mathrm{Sources}}\}$
Odor = property odor
pH = potential of hydrogen
R = electric resistivity
R_∞ = paper reflectivity
REC = recovery of a hazardous component
RVP = Reid vapor pressure
TAC = total annual cost
Tox or TOX = toxicity
W_i = total flow rate for the process sources i
w_i^{int1} = segregated flow rate from process source i to interceptor int^1
$w_i^{\mathrm{int1},\ldots,\mathrm{int}N}$ = segregated flow rate from process source i to interceptors $\mathrm{int}^1,\ldots, \mathrm{int}^N$
waste = total flow rate for the waste stream discharged to the environment
z = composition or concentration

Greek letters

$\alpha_{b,k}$ = damage caused by category k per unit of chemical b released to the environment
$\alpha_p^{\mathrm{int1},\ldots,\mathrm{int}N}$ = efficiency of property interceptor for property p
β_b = total amount of chemical b released per unit of flow due to direct emissions
δ_d = normalization factor for the damage category d
$\delta_{\mathrm{TAC}}^{+}$ = positive deviation for target $\mathrm{TAC}^{\min}$
$\delta_{\mathrm{TAC}}^{-}$ = negative deviation for target $\mathrm{TAC}^{\min}$
δ_{EI}^{+} = positive deviation for target $\mathrm{EI}^{\min}$
δ_{EI}^{-} = negative deviation for target $\mathrm{EI}^{\min}$
ε = parameter for the constraint method
ψ_p = property operator for the mixing rule for property p
ρ = density
μ = viscosity
ω_d = weighting factor for the damage category d

Indices

b = chemical released to the environment
Env = environment
i = process source
In = inlet
j = sink
k = impact category for the eco-indicator 99
LO = lower value
max = maximum
min = minimum
Out = out
p = property
PIN = property interceptor network
r = fresh source
Sink = sink
Source = source
UP = upper value
waste = waste discharged to the environment

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