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Synthesis of mass exchange networks: A novel mathematical programming approach

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ABSTRACT

Mass integration is an efficient tool to prevent pollution derived from chemical processes. In recent years, several advances have been reported in methodologies for the design of mass exchange networks (MENs), using approaches as the pinch point and mathematical programming. Recently, simultaneous design and optimization methodologies have been proposed. The design methods based on simultaneous optimization offer the possibility of synthetizing MENs in a single step, formulating the synthesis problem as a mixed-integer nonlinear programming problem (MINLP). In this work, a MINLP model for the synthesis of mass exchange networks is presented. The model is based on a superstructure represented with disjunctions. The proposed superstructure is obtained from a state-task-network representation and is applied to a process for copper removal from an etching process. The obtained mass exchange network showed a lower total annual cost than the networks previously reported for the same process.

1. Introduction

The industrial processes are important in modern society. Nowadays, the process designer must be concerned about the rational use of the natural resources and the preservation of the environment. New processes must be efficient, economically competitive, sustainable, and flexible. Of course, the design of such processes requires the availability of proper conceptual methodologies and powerful computational tools. An approach for reducing the environmental impact of a process implies the use of mass exchange networks (MENs), originally proposed by El-Halwagi and Manousiouthakis (1989). The MENs are systems of direct contact mass transfer units, which use process streams of external mass separation agents (MSA, poor streams) to selectively remove pollutants from waste process streams (rich streams). A schematic representation of a MEN is shown in Fig. 1. The optimal synthesis of the MEN is especially important in the design of wastewater treatment networks. Some works in the area involve the development of wastewater treatment networks with recycles and rerouting (Sueviriyapan et al., 2016), the synthesis of non-isothermal networks (Ibric et al., 2016), the design of wastewater networks including uncertainties (Lira-Barragán et al., 2016), and the analysis of wastewater networks from a macroscopic point of view (Garibay-Rodríguez et al., 2017), among others.

El-Halwagi and Manousiouthakis (1989) proposed a sequential methodology to synthesize MENs; first, a network of external separation agents with a minimum cost is generated through thermodynamic considerations; then, the minimum capital cost is obtained through heuristic rules. Other approaches to synthesize MENs are based on the development of superstructures and modeled as mixed-integer non-lineal programming problems (El-Halwagi and Manousiouthakis, 1990a,b; Papalexandri et al., 1994), based on techniques for the design of heat exchange networks. Alva-Argáez et al. (1999) reported an approach to consider multiple pollutants in the synthesis of water networks for wastewater minimization. Chen and Hung (2005) developed a methodology for the synthesis of MENs based on the mathematical programming technique reported for the design of heat exchange networks, which makes use of the concept of a stage-wise superstructure. Isafiade and Fraser (2008) formu-

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Nomenclature

Q_i [kg/s]	mass flowrate of sub-stream *i* from SR_1
x_i [kg/kg]	mass fraction of sub-stream *i* from SR_1
T_i [kg/s]	mass flowrate of sub-stream *i* from SR_2
w_i [kg/kg]	mass fraction of sub-stream *i* from SR_2
R_i [kg/s]	mass flowrate of sub-stream *i* from SS_1
z_i [kg/kg]	mass fraction of sub-stream *i* from SS_1
S_i [kg/s]	mass flowrate of sub-stream *i* from SS_2
y_i [kg/kg]	mass fraction of sub-stream *i* from SS_2
SS_1 [kg/s]	total mass flowrate for solvent 1
SS_2 [kg/s]	total mass flowrate for solvent 2
m_{je} []	slope for the lineal equilibrium relationship in the mass transfer device *j*
b_j []	intercept for the lineal equilibrium relationship in the mass transfer device *j*
Y_j []	binary variable associated to the mass transfer device *j*
Y_j' []	binary variable associated to the absorption factor of the mass transfer device *j*
N_j []	number of theoretical stages for the mass transfer device *j*
$\Delta_j y$ []	difference between the input and output compositions for the trayed device *j*
$\Delta_j y_e$ []	difference between the input and output equilibrium compositions for the trayed device *j*
$\Delta_j y_1$ []	difference between the input composition and the output equilibrium composition for the trayed device *j*
$\Delta_j y_2$ []	difference between the input equilibrium composition and the output composition for the trayed device *j*
H_j [m]	packing height for the mass transfer device *j*
HTUj [m]	global height of a mass transfer unit for the mass transfer device *j*
NTU_j []	number of mass transfer units
k_{yj} [kg/m^2·s]	mass transfer coefficient in the mass transfer device *j*
a_j [m^2/m^3]	interfacial area per unit volume of packing in the mass transfer device *j*
$Area_j$ [m^2]	cross-sectional area for the mass transfer device *j*
M_j [kg/s]	mass transferred from the rich stream to the poor stream in the unit *j*
C_{op} [USD/y]	operational costs
C_{SS1} [USD/kg·y]	unitary cost for the solvent SS1
C_{SS2} [USD/kg·y]	unitary cost for the solvent SS2
C_{in} [USD/y]	investment costs
C_j [USD/y]	unitary cost for the mass transfer device *j*

lated the synthesis of MENs through the use of a superstructure based on intervals of composition, defined in terms of the inlet and target compositions for the rich and poor streams. Torkfar and Avami (2016) reported an approach for synthesizing integrated water and energy networks, involving pressure drop considerations. Other methodologies for the synthesis of MENs have been reported, such as graphical methods (Gadalla, 2015), Process Graph Theory (Lee and Park, 1996), genetic algorithms (Garrard and Fraga, 1998), and Infinite DimEnsioAl State-Space (IDEAS), by Wilson and Manousiouthakis (2000). The synthesis of multi-component mass exchange networks has also been reported (Liu et al., 2013). Recently, Ghazouani et al. (2017) reported a model for the determination of mass allocation and heat exchanger networks, resulting in a MILP problem.

A proper synthesis method for a MEN requires an accurate strategy for the design of the mass transfer units. It has been demonstrated that minimizing the number of mass transfer units will not necessarily lead to a minimum in the capital cost. Thus, besides the number of units, the design parameters of the units (diameter of column, distance between trays, etcetera) must be considered (Hallale and Fraser, 2000a, b). Shenoy and Fraser (2003) proposed a reformulation of the Kremser equation to eliminate the involved singularities. This modification is useful for promoting convergence in MEN synthesis methodologies based on mathematical programming techniques.

An alternative way of representing superstructures involves the use of generalized disjunctive programming (GDP), which makes use of disjunctions and logic propositions to model the superstructure. The GDP is constituted by three basic elements: states, tasks and equipment, which can be combined in two kinds of representations: state-task-network (STN) and state-equipment-task (SET). The STN representation has been previously used for making decisions in fusion fuel cycle (Lee et al., 2016), modeling energy supply chains (Kalaitzidou et al., 2016), and scheduling in pharmaceutical manufacturing (Casola et al., 2016), among others. Lee et al. (2016) stated that the network-based representations, including STN, allow representing complex system configurations with several operational conditions. Besides, Casola et al. (2016) stated that, for the type of problem that they reported, the STN representation results in models that require relatively low computational times. Other network-based representations have also been reported, such as the resource-task-network (RTN), which is widely used for scheduling and scheduling/design problems (Barbosa-Póvoa and Pantelides, 1997;1999).

In this work, the synthesis problem of a MEN is studied using a state-task-network superstructure. The superstructure is modeled through general disjunctive programming and then re-formulated as a MINLP. The mass transfer units are modeled using the number of transfer units (NTU) approach. The proposed superstructure allows mixing and splitting the streams, increasing the number of feasible exchanges in the superstructure. This can also be obtained through the stage-based methods, which include most of the previously reported approaches. For some stage-wise superstructures, a parameter which may affect the results is the number of stages (Chen and Hung, 2005). In the methodology proposed in this work, this parameter is not necessary. Moreover, the use of general disjunctive programming allows a more logical modeling for the discrete decisions. The present strategy is tested using a well-known case of study for the removal of copper in an etching plant. The results are similar to those reported in previous works (Chen and Hung, 2005), overcoming the non-linearities and non-convexities in the model. Thus, the use of STN superstructures is a feasible alternative to model the MEN synthesis problem.

2. State-task-network superstructure

In a given process, the flowsheet has three main elements: states, tasks and equipment. Taking those elements into account, Yeomans and Grossmann (1999) developed a scheme to represent problems of process synthesis in two stages. In the first stage, the superstructure is constructed in terms of two basic complementary representations: state-task-network (STN) and state-equipment-task (SET). In the second stage, the selected representation is modeled through general disjunctive programming and reformulated as a mixed-integer problem.

In the aforementioned representations (STN and SET), the states represent the set of physical and chemical properties identifying the process streams (e.g., composition, temperature, pressure,

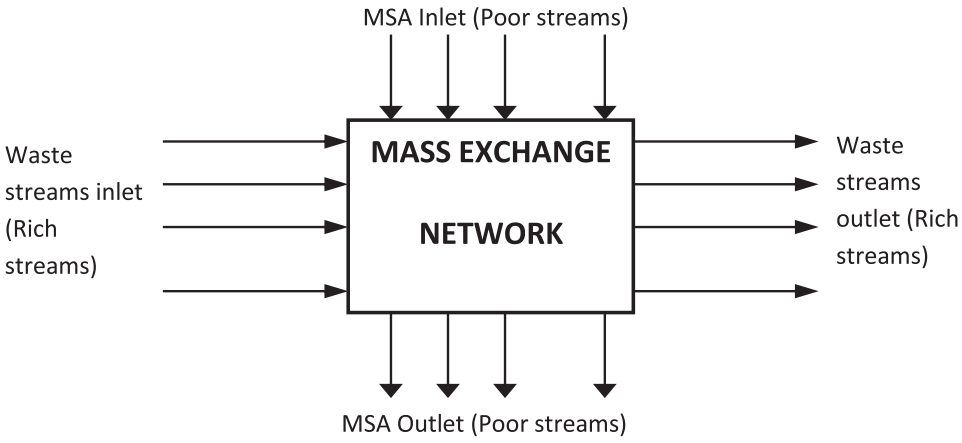

Fig. 1. Schematic representation of a MEN.

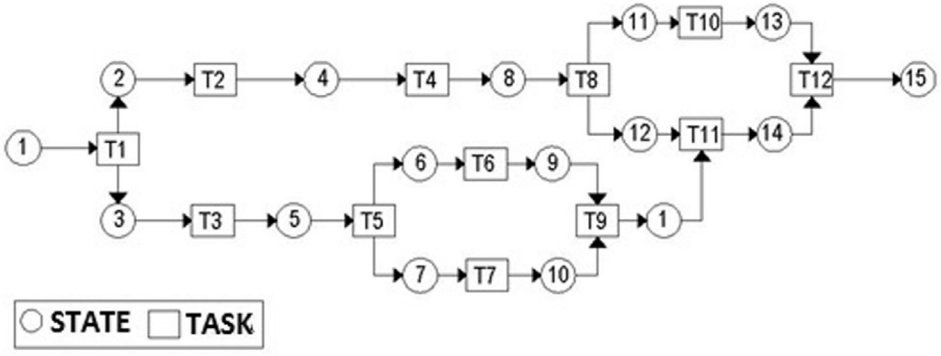

Fig. 2. General scheme of a state-task-network representation.

flowrate, etcetera). Some tags can also be used to identify a state, as hot/cold stream, poor/rich stream, extractant, adsorbent, laminar/turbulent flow, etcetera. The tasks are related to the physical and chemical transformations occurring between adjacent states. The tasks correspond to mass, energy, or momentum transfer operations, such as distillation and adsorption. Finally, equipment are the elements in the flowsheet corresponding to the physical devices where a given task will occur (reactors, absorption columns, heat exchangers, etcetera).

In the STN representation, tasks and states are defined, while the assignation of equipment is unknown. In Fig. 2, a general scheme of a STN representation is shown. Some of the tasks may be conditional, while others may exist in all the design alternatives.

Once the states and tasks are identified, it is necessary to assign these tasks to a given equipment. Two cases can be distinguished:

(1) One task to one equipment (OTOE): in this case, each task is assigned to a single equipment. Thus, the tasks are redefined to distinguish one from the other.
(2) Various tasks to one equipment (VTE): first, an equipment which may perform all the required tasks in the flowsheet is identified. In this way, a single unit can be assigned to different tasks, and a single task can be assigned to different equipment. Using this approach, the assignment of equipment to the different tasks can be assumed as a part of the optimization problem.

3. Case study

The methodology proposed here is applied to a mass exchange network formed by two rich streams and two poor streams for the removal of copper in an etching plant. This problem has been previously reported by El-Halwagi and Manousiouthakis (1990a) and Chen and Hung (2005). A representation of the problem is shown in Fig. 3. One of the rich streams (SR_1) is an ammonia solution, while the other rich stream (SR_2) comes from a washing stage. These two streams are rich in copper and must be treated to reach the concentrations allowed by both, the environmental regulations, and the process economy. Two external mass separation agents, SS_1 and SS_2, are available for the copper recovery. Mass flow rates and copper concentrations for the involved streams are shown in Table 1. Most of the data presented in Table 1 has been reported by El-Halwagi and Manousiouthakis (1990a). Only the cost for solvents is modified, according to the proposal of Papalexandri et al. (1994) used by Chen and Hung (2005).

Table 1
Data for the streams in the etching process.

Rich streams			
Stream	y^{in}	y^{out}	Mass flowrate (kg/s)
SR_1	0.13	0.10	0.25
SR_2	0.06	0.02	0.10
Poor streams			
Stream	x^{in}	x^{out}	Cost (USD/kg·y)
SS_1	0.03	0.07	58,680
SS_2	0.001	0.02	704,160

4. Description of the superstructure

To develop the model, a superstructure based on a state-task-network representation is proposed. This superstructure must

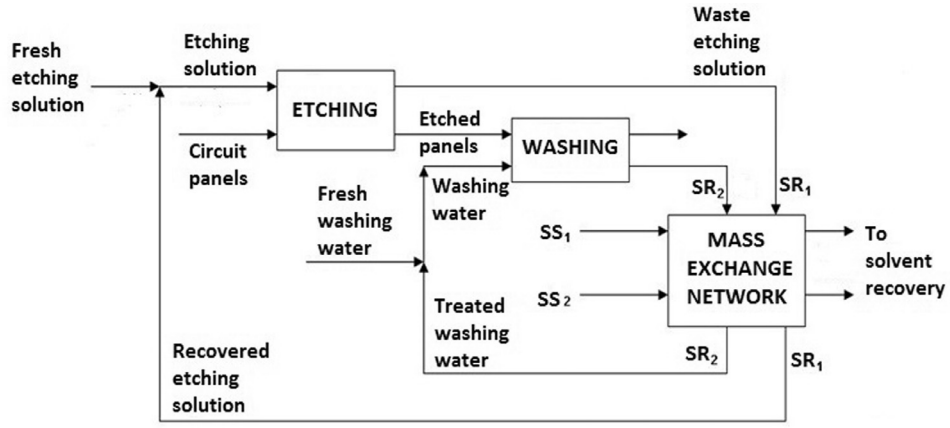

Fig. 3. Copper recovery in an etching plant.

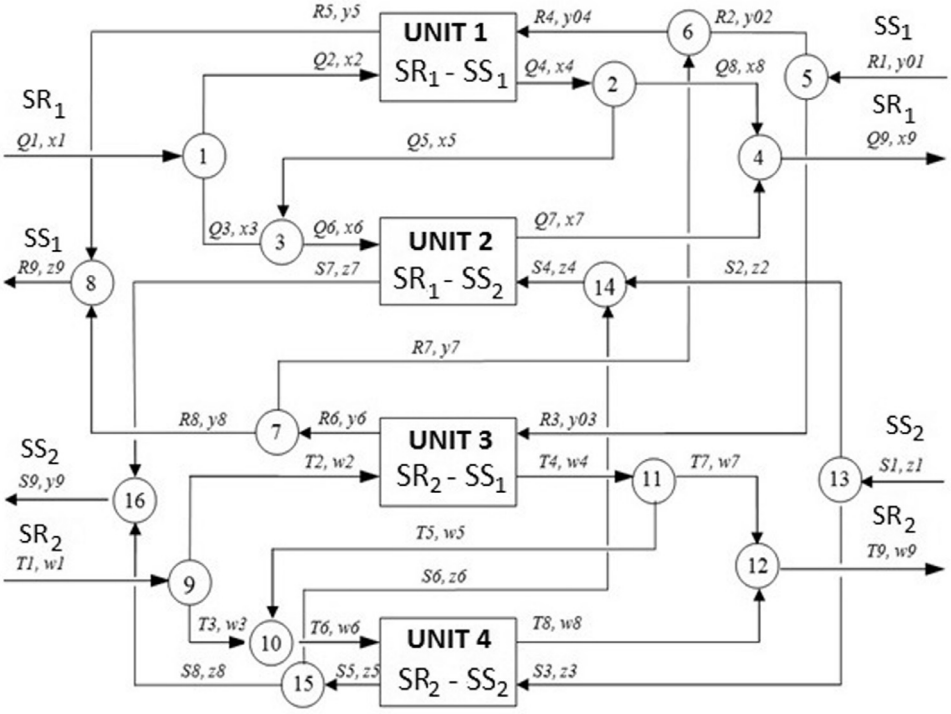

Fig. 4. Superstructure for the mass exchange network between two rich streams (R_1 and R_2) and two poor streams (S_1 and S_2).

Table 2
Comparison with a previously reported solution.

	SS_1 flow rate (kg/s)	SS_2 flow rate (kg/s)	N_1	H_2 (m)	N_3	H_4 (m)	TAC (USD/y)
This work (BARON)	0.30	0.021	1	0	3	0.309	52,068
This work (SBB)	0.2769	0.0221	0.788	0	3.09	0.319	50,855
Chen and Hung (2005)	0.276	0.023	1	0	3	0.457	52,300

show all the feasible combinations between streams and equipment, as shown in Fig. 4. Two possible mass transfer units are considered: trayed columns (Units 1 and 3) and packed columns (Units 2 and 4). The circles represent units for the combination or separation of streams. The representative states for the streams are defined by the mass flowrates (Q_i, R_i, S_i and T_i) and by the mass compositions (x_i, y_i, z_i).

Each stream entering the network is divided and directed to different mass exchange units, for a potential combination between a rich stream and a poor stream. The streams leaving a mass exchange unit have different compositions from those entering the same unit. In the nodes where a stream division occurs, the compositions are the same for the inlet and outlet streams. A zero-mass flowrate in the model solution will represent the absence of that stream in the final configuration. The resulting topologies include parallel arrangements, series arrangements, or combinations of both, as well as split streams.

5. Methodology

Once the superstructure has been obtained, the mathematical model is developed. This include the following equations:

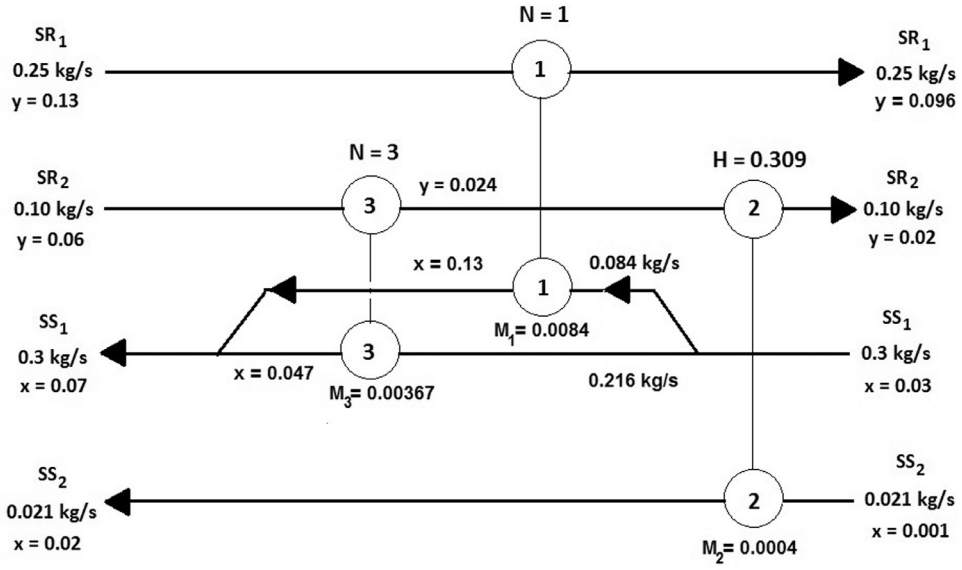

Fig. 5. Optimized mass exchange network.

1. *Mass balances in nodes*: Total mass balances, together with mass balances for each component, are applied to the points where streams are mixed or split. It is important to mention that there are bilinear terms in these equations, which cause non-linearities in the model.
2. *Mass balances in the separation units*: A mass balance for every component is required in each mass exchanger.
3. *Equations for mass transfer feasibility*: The feasibility for mass transfer is represented through the thermodynamic equilibrium relationships. A binary variable Y_j is used for each unit. Y_j is equal to zero when there is no interaction between a given rich stream and a poor stream. To ensure a composition difference greater than zero between the operation line and the equilibrium line in the extreme zones of the mass exchanger, a minimum allowed difference on composition, εj, is defined, where $\varepsilon j = 0.0001$. This will allow obtaining a finite number of equilibrium stages in the trayed columns and a finite packing height in the packed columns.
4. *Dimensioning of mass exchangers*: Units 1 and 3 are trayed columns, whose number of stages is computed through the use of the Kremser equation with the Chen approximation, replacing the concentration logarithmic mean by a concentration geometric mean. Two cases are defined: when the absorption factor, A_j, is different to one, and when it takes the value of 1.
   Units 2 and 4 are packed columns, where the packing height (H_j) required for separating the component from the rich stream to the poor stream is a function of the number of transfer units (NTU_j) and the global height of a transfer unit (HTU_j). Following the proposal of Chen and Hung (2005), diameter for packed and trayed columns has been fixed as 1 m.
5. *Disjunctions and logical propositions*: The disjunction equations determine the existence or absence of each mass exchanger in terms of logical variables. The logical propositions describe the relationships between the mass exchangers. In this case, it is allowed for every mass exchanger to exist, independently of the existence or absence of the other exchangers.
6. *Equations for the total annual cost*: The total annual cost is divided in two terms: operational costs (C_{op}) and investment costs (C_{in}). For the operational costs, the cost of using the two solvents, S_1 and S_2, is considered. For the investment costs, simplified correlations have been used in terms of the number of stages for the trayed columns or in terms of the packing height for the packed columns.
7. *Objective function*. The objective function implies the minimization of the total annual cost.

4 Once the optimization problem has been set, the disjunctions are re-formulated through the Big-M strategy, obtaining a MINLP problem. The MINLP model is coded in the GAMS software and solved using the BARON solver.

5. Results

The MINLP model has 93 continuous variables and 4 binary variables, with 148 equations, and it has been solved using the BARON solver of the GAMS software. The execution time is lower than 1×10^{-3} s, with a relative gap of 0.1. The resulting MEN showed a minimum total cost value from the objective function of 52,068 USD/y, requiring 0.3 kg/s of solvent S1 and 0.021 kg/s of solvent S2. Operational costs represent about 63% of the total annual cost. The binary variables indicate that the units required are Unit 1, Unit 3 and Unit 4. The resulting network is shown in Fig. 5, including the distribution of the mass exchangers and the interconnections between the streams. In Fig. 5, M_j indicates the quantity of mass transferred in each unit. In Fig. 6, the arrangement of the network for the etching process is shown. It can be seen that the synthetized network has an arrangement in parallel for the R1-S1 and the R2-S2 exchanges, while the exchanges for R2-S1 and R2-S2 imply a serial arrangement. This shows the capability of the methodology to obtain networks where the streams can be split.

A comparison between the results reported by Chen and Hung (2005) and the results obtained in this work is shown in Table 2. An additional solution has been obtained through the use of the solver SBB, which is also reported in Table 2. In the case of SBB, the execution time is 0.08 s, with a relative gap lower than 1×10^{-6}. Although the configuration obtained with both, SBB and BARON, is similar, the solution with BARON showed integer values for N1 and N3. Due to the nature of the Kremser equation, such variables are, in principle, stated as continuous. Nevertheless, physically they must be integer; thus, the result obtained with BARON is more accurate, and is taken as the right one. It is observed that the selected solution shows a total annual cost slightly lower than that reported by Chen and Hung (2005), although the network obtained in this work is similar to the one of Chen and Hung (2005).

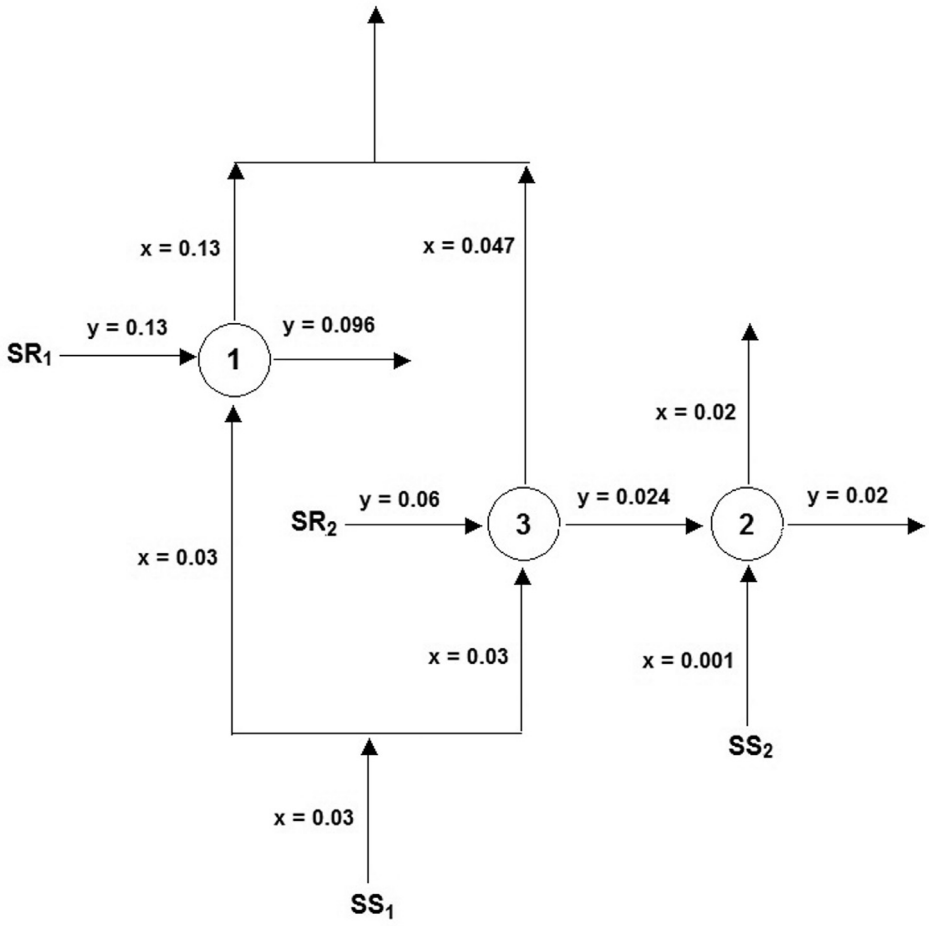

Fig. 6. Mass exchange network for copper recovery.

The difference between the numerical results can be attributed to the difference in the model for the calculation of the number of transfer units for the packed columns, since a geometric mean is used in this work for the concentrations, according to the proposal by Chen (1987), while Chen and Hung (2005) used a logarithmic mean.

6. Conclusions

A strategy for the modeling and optimization of mass exchange networks has been proposed, which is based on the use of state-task-network superstructure and its modeling using general disjunctive programming. The methodology has been applied to a copper recovery case of study. The proposed superstructure allows testing all feasible exchanges between streams. Optimal designs for the mass exchange networks have been obtained, with the simultaneous determination of the network structure and the dimensioning of the mass transfer units. It has been shown that the proposed state-task-network superstructure allowed obtaining results comparable to those reported in the literature, without the necessity of defining the number of stages. Moreover, the superstructure can be easily extended to a case with a higher number of streams. Finally, the use of generalized disjunctive programming allows developing the mathematical model following a logic-based structure.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2018.04.012.

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