Anton Friedl, Jiří J. Klemeš, Stefan Radl, Petar S. Varbanov, Thomas Wallek (Eds.)
Proceedings of the 28th European Symposium on Computer Aided Process Engineering
June 10th to 13th, 2018, Graz, Austria.
http://dx.doi.org/10.1016/B978-0-444-64235-6.50061-9

Optimal synthesis of mass exchange networks through a state-task representation superstructure

Miguel Ángel Velázquez-Guevara, [a*] Agustín Ramón Uribe-Ramírez, [a] Fernando Israel Gómez-Castro, [a] Juan Gabriel Segovia-Hernández, [a] Salvador Hernández, [a] José María Ponce Ortega [b]

[a]*Departamento de Ingeniería Química, División de Ciencias Naturales y Exactas, Campus Guanajuato, Universidad de Guanajuato, Noria Alta S/N, Guanajuato, Gto., 36050, México*

[b]*División de Estudios de Posgrado, Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, Francisco J. Múgica S/N, Morelia, Mich., 58060, México*

guevaraf@ugto.mx

Abstract

The use of mass exchange networks is a strategy that allows the recovery and reuse of dangerous components from effluents of industry, reducing, or even avoiding, the pollution derived from the release of such components to the environment. The most common strategy for the synthesis of mass exchange networks involves the use of analogies to the pinch point method for heat exchange networks, and some approaches have been reported on the use of mathematical methods to solve the synthesis problem following a super-structure based on stages. Nevertheless, such super-structure requires deciding the proper number of stages. In this work, a superstructure is proposed to represent the synthesis of a mass exchange network for the recovery of copper in an etching process. The superstructure is developed following a state-task representation, using the concepts of transfer units for the design of the mass exchangers. This representation allows obtaining a wide search space, with no need of assuming additional parameters related to the formulation. The disjunctive mathematical model is developed and its MINLP equivalent is obtained through the convex hull strategy. The MINLP is then solved using the DICOPT solver of GAMS.

Keywords: mass exchange networks, state-task representation, mathematical programming

1. Introduction

Mass exchange networks are structures with many direct-contact mass transfer units, on which waste process streams (so-called rich streams) are treated to remove pollutants. This removal task is usually performed through external mass separation agents (so-called poor streams). The selection of which rich streams must exchange mass with which poor streams is one of the main challenges in the design of mass exchange networks. One of the first methodologies to synthesize mass exchange networks has been proposed by El-Halwagi and Manousiouthakis (1989), where the minimum capital cost is obtained through heuristics. The use of superstructures to represent the set of possible configurations for the network has been widely developed in the last years. Chen and Hung (2005) proposed a synthesis methodology based on the design of heat exchange networks. On the other hand, Isafiade and Fraser (2008) used a superstructure based on intervals of composition. Liu et al. (2013) reported a superstructure for the synthesis of mass exchange networks, involving the recovery of multiple components. Isafiade and Short (2016) proposed the use of more rigorous cost functions to solve the synthesis problem of mass exchange networks. Ghazouani et al. (2017) proposed a superstructure for the simultaneous design of mass and heat exchange networks, with a simplified model, obtaining a MILP problem. Other design approaches have been also reported, based on graphical methods and the pinch point analysis (Gadalla, 2015).

Most of the previously mentioned works report the use of a stage-based superstructure. Nevertheless, an important parameter to choose when obtaining such a superstructure is the number of stages, whose proper value is unknown at the beginning of the solution, although some approaches have been reported to this end (Chen and Hung, 2005). An alternative way to propose the superstructure is through the development of a state-task-network based superstructure. In this approach, the tasks (physical or chemical transformations) and the states (properties for the streams) are defined, while the assignation of equipment is unknown. In this work, a state-task-network based superstructure is developed for a classic mass exchange network synthesis problem. The problem is modelled through general disjunctive programming, relaxed into a MINLP and solved with the software GAMS. The non-linear terms are involved mainly in the design equations for the mass transfer units.

2. Case study

The design of a mass exchange network for the removal of copper in an etching plant is studied (Chen and Hung, 2005). This problem involves the integration between two rich streams and two poor streams. Figure 1 shows a simplified representation of the network. Stream R_1 is a solution with ammonia, while stream R_2 comes from a washing stage. Both, R_1 and R_2, have a high concentration of copper, so they must be treated to reach the environmental regulations with little affection to the process economy.

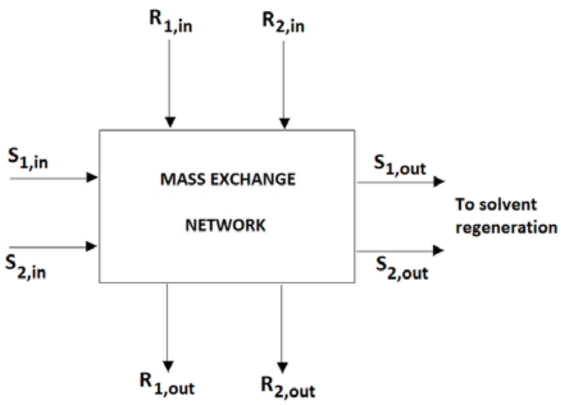

Figure 1. Simplified representation of the mass exchange network.

R_1 has a flowrate of 0.25 kg/s, with initial composition of copper of 0.13. On the other hand, flowrate for R_2 is 0.10, with initial composition of copper of 0.06. It is desired to reach compositions of 0.10 and 0.02 for streams R_1 and R_2, respectively. To perform this task, there are two external mass separation agents, S_1 and S_2, where S_1 has a unitary cost of 58,680 USD/kg·y, while the unitary cost of S_2 is 704,160 USD/kg·y (Papalexandri et al., 1994).

3. Superstructure and mathematical modelling

Figure 2 shows the superstructure representing the feasible combinations between streams and equipment. Such superstructure is based on a state-task-network representation. In Figure 2, the circles are units for mixing or separation of streams, which allows to split a single stream and treat its sub-streams in different equipment, or mixing to streams to be treated in a single equipment. Units 1 and 3 are trayed columns, while Units 2 and 4 are packed columns. Variables written in capital letters (Q_i, R_i, S_i and T_i) are mass flowrates, while variables in lowercase letters (x_i, y_i, z_i) are mass compositions. The superstructure is arranged in a way to allow parallel and serial arrangements, or combinations of both. Moreover, as abovementioned, this superstructure allows the split of the streams, which is one of the major advantages of this approach.

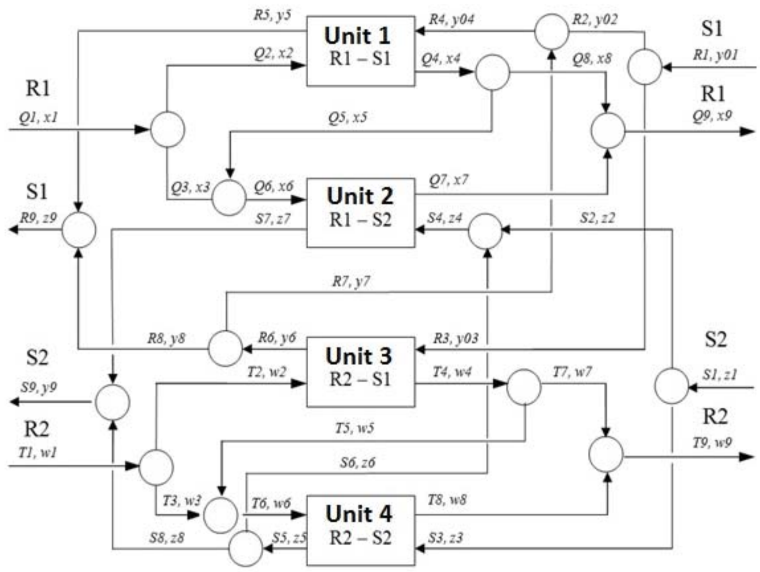

Figure 2. State-task-network based superstructure.

The mathematical model for the superstructure includes the mass balances in the nodes, the mass balances in the separation units, relationships for thermodynamic equilibrium, equations for dimensioning of the mass exchangers, disjunctions and logical propositions, and equations for the calculation of total annual cost. The mass balances in the nodes are applied in each point where streams are mixed or split. The bilineal terms in these balances contribute to the non-convexity of the model. The mass balances in the separation units are applied for each component. The relationships for thermodynamic equilibrium are used to establish the feasibility for mass transfer in each exchange. Here, a minimum allowed difference in composition is used to ensure a finite number of stages in the trayed columns and/or a finite packing height in the packed columns. In the case of the dimensioning of the mass exchangers, the Kremser equation with the approximation of Chen has been used for the trayed columns. As aforementioned, for the packed columns, the concept of height of transfer unit is used. The logical propositions are established to allow independence between the mass exchangers, i.e., the selection of one unit does not affect the possibility of selection or not selection of a second unit. The objective function for the optimization is given by the minimization of the total annual cost, which is the sum of the annualized capital costs and the operational costs. For this network, the operational costs are given by the solvents. The disjunctions have been relaxed through the convex hull strategy, and the resulting MINLP model is solved using the DICOPT solver of GAMS.

4. Results

The MINLP model to be solved has 93 continuous variables, 4 binary variables and 148 equations. Figure 3 shows the resulting network. The numbers in the rectangles with dotted lines represent the quantity of mass transferred in each unit. The exchanges R1-S1 and R2-S2 have parallel arrangement, while the exchanges R2-S1 and R2-S2 have a serial arrangement. From Figure 3, it can be seen that the stream S1 is divided, so a fraction of S1 exchanges mass with R1, while the other fraction performs the exchange with R2. The total annual cost for the network is 50,855 USD/y, where 63% of the total annual cost is given by the operational costs.

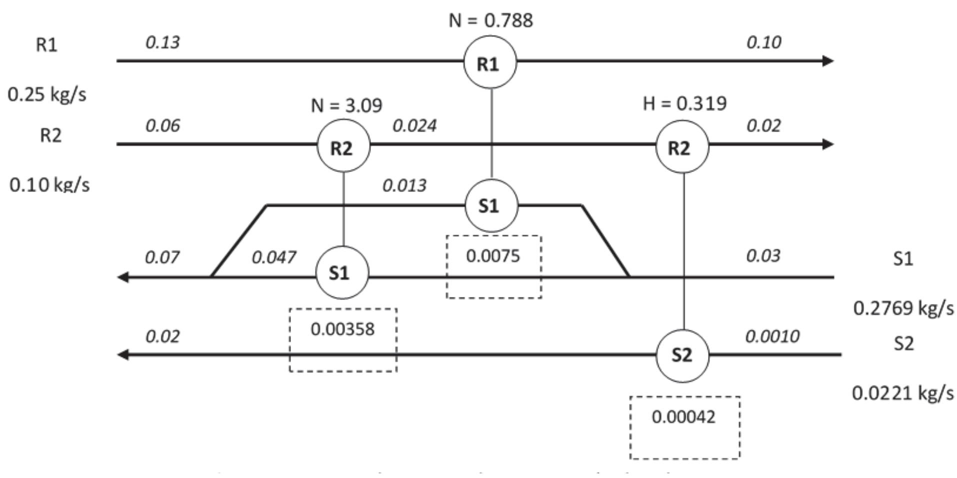

Figure 3. Optimal mass exchange network.

Table 1. Comparison of the results with a previous work.

	S1 (kg/s)	S2 (kg/s)	TAC (USD/y)
This work	0.2769	0.0221	50,855
Chen and Hung (2005)	0.276	0.023	52,300

The obtained solution has been compared with that reported by Chen and Hung (2005), this comparison is shown in Table 1. In terms of the use of solvent, the results for the base work are very similar to those obtained by the proposed alternative. Nevertheless, the total annual cost obtained through the method reported here is around 3% lower that that obtained by Chen and Hung (2005). Thus, the state-task-network based superstructure has allowed obtaining a similar solution to that previously reported for the same case study, with a lower total annual cost and making use of the possibility of split streams.

5. Conclusions

A state-task-network based superstructure has been proposed to solve the synthesis problem of a mass exchange network. This approach opens the possibility of split for a given stream to exchange mass with more than one stream. Moreover, the dimensioning of the columns is performed through semi-rigorous approaches, namely the Kremser equation and the high of transfer unit concept. This allows obtaining proper designs of the mass transfer equipment. The superstructure has been modelled through general disjunctive programming, and relaxed to a mixed-integer non-lineal problem through the convex hull method. The proposed superstructure has been applied to a classic problem for the removal of copper in an etching facility. The relaxed problem has been solved using the software GAMS, with a proper selection of the initial values for the degrees of freedom, obtaining a solution similar to that reported in the literature. Moreover, the resulting network makes use of the split of one of the solvent streams to satisfy the requirement of one of the rich streams.

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