Multiproduct Batch Plants Design Using Linear Process Performance Models

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In this contribution, a novel linear generalized disjunctive programming (LGDP) model is developed for the design of multiproduct batch plants optimizing both process variables and the structure of the plant through the use of process performance models. These models describe unit operations using explicit expressions for the size and time factors as functions of the process variables with the highest impact. To attain a linear formulation, values of the process variables as well as unit sizes are selected from a set of meaningful discrete values provided by the designer. Regarding structural alternatives, both kinds of unit duplications in series and in parallel are considered in this approach. The inclusion of the duplication in series requires different detailed models that depend on the structure selected. Thus, in a new approach for the multiproduct batch plant design, a set of potential structural alternatives for the plant is defined. *AIChE J,* 57: 122–135, 2011
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Introduction

A large number of optimization models for the design of multiproduct batch plants have been developed over the last decades.[1] This kind of plants produces a number of related products using the same equipment in the same operation sequence. Mainly, approaches with constant time and size factors are the most used in the modeling of such plants.[2–11] Similar approaches using constant factors have also been presented in the field of multipurpose batch plant design.[12–16] However, these models fix the process variables to get a determined process recipe avoiding the evaluation of various economic trade-offs involved in the design decisions. To attain more detailed formulations, process performance models have been included into the design of multiproduct batch plants. The performance models describe size and time factors as a function of the process decision variables (i.e., variables with the highest economic impact on the process) selected for the optimization. Several contributions[17–23] have tackled performance models instead of fixed recipes to incorporate information about the production process in the plant design. Specifically, the performance models entail additional algebraic equations obtained from mass balances and simplified kinetic equations that describe every unit operation in the process. They may be constant values, an equation, or even a system of equations in accordance with the selected level of detail.

In all of the aforementioned problem formulations, the final model is nonlinear and, generally, depending on the proposed representation for the unit operations, nonconvex.

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Typically, the most common approach used to solve this problem has been to formulate it as a mixed-integer nonlinear programing (MINLP) model. It is well-recognized that nonlinear nonconvex models are difficult to solve and, with the available solvers, they cannot guarantee global optimal solutions.

An option to guarantee global optimality in the solution of the batch design problem is based on the development of linear models as was suggested by Voudouris and Grossmann.[3] They show that many nonlinear models for batch design, which are based on the assumption of continuous sizes, can be reformulated as MILP problems when sizes are restricted to discrete values. Although the precision of the model is reduced, a superior performance is achieved.[24]

A fundamental aim of this work is the integration of the process decision variables in multiproduct batch plant design problems using linear models. To obtain a linear formulation, besides considering the units available in discrete sizes, process decision variables are assumed to take values from a set of meaningful discrete values provided by the designer. Although this may reduce the detail level of the models, linear formulations are obtained that can be solved to assure global optimality. This approach may be considered an extension of the previous work by Moreno et al.,[23] where a general nonconvex MINLP model that simultaneously optimizes process and design variables of a multiproduct batch plant was proposed. In that work, the unique binary variables are the ones that selects the structure of the plant. The drawbacks of such approach come from the detailed nonlinear nature of the modeling. General expressions are used to model the plant and then a nonconvex formulation is attained. Therefore, the optimal solution cannot be guaranteed, the solution depends on the starting point, and, sometimes, solvers can miss the optimal solution.

From the structural point of view, to improve the productivity of the batch plants, the duplication of units in parallel working out-of-phase and the duplication of units in series are incorporated in the formulation. In the last one, an operation is performed with different number of units.[25,26] In this way, the number of stages in the operations, and, therefore, in the process, is unknown and will be determined in the optimization. Although parallel units can be applied to any stage of a batch process to reduce idle times in the processing units, the duplication in series is only used in specific operations and its effect on the process depend on the unit operation. For instance, the operation of extraction is carried out with several stages that permit to overcome disadvantages such as high solvent consumption, long extraction time, and low extraction efficiency of a single unit extraction. Furthermore, the duplication of units in series in an operation not only affects that operation but also the upstream and downstream operations in the plant. Thus, the usual approaches with constant time and size factors or with fixed process performance models are not possible, unless additional assumptions are introduced. For example, Moreno and Montagna[25] supposed that, for each operation, the yield at the end of all possible configurations in series had to be the same.

In this work, to obtain general linear formulations including duplication in series and process performance models, a new approach is proposed using a set of potential structural alternatives for the plant. Each one is defined determining the number of units duplicated in series for each operation. Thus, process performance models can be generated for each operation in the process for a specific plant structure. Generally, in a given batch process, the amount of operations that can be duplicated in series is low; hence, the number of structural alternatives is also small.

With this approach, a set of nested discrete decisions is posed. First, the structural alternative for the plant must be selected. Then, process decision variables have to be chosen. Finally, the number of units in parallel in each stage and their sizes must be determined. Taking into account this set of decisions, linear generalized disjunctive programing (LGDP) result a reasonable option to represent this problem. LGDP uses disjunctions and logic propositions in terms of Boolean variables to formulate problems, facilitating the representation of discrete choices and a better understanding of complex models with many embedded disjunctions.[6,27–29]

Therefore, a linear model is proposed for the multiproduct batch plant design, including detailed description of the operations through process performance models. Duplication in parallel and in series are allowed. This last option requires specific models for all the operations depending on the selected number of units in series. Then, a new approach is proposed based on structural alternatives for the plant.

The remainder of the article is organized as follows. The next section describes the characteristics of the problem, whereas, in the following section, the general model using LGDP is presented. Then, the fourth section is devoted to describe the design of a plant that manufactures herbal extracts, specifically oleoresins. A numerical example is given in fifth section. Finally, the last section summarizes some concluding remarks.

Problem Description

A multiproduct batch plant manufactures I products through P batch operations. For each product i ($i = 1, 2, \ldots, I$), the required demand q_i to be satisfied in a time horizon H is known. Every operation p ($p = 1, 2, \ldots, P$) can be performed by different configurations of units in series h. Let H_p be the set of possible configurations h to perform the operation p. It should be emphasized that the units belonging to a configuration in series can take equal or different sizes, depending on the unit operation being performed.

As mentioned in previous section, the selected option for the duplication of units in series in every operation not only affects itself but also the rest of the operations in the plant. Consequently, the concept of structural alternative of plant a, introduced by Moreno et al.,[23] is used in this work. A structural alternative allows to define a set of process performance models that corresponds to that configuration. Different structural alternatives require different process performance models. Thus, A, the total number of structural alternatives of the plant, is determined by all the possible combinations among every configuration in series h in each operation p of the plant $\left(A = \prod_{p=1}^{P} H_p\right)$. Figure 1 shows an example with a plant with two operations where the first operation can be duplicated in series up to two units ($H_1 = 2$) and the second one up to three units ($H_2 = 3$). Hence, the total number of structural alternatives of this plant is $A = 6$.

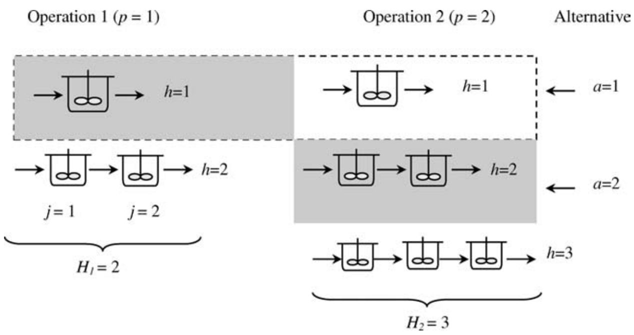

Figure 1. Structural alternatives a in the plant.

Also, in Figure 1, two of the six possible structural alternatives in this plant are highlighted. The first structural alternative of the plant ($a = 1$) is closed by the dashed line and corresponds to one unit in the first operation ($p = 1$ and $h = 1$) and one unit in the second operation ($p = 2$ and $h = 1$). The second alternative ($a = 2$) corresponds to one unit in the first operation ($p = 1$ and $h = 1$) and two units in series in the second one ($p = 2$ and $h = 2$), that is, the structure in gray in Figure 1.

In this way, when a particular structural alternative a is selected in a plant, a sequence of stages j for every operation p is determined. Let J_{pa} be the set of stages j included in the operation p for the structural alternative a. Now, each stage j in the operation p can be duplicated in parallel, working out-of-phase. Let M_p^{U} be the maximum number of units that can be added in parallel in the operation p.

To formulate an optimization model, the following assumptions are adopted.

(1) The plant operates in single product campaign (SPC) mode.

(2) A zero wait (ZW) transfer policy between batch stages is adopted.

(3) Parallel units operating out of phase are identical.

(4) Equipment items are available in discrete sizes.

(5) Allocation of intermediate storage tank is not allowed.

The first assumption is usually adopted in batch plant design: all the batches of a product are successively processed without overlapping with other products. Also, the second assumption means that a batch processed in a unit is immediately transferred to the following unit. Parallel units operating out-of-phase allow to decrease the cycle time, increasing the production rate of the products.

Assumption (4) follows the usual procurement policy. The equipment size for any stage j of the batch operation p, V_{jp}, is restricted to take values from the set $SV_{jp} = \{v_{jp1}, v_{jp2}, \ldots, v_{jp,n_{jp}}\}$, where v_{jps} represents a discrete size s for the batch unit at stage j in operation p and n_{jp} is the given number of available discrete sizes from the commercial point of view for that operation.

On the other hand, the process decision variables that have the largest impact on the economics of the process for each product have been selected. As multiple products are produced in the plant, the variable e_{il} is used to represent the process variable l for the product i, where $l = 1, 2, \ldots, L$. Then, L corresponds to the total number of process variables for product i. In this work, it is assumed that all the product recipes are similar and the same decision variables have been selected for all the products. More detailed models can be formulated where this number is different for each product and L_i must be used. Each variable e_{il} can affect either just the operation that introduces it, or other operations of the process. Then, size and time factors of every product for each stage of every operation can be expressed as a function of these process decision variables. As the duplication of units in series adopted in an operation not only affects itself but also the models corresponding to other operations in the plant, these factors are different functions depending on the structural alternative of the plant a.

Thus, each structural alternative a determines an expression for the size S_{ijpa} and time t_{ijpa} factors of each product i in every stage j of the operations p. Each expression is a function of the process variables e_{il}.

To attain a linear model, it is assumed that each process variable e_{il} is restricted to take values from a set of discrete values $SL_{il} = \{g_{il1}, g_{il2}, \ldots, g_{ild_{il}}\}$ where g_{ilr_l} represents the discrete value r_l of the process variable l for the final product i and d_{il} is the number of available values for that variable. These values are good estimates of the process variables based on the experience of the designer for that particular batch process.

The linear model proposed in the following section optimizes the process variables simultaneously with the plant structure of a batch process, that is, duplication in series in each operation, duplication in parallel in each stage, and the selection of unit sizes, minimizing the total costs of the plant.

Mathematical Formulation

In this section, a detailed LGDP model for the aforementioned problem is formulated. The discrete choices involved in this formulation are represented by means nested disjunctions presented in Eq. 1.

$$\bigvee_{a\in A}\left[\begin{array}{c} Z_a \\ \bigvee_{\substack{r_l\in SL_{il}\\ l=1,\ldots,L}}\left[\begin{array}{c} O_{\mathrm{air}_1,r_2,\ldots,r_L} \\ S_{ijp}=f_a^S(g_{ilr_l}) \quad \forall j\in J_{pa},p \\ t_{ijp}=f_a^t(g_{ilr_l}) \quad \forall j\in J_{pa},p \end{array}\right] \quad \forall i \\ \bigvee_{s\in SV_{jp}}\left[\begin{array}{c} W_{jpsa} \\ n_i \ge \left(\frac{S_{ijp}}{v_{jps}}\right) q_i \quad \forall_i \\ \mathrm{CO}_{jp}=\alpha_p v_{jps}^{\beta_p} \end{array}\right] \quad \forall j\in J_{pa},p \\ \bigvee_{m\in M_p}\left[\begin{array}{c} Y_{jpma} \\ T_i \ge \frac{\sigma_{ijp}}{m} \quad \forall i \\ \mathrm{CB}_{jp}=m\mathrm{CO}_{jp} \end{array}\right] \quad \forall j\in J_{pa},p \\ C_p=\sum_{j\in J_{pa}} \mathrm{CB}_{jp} \quad \forall p \end{array}\right] \quad (1)$$

The main disjunction in Eq. 1 is formulated to model the structural alternatives of the plant. It has a term for each possible structural alternative $a \in A$ that the plant can adopt to carry out the whole process. In the optimal solution, only one alternative will be selected and just the constraints included in the corresponding term must be satisfied. The variable Z_a is a Boolean variable, which is true if alternative a is the one to be in the plant and is false in the opposite case. Once the plant structure is selected, three new decisions have to be made through nested disjunctions: the first one is valid for each product i, whereas the other two are valid for each stage j in every unit operation p.

In the first inner disjunction in Eq. 1, the discrete values for the process variables are selected for every product. Here, the Boolean variable $O_{air_1,r_2,\ldots,r_L}$ is true when the discrete value r_1 is adopted for the first process variable ($l = 1$), the discrete value r_2 is adopted for the second process variable, and continuing in the same way, until the discrete value r_L is adopted for the last process variable of the product i. Thus, a unique combination of discrete values is adopted for all the process variables. In the second inner disjunction, Boolean variables W_{jpsa} are defined to determine the standard size of the batch units in the plant. If W_{jpsa} is true, the discrete size s is selected for process equipment at stage j in operation p. Finally, in the last nested disjunction, the Boolean variable Y_{jpma} is defined to decide the duplication in parallel. If Y_{jpma} is true, m units in parallel working out-of-phase at stage j are chosen to carry out that stage of the operation p for alternative a.

Now, the description of individual constraints included in each disjunction is discussed. As was previously mentioned, the complete formulation includes process performance models for the unit operations in the plant. These models describe time and size factors as functions of the process variables selected for optimization. These functions are expressed as algebraic equations obtained from the analytical integration of simplified mass balances and kinetic expressions that describe each unit operation. They are kept as simple as possible while retaining the influence of the process variables selected to optimize the plant. Thus, in the first embedded disjunction the performance models are included as follows:

$$S_{ijp} = f_a^S(g_{ilr_l}) \quad \forall\, i, j \in J_{pa}, p, a \tag{2}$$

$$t_{ijp} = f_a^t(g_{ilr_l}) \quad \forall\, i, j \in J_{pa}, p, a. \tag{3}$$

The functions f_a^S and f_a^t corresponding to the size and time factors, respectively, indicate that their expressions depend on the structural alternative a, that is, the functionality of the size and time factors with the process variables is different for each structural alternative of the plant. To tackle this situation, LGDP formulation offers the advantage of representing each alternative separately.

If the variable $O_{air_1,r_2,\ldots,r_L}$ is true in the optimal solution, then discrete values g_{ilr_l} are selected for all process variables e_{il}. In this way, Eqs. 2 and 3 allow calculating the values of size and time factors for the chosen alternative a.

In a batch plant, the sizing equation that determines the size V_{jp} of the process equipment at stage j performing operation p is given by:

$$V_{jp} \geq S_{ijp} B_i \quad \forall\, i, j, p. \tag{4}$$

For each product i, the amount produced q_i, the batch size B_i, and the number of batches n_i, are related by means of the following equation:

$$B_i = \frac{q_i}{n_i} \quad \forall\, i. \tag{5}$$

By substituting Eq. 5 into Eq. 4, the constraint takes the following form:

$$n_i \geq \left(\frac{S_{ijp}}{V_{jp}}\right) q_i \quad \forall\, i, j, p. \tag{6}$$

As mentioned earlier, equipment sizes V_{jp} are assumed available in a set of standard and discrete sizes v_{jps}. Thereby, the following linear constraint is posed in the second nested disjunction to determine the volume of the units in every operation.

$$n_i \geq \left(\frac{S_{ijp}}{v_{jps}}\right) q_i \quad \forall\, i, j, p, s \tag{7}$$

where the size of the unit v_{jps} is a constant value. It should be noted that in each operation and in each stage, only one option W_{jpsa} will be true, so only one expression in Eq. 7 must be satisfied. In other words, if the variable W_{jpsa} is true in the solution, the discrete size v_{jps} is selected at stage j in operation p for the structural alternative a. Otherwise, if W_{jpsa} is false, the corresponding expression will not be considered.

Furthermore, in these embedded disjunctions, the constraint in Eq. 8 calculates the investment cost CO_{jp} of the unit size at stage j in each operation p for the alternative selected. Parameters α_p and β_p are cost coefficients distinctive of each batch operation p.

$$\mathrm{CO}_{jp} = \alpha_p v_{jps}^{\beta_p} \quad \forall\, j \in J_{pa}, p, s. \tag{8}$$

Taking into account that v_{jps} is a discrete size, CO_{jp} can be directly assessed using the value provided by the supplier. In this formulation, Eq. 8 has been expressed maintaining the traditional notation used in previous works of this area.

Constraints in the last inner disjunction consider the addition of parallel units at each stage j in operation p, taking into account all the stages included in the structural alternative a selected previously in the outer disjunction. The limiting cycle time for product i, TL_i, is the shortest possible time between two consecutive batches of product i leaving the plant. It is given by the longest processing time among all the stages in the plant for product i. To reduce the cycle time for a particular product, duplicated units working out-of-phase can be introduced. If the Boolean variable Y_{jpma} is true, m identical units in parallel are selected for stage j associated with operation p. Then, the cycle time of product i in period t is determined by:

$$\mathrm{TL}_i \geq \frac{t_{ijp}}{m} \quad \forall\, i, j, p, m \tag{9}$$

taking into account that only one option will be selected through Boolean variables Y_{jpma}. The total time for producing product i is defined as:

$$T_i = n_i \mathrm{TL}_i \quad \forall\, i. \tag{10}$$

By multiplying Eq. 9 by the number of batches n_i, and, substituting for T_i from Eq. 10, gives:

$$T_i \geq \left(\frac{t_{ijp}}{m}\right) n_i \quad \forall i, j, p, m. \tag{11}$$

Constraint in Eq. 11 is nonlinear because of the product of the variables t_{ijp} and n_i. To eliminate this cross-product, a new variable σ_{ijp} is defined to represent these bilinear terms.

$$\sigma_{ijp} = t_{ijp} n_i \quad \forall i, j, p. \tag{12}$$

This substitution is enabled taking into account the disjunctive formulation adopted. Considering that only one variable $O_{air_1, r_2, \ldots, r_L}$ is true, then particular values have been selected for the process variables. Therefore, Eq. 12 is expressed using only variable n_i since the variables that define t_{ijp} are constant in each term of the disjunction. Thus, a linear expression is attained. In this presentation, it has been preferred to maintain the time factors in the first inner disjunction to simplify the explanation. However, in the real mathematical formulation, variables σ_{ijp} are included in the first inner disjunction, involving linear expressions with n_i.

Thus, the expression takes the form used in the last embedded disjunction:

$$T_i \geq \frac{\sigma_{ijp}}{m} \qquad \forall i, j, p, m. \tag{13}$$

In this expression, m is a constant value for each option. When the Boolean variable Y_{jpma} is true, then the corresponding discrete value m is used.

Moreover, the Eq. 14 introduced in this disjunction corresponds to the total investment cost CB_{jp}, which accounts for the cost of the unit size, CO_{jp}, and the number of parallel units m selected at every stage j in each operation p.

$$\mathrm{CB}_{jp} = m\mathrm{CO}_{jp} \qquad \forall j, p, m. \tag{14}$$

Finally, the last constraint (Eq. 15) in the outer disjunction in Eq. 1 allows for calculating the investment cost value C_p in each operation for the structural alternative a selected for the batch plant (Z_a = True). This cost takes into account all the stages j included in the operation p.

$$C_p = \sum_{j \in J_{pa}} \mathrm{CB}_{jp} \quad \forall p. \tag{15}$$

Whereas the above equations and inequality constraints are contained in disjunctions of Eq. 1, there are further inequality constraints (Eq. 16) that remain irrespective of discrete alternatives. Considering the SPC-ZW policies, all products must be produced within production horizon H, which is expressed by the following constraint:

$$\sum_i T_i \leq H. \tag{16}$$

The objective function for the multiproduct batch plant design problem consists in minimizing the total investment cost CT, which is written as:

$$\min \mathrm{CT} = \sum_p C_p. \tag{17}$$

In summary, the final model LGDP implies minimizing the investment cost represented by Eq. 17 subject to Eqs. 1 and 16 plus bound constraints on the model variables.

Before solving the above LGDP model, the disjunctions and propositions need to be converted to a mixed integer linear program (MILP). This reformulation can be done in different ways, including the two most common alternatives, big-M (BM) and convex hull (CH). Following the results of Vecchietti et al.[28] that have analyzed the advantages and disadvantages of the available approaches, in this work, the CH reformulation has been used because it provides a tighter relaxation. Appendix B details all the equations of this relaxation.

Application to Oleoresin Production

The considered example is a batch plant for the production of multiple oleoresins to be manufactured by solid–liquid extraction.[23] This plant involves six unit operations as is shown in the flowsheet of Figure 2. In practice, the batch process for the production of oleoresins consists of a series of batch and semi-continuous operations. In contrast with a batch operation, where units operate discontinuously, in a semi-continuous operation, the unit runs continuously with periodic start-ups and shutdowns. It should be stressed that extraction, pressing, and blending operations are performed by batch units whereas the rest of the operations use semi-continuous units. Also, it must be noted that only the batch operation of extraction admits the duplication of units in series in this particular example.

In the following paragraphs, the operations involved in the manufacture of oleoresins are described and the process decision variables with the largest impact on the process are selected. For a detailed analysis of the selection criteria of the process decision variables, see Moreno et al.[23]

In the grinding operation, the particle size of raw material that enters into the mill da is reduced to a particle size db. This size reduction is carried out to increase the surface area (i.e., greater contact area) because it increases the extraction rate in the next operation. However, further size reduction requires much more power of the mill. Thus, the particle size db is selected as an optimization variable due to the trade-off between smaller sizes that allow increasing the extraction rate in the next operation and the greater power of the mill needed to produce such size reduction.

Extraction operation involves the separation of a soluble constituent (oleoresin) of a solid phase (herbs or spices) with an organic solvent (ethanol). This type of operation may be performed in one or multiple stages. A pure solvent enters to the first unit in the battery of extractors and flows in the opposite direction to the solid. Therefore, a series of units or stages in a countercurrent arrangement is used. This task

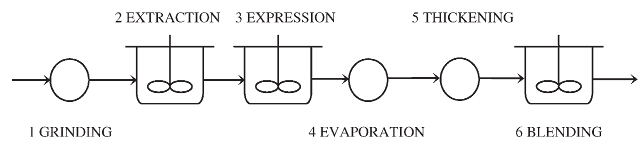

Figure 2. Operations in the batch plant for the production of oleoresins.

introduces the mass ratio of solvent to solid, E, and the extent of the extraction, η, as optimization variables. Both variables have an economic impact on the process. For example, larger ratios of solvent to solid increase the yield of the extracted solute per kilogram of raw material, but the cost of recovery of the spent solvent is increased.

The separation of the solution (liquid extract) from the insoluble solid is carried out by means of hydraulic pressure in the operation of expression. A larger amount of the desired product can be obtained by increasing the extent of the expression, ε, but the time used to carry out the operation is increased. On the contrary, if the extent is small, both desired product and solvent are lost with the solid residues of the plant.

In the operation of evaporation, given a specified maximum mass fraction of solvent in the product $y_{i,\mathrm{eva}}^{\mathrm{out}}$, a falling-film evaporator is used to separate the solvent of the fluid final product. The higher the solvent to solid mass ratio E used in the previous extraction operation, the bigger the amount of solvent to evaporate (i.e., the greater the evaporation cost).

The concentration of the product is increased by a rotary drum evaporator in the operation of thickening. Here, the residual solvent is separated from the final semi-solid product.

In the last operation, the oleoresin must be mixed with soluble agents, polysorbate 80, and/or fluid additives to give a final product with the desired specifications. The proportions are variables and obtained from product development, but in this case they are estimated in 20%.

To sum up, the process decision variables selected in this example are the particle size leaving the mill (db), the mass ratio of solvent to solid (E), the extent of the extraction (η), and the extent of the expression (ε).

The process performance models involve additional equations to determine size and time factors which depend on the previously mentioned process variables. In Appendix A, the algebraic equations that describe them for each unit operation of this process are presented. In this section, only general expressions of each size and time factor as a function of the involved process variables are presented. Taking into account the aforementioned relations, the following equations can be posed:

$$S_{i,\mathrm{ext}} = f_a^S(E_i, \varepsilon_i, \eta_i) \quad \forall\, i, a \tag{18}$$

$$S_{i,\mathrm{pre}} = f_a^S(E_i, \varepsilon_i, \eta_i) \quad \forall\, i, a \tag{19}$$

$$D_{i,\mathrm{gri}} = f_a^D(E_i, \varepsilon_i, \eta_i, db_i) \quad \forall\, i, a \tag{20}$$

$$D_{i,\mathrm{eva}} = f_a^D(E_i, \eta_i) \quad \forall\, i, a \tag{21}$$

$$t_{i,\mathrm{ext}} = f_a^t(E_i, \eta_i, db_i) \quad \forall\, i, a \tag{22}$$

$$t_{i,\mathrm{pre}} = f_a^t(\varepsilon_i) \quad \forall\, i, a. \tag{23}$$

The remaining unit operations are described through fixed size and time factors.

As was previously mentioned, in this process, some operations are performed by semi-continuous units. Considering that the constraints for calculating the capacity of the units in semi-continuous operations are different from the batch ones, the subscripts k will be used for the semi-continuous operations of grinding, evaporation, and thickening included in this process. Thus, in the above equations, D_{ik} is used to represent the size factor, known as the duty factor of product i for semi-continuous operation k. Similar to batch operations, it is a function of the process decision variables and depends on the adopted structural alternative for the plant.

To formulate the LGDP model for this process, first some further definitions and assumptions have to be made. First, each process decision variable is assumed to be restricted to take values from a set of discrete values. In this way, the mass ratio of solvent to solid for each product, E_i, can take values from the set $SC_i = \{E_{i1}, E_{i2}, \ldots, E_{i,nE_i}\}$, where E_{ic} represents the discrete value c for product i and nE_i is the given number of discrete values available for product i. An analogous situation occurs for the other process variables, that is η_i, db_i, and ε_i take values from the sets $SB_i = \{\eta_{i1}, \eta_{i2}, \ldots, \eta_{i,n\eta_i}\}$, $SD_i = \{db_{i1}, db_{i2}, \ldots, db_{i,ndb_i}\}$, and $SF_i = \{\varepsilon_{i1}, \varepsilon_{i2}, \ldots, \varepsilon_{i,n\varepsilon_i}\}$, respectively. Thereby, η_{ib} represents the discrete value b that adopts the extent of the extraction for product i in the operation of extraction; db_{id} is the value d that adopts the particle size of product i leaving the mill, and ε_{if} is the discrete value f adopted for the extent of the expression for product i.

On the other hand, it is necessary to add the sizing of semi-continuous operations to the general model proposed in the previous section. In a similar way to batch operations, the unit size R_k in the semi-continuous operation is restricted to take discrete values from the set $SR_k = \{\omega_{k1}, \omega_{k2}, \ldots, \omega_{km_k}\}$, where ω_{ku} denote the size u for the unit in the semi-continuous operation k.

Considering previous definitions, the LGDP model for the multiproduct batch plant that produces oleoresins can be written as:

$$\bigvee_{a\in A}\left[\begin{array}{c}
Z_a \\
\bigvee_{\substack{c\in SC_i\\ b\in SB_i\\ f\in SF_i\\ d\in SD_i}}\left[\begin{array}{c}
O_{aicbfd} \\
D_{i,\mathrm{gri}} = f_a^D(E_{ic}, \varepsilon_{if}, \eta_{ib}, db_{id}) \\
S_{i,j,\mathrm{ext}} = f_a^S(E_{ic}, \varepsilon_{if}, \eta_{ib}) \\
t_{i,j,\mathrm{ext}} = f_a^t(E_{ic}, \eta_{ib}, db_{id}) \\
S_{i,j,\mathrm{pre}} = f_a^S(E_{ic}, \varepsilon_{if}, \eta_{ib}) \\
t_{i,j,\mathrm{pre}} = f_a^t(\varepsilon_{if}) \\
D_{i,evap} = f_a^D(E_{ic}, \eta_{ib}) \\
CM_i = \kappa_i f_a^{CM}(E_{ic}, \eta_{ib}) \\
CS_i = c_{\mathrm{solv}} f_a^{CS}(E_{ic}, \eta_{ib})
\end{array}\right] \quad \forall i \\
\\
\bigvee_{s\in SV_p}\left[\begin{array}{c}
W_{jpsa} \\
n_i \geq \left(\frac{S_{ijp}}{v_{jps}}\right) q_i \quad \forall i \\
\mathrm{CO}_{jp} = \alpha_p v_{jps}^{\beta_p}
\end{array}\right] \quad \forall j \in J_{pa}, p \\
\\
\bigvee_{u\in SR_k}\left[\begin{array}{c}
G_{kua} \\
\xi_{ib} \geq \left(\frac{D_{ik}}{\omega_{ku}}\right) q_i \quad \forall i, b \\
CR_k = \gamma_k \omega_{ku}^{\delta_k}
\end{array}\right] \quad \forall k \in b \\
\\
\bigvee_{m\in M_p}\left[\begin{array}{c}
Y_{jpma} \\
T_i \geq \frac{\xi_{ib_p^u} + \sigma_{ijp} + \xi_{ib_p^d}}{m} \quad \forall i \\
\mathrm{CB}_{jp} = m\,\mathrm{CO}_{jp}
\end{array}\right] \quad \forall j \in J_{pa}, p \\
C_p = \sum_{j\in J_{pa}} \mathrm{CB}_{jp} \quad \forall p
\end{array}\right] \tag{24}$$

Next, all the expressions will be explained for this particular example. Here, in the first nested disjunction in Eq. 24, the Boolean variable O_{aicbfd} is true if the mass ratio of solvent to solid, the extent of the extraction, the extent of the pressing, and the particle size take discrete values c, b, f, and d, respectively. Otherwise, the variable O_{aicbfd} is false. Thus, in each term, all the variables E_{ic}, η_{ib}, db_{id}, and ε_{if} take discrete values. Then, the size and time factors can be calculated through different and specific expressions for each structural alternative a selected for the plant. In this way, each term of the first nested disjunction corresponds to a specific combination of discrete values of the process variables to determine the time and size factors. Therefore, when the variable O_{aicbfd} is true, specific time and size factors are attained whereas all the remaining expressions with O_{aicbfd} false are discarded. Thus, only one set of size and time factors is determined to be used in the remaining disjunctions.

The above disjunction in Eq. 24 presents an additional embedded disjunction with respect to Eq. 1. The third nested disjunction is used to consider the selection of the equipment size for semi-continuous operations of the process and is formulated in the same way as the second one (batch units). The Boolean variable G_{kua} is true when the standard discrete size u is used to carry out the semi-continuous operation k and the structural alternative a is selected for the plant. In the following discussion, details of the constraints within this disjunction are explained.

The processing time of product i for semi-continuous unit k, θ_{ik}, can be calculated by[30]:

$$\theta_{ik} \geq \frac{D_{ik}B_i}{R_k} \quad \forall\, i,k. \tag{25}$$

Furthermore, a semi-continuous subtrain b consists of a sequence of semi-continuous units with no batch unit among them. To avoid accumulation of material, all the units belonging to subtrain b must operate for the same length of time. In this way, the operating time of a semi-continuous subtrain ϕ_{ib} is the maximum processing time of all semi-continuous units k that belong to that subtrain, then:

$$\phi_{ib} \geq \frac{D_{ik}B_i}{R_k} \quad \forall\, i,b,k \in b. \tag{26}$$

Multiplying both sizes by n_i and taking into account Eq. 5 gives:

$$\phi_{ib}n_i \geq \frac{D_{ik}}{R_k}q_i \quad \forall\, i,b,k \in b. \tag{27}$$

Constraint in Eq. 27 is nonlinear because of bilinear terms $\phi_{ib}\, n_i$. To reformulate this equation as a linear expression, a new variable has to be introduced in the formulation:

$$\xi_{ib} = \phi_{ib}n_i \quad \forall\, i,b. \tag{28}$$

Furthermore, as pointed out in previous sections, variables R_k are considered available in a set SR_k of discrete sizes ω_{ku}. In this way, Eq. 27 can be posed as a linear expression in Eq. 24 as follows:

$$\xi_{ib} \geq \left(\frac{D_{ik}}{\omega_{ku}}\right)q_i \quad \forall\, i,b,k \in b,u. \tag{29}$$

Equation 30 in the third nested disjunction represents the investment cost for the unit in semi-continuous operation k, CR_k. Here, the parameters γ_k and δ_k are cost coefficients for semi-continuous operations.

$$CR_k = \gamma_k \omega_{ku}^{\delta_k} \quad \forall\, u,k. \tag{30}$$

Following the comment in Eq. 8, this expression can be replaced by the cost provided by the supplier.

Finally, the last embedded disjunction in Eq. 24 considers the addition of units in parallel in each operation p. Here, the constraint for calculating the total time for producing product i is different from the one presented previously because of the presence of semi-continuous units in the process. Thus, the limiting cycle time is given by the following expression:

$$\mathrm{TL}_i \geq \frac{\phi_{ib_p^u} + t_{ijp} + \phi_{ib_p^d}}{m} \quad \forall\, i,j,p \tag{31}$$

where $\phi_{ib_p^u}$ is the feeding time and $\phi_{ib_p^d}$ is the discharging time, corresponding to the upstream and downstream semi-continuous subtrains, of the batch operation p. The total time for producing product i, T_i, can be then calculated by multiplying the above constraint by the number of batches n_i, as shown by the following expression:

$$T_i \geq \frac{\phi_{ib_p^u}n_i + t_{ijp}n_i + \phi_{ib_p^d}n_i}{m} \quad \forall\, i,j,p. \tag{32}$$

Then, substituting from Eq. 28 into Eq. 32, and considering the variable defined in Eq. 12, the expression into the last nested disjunction in Eq. 24 is attained:

$$T_i \geq \frac{\xi_{ib_p^u} + \sigma_{ijp} + \xi_{ib_p^d}}{m} \quad \forall\, i,j,p. \tag{33}$$

On the other hand, when semi-continuous units are included in the process, the limiting cycle time, TL_i, is obtained considering the maximum time of all operations in the process, that is, both batch and semi-continuous operations. Thus, the following expression has to be also included:

$$\mathrm{TL}_i \geq \phi_{ib} \quad \forall\, i,b. \tag{34}$$

Multiplying Eq. 34 by the number of batches n_i and considering Eq. 12, an additional expression for the total time T_i is obtained:

$$T_i \geq \xi_{ib} \quad \forall\, i,b. \tag{35}$$

Furthermore, it can be seen in the first nested disjunction of Eq. 24 that additional constraints are included corresponding to the cost of the raw material, CM_i, and the cost of the solvent, CS_i. The amounts of raw material and the solvent fed to the extractor affect the total cost in this process.

Table 1. Product Data for the Example

Product	Name	Production q_i (kg year^{-1})	Initial Concentration x_i^{in}	Raw Material Cost (\$ kg^{-1})
A	Sweet bay	12,000	0.10	1.00
B	Rosemary	14,000	0.05	0.80

Hence, they must be included in the objective function. Thereby, the trade-offs between process decision variables, unit sizes, and the resources used in the process are considered simultaneously.

The variables $x_{i,\text{ext}}^{\text{in}}$ and $x_{i,\text{ext}}^{\text{out}}$ are the mass fractions of product i in the solid at the entry and the exit of the extractor, respectively. Moreover, the variable $y_{i,\text{ext}}^{\text{out}}$ is the mass fraction of product i (solute) in the liquid extract at the exit of the battery of extractors. To get a more compact formulation, the variables $x_{i,\text{ext}}^{\text{out}}$ and $y_{i,\text{ext}}^{\text{out}}$ are kept as intermediate process variables of the extraction operation in the formulation. They are functions of the process decision variables E_i and η_i. Also, as it is detailed in Appendix A, they are expressed by different functions depending on the structural alternative a that is selected in the plant according to the configuration in series in the extraction operation (p = ext).

Thus, the amount of total solid raw material fed to the extractor, RM_i, used to elaborate the demand of the product i, q_i, is given by:

$$\text{RM}_i = \frac{q_i}{\left(x_{i,\text{ext}}^{\text{in}} - x_{i,\text{ext}}^{\text{out}}\right)} \quad \forall\, i. \tag{36}$$

The cost of the raw material necessary for the production is then estimated by multiplying RM_i by the parameter κ_i, the purchase price per kg of the raw material used to elaborate oleoresin i.

$$CM_i = \kappa_i RM_i \quad \forall\, i. \tag{37}$$

Also, the required amount of solvent Solv_i (kg) can be calculated through the process variable E_i, which relates it to the amount of solid raw material RM_i, by means of the following expression:

$$\text{Solv}_i = E_i \text{RM}_i \quad \forall\, i. \tag{38}$$

Ethanol was used as the extraction solvent for all products in this process. Then, the total cost of the solvent may be written as:

$$CS_i = c_{\text{solv}} E_i \text{RM}_i \quad \forall\, i \tag{39}$$

Table 2. Cost of Equipment

Operation	Size	Cost
Grinding	R_k (kW)	5700 $R^{0.45}$
Extraction	V_p (L)	6920 $V^{0.6}$
Expression	V_p (L)	6820 $V^{0.6}$
Evaporation	R_k (m^2)	5500 $R^{0.5}$
Thickening	R_k (m^2)	5100 $R^{0.55}$
Blending	V_p (L)	5570 $V^{0.6}$

Table 3. Discrete Values for the Process Variables of Each Product

	Product A				Product B			
Option	E_{ic}	η_{ib}	ε_{if}	db_{id}	E_{ic}	η_{ib}	ε_{if}	db_{id}
1	1.00	0.38	0.40	0.01	1.00	0.39	0.40	0.01
2	2.50	0.50	0.55	0.03	2.50	0.50	0.55	0.03
3	3.50	0.65	0.75	0.05	3.50	0.65	0.75	0.05
4	5.00	0.70	0.85	0.10	5.00	0.80	0.85	0.10

where c_{solv} is the recovery cost per kg of solvent. From Eqs. 36,37, and 39 it may be noted that CM_i and CS_i are functions of the process variables E_i and η_i. Hence, these constraints can be expressed as a function of these variables. Then, they are included into the first nested disjunction where the discrete values for the process variables are chosen.

Therefore, the final objective function for the presented process consists of minimizing the total cost of the process CT in the time horizon H.

$$\min \text{CT} = \sum_p C_p + \sum_k CR_k + \sum_i CM_i + \sum_i CS_i. \tag{40}$$

The last two terms in the objective function correspond to the cost of raw material and the cost of solvent, respectively, used in the process to manufacture the required quantities of products in the production time horizon.

To sum up, the whole model for the design of the multiproduct batch plant that produces oleoresins through a linear generalized disjunctive problem (LGDP) is defined by minimizing the objective function in Eq. 40 subject to Eqs. 16, 24, and 35 plus bounds constraints that may apply.

Numerical Results and Discussion

In this section, the results of the proposed model are analyzed and discussed. The problem is modeled and solved within the GAMS modeling environment using the code CPLEX 9.0 as the MILP solver, with a 0% integrality gap. The computations were carried out on a PC Intel (R) Core2, 1.86 GHz with a 2.00 GB of RAM.

In this work, the same batch plant considered in Moreno et al.[23] is taken as illustrative example. The plant produces two oleoresins, namely sweet bay (A) and rosemary (B), using pure ethanol as the solvent. A global time horizon of 1 year (6000 h) has been considered. Table 1 shows the demand and mass fraction in every raw material to manufacture each product.

The cost coefficients α_p and β_p for batch operations, and γ_k and δ_k for semi-continuous operations to be considered in

Table 4. Standard Available Sizes for Each Operation

	Discrete Volumes (v_{ps})			Discrete Sizes (ω_{ku})		
Option	2	3	6	1	4	5
1	100	30	5	7	0.5	0.2
2	300	100	10	10	1	0.5
3	500	200	20	20	2	1
4	1000	500	30	25	3	1.5
5	2000	1000	50	30	5	2

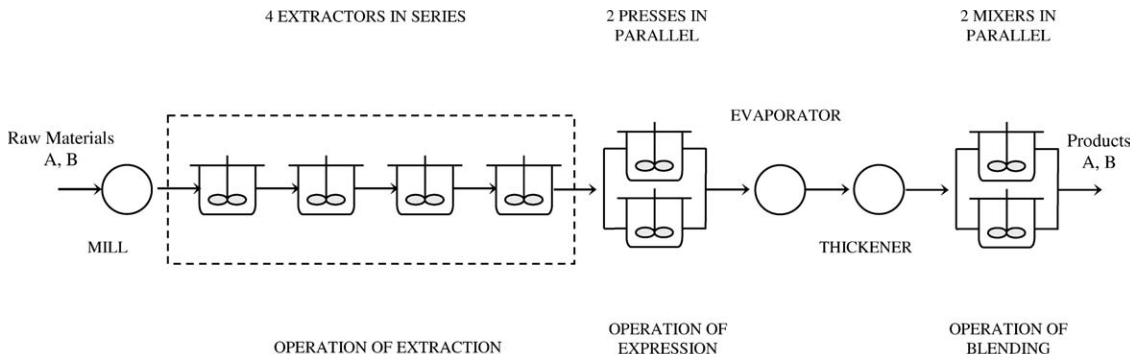

Figure 3. Optimal plant structure for the production of oleoresins.

the design are listed in Table 2. The recovery cost c_{solv} of the solvent is assumed to be 0.05 \$ kg^{-1}.

The upper bound for the number of stages in the battery of extractors is six. Thus, there are six possible configurations of units in series to carry out this operation ($H_2 = 6$). It should be reminded that the number of structural alternatives for the plant is calculated by ($A = \prod_{p=1}^{P} H_p$). Therefore, there are six potential plant structures $A = 6$. Furthermore, all batch operations can be duplicated in parallel up to four units ($M_p^{\text{U}} = 4$) working out-of-phase.

The estimated values that can be taken by each decision process variable are given in Table 3. Table 4 shows the available discrete sizes for each operation.

The objective function for this problem has a value of \$1,818,411. The convex hull reformulation involves 3120 binary variables out of a total of 15,685 variables, whereas the number of constraints is 18,872. The results for the optimal structure for the plant of this example are shown in Figure 3, where it can be seen that four stages in series were selected to carry out the extraction operation. Also, there are two units in parallel working out of phase in the batch operations of pressing and blending. It is interesting to note that the optimal plant structure found is the same as that obtained by Moreno et al.[23]

Comparison of MILP and MINLP models

Taking into account the previous contribution with detailed performance MINLP models by Moreno et al.[23] where the same problem has been solved, a comparison between both approaches is addressed. Therefore, the results of the proposed MILP formulation are jointly presented with the ones of the predecessor contribution to achieve an effective appraisal of both works. Table 5 lists the values of decision variables attained in the optimal solution whereas Table 6 reports optimal sizes selected for each unit used to carry out the operations and the plant structure for this process. The summary of the processing times in each operation and the limiting cycle time for every product are shown in Table 7. Finally, Table 8 reports data about the performance of the models: numbers of variables and constraints and required CPU times. In Table 5, the results for the MINLP problem are expressed with four decimal digits while the MILP ones with only two because the first ones have been obtained from a continuous range while the second ones have been selected from a set of discrete values proposed by the designer.

By examining the results reported in Tables 5–8, a comparison between MILP and MINLP models can be made. First, the selected values for the process variables are approximate to the values of the previous formulation. Also, the unit sizes chosen in the solution of the MILP problem are the closest discrete values to the continuous ones found in the nonlinear model. Therefore, the resulting total cost of the plant in this case is ~4% higher than the value of the original MINLP solved in the previous work (\$1,748,080). Taking into account these results, operation times and cycle times are relatively similar to the exact values (Table 7).

Though both contributions solve the same problem, the results must be carefully assessed, including the performance indicators (Table 8). First, as Moreno et al.[23] have remarked, the MINLP model is nonlinear and nonconvex; hence, the obtained solution will depend on the starting point and global optimality cannot be guaranteed. The available MINLP algorithms (for example DICOPT, based on the extensions of the outer-approximation algorithm for the equality relaxation strategy[31]) can miss the optimal solution through the application of linear cuts to nonconvex regions. MINLP problems are usually solved through methodologies that successively solve mixed integer linear (MILP) approximations to the model, and NLP problems for fixed configurations, where the values of binary variables have been fixed. For the case of nonconvex problems, this mechanism presents the drawback that successive linearizations usually cut part of the feasible region. In this way, some solutions to the problem can be lost. In addition, many plant configurations, which are found through MILP subproblems, correspond to nonfeasible structures, that do not fulfill production requirements.

Table 5. Discrete Values Adopted for the Process Variables in the Optimal Solution

Model	Product	E_i	η_i	ε_i	db_i (cm)
MILP	A	1.00	0.38	0.75	0.01
	B	1.00	0.39	0.75	0.01
MINLP[23]	A	1.0000	0.3763	0.7017	0.0100
	B	1.0000	0.3838	0.7327	0.0100

Table 6. Optimal Sizes and Duplication of Units in Each Operation

Model		Operations 1	2	3	4	5	6
MILP	Sizes	30.00 (kW)	300.00 (L)	100.00 (L)	5.00 (m^2)	0.20 (m^2)	5.00 (L)
	Units in parallel	–	1	2	–	–	2
	Units in series	–	4	1	–	–	1
MINLP[23]	Sizes	22.371 (kW)	280.068 (L)	69.735 (L)	5.000 (m^2)	0.200 (m^2)	5.000 (L)
	Units in parallel	–	1	2	–	–	2
	Units in series	–	4	1	–	–	1

Table 7. Operating Times per Product in Each Operation (h) in the Optimal Solution

Model	i	Operations 1	2	3	4	5	6	TL_i
MILP	A	0.081	0.352	0.479	0.421	0.306	0.423	0.450
	B	0.035	0.463	0.479	0.496	0.256	0.423	0.498
MINLP[23]	A	0.0756	0.3356	0.4331	0.3893	0.2811	0.4225	0.4112
	B	0.0325	0.4287	0.4612	0.4612	0.2359	0.4225	0.4612

Using the MILP approach presented here, the discrete proposed values are selected by the designer that can provide physically meaningful suggestions, thus increasing the robustness and usefulness of the optimization models. Here, to present an unbiased solution, the proposed values have been selected dividing the allowed range in equal parts. However, more precise solutions can be attained if the proposals are focused on desired regions using the knowledge of the designer. Also, the MILP formulation assures the optimal solution can be achieved, although this simplified model is significantly larger than the MINLP formulation. Finally, the MILP model is a simplified approach and the optimal solution must be considered from this point of view.

Obviously, the results and the performance shown in Table 8 depend on the starting point, the number of discrete values proposed, the computer used, etc. However, they are shown in this section to give a wider perspective about both approaches.

Conclusions

In this work, a novel LGDP optimization model for the design of multiproduct batch plants that simultaneously optimizes the plant structure and the process variables has been presented. Process performance models have been handled as extra equations which express size and time factors in function of the process variables with the highest impact on the economic of the process.

The proposed approach is capable of handling different embedded levels of decisions. First, structural decisions include the duplication of units in series and the duplication of units in parallel working out-of-phase in each operation of the process. Second, design decisions comprise the determination of the unit sizes, the number of batches, and the processing times. Finally, process decisions involve the selection of the process variables, for instance, in the production of oleoresins presented in this work, the mass ratio of solvent to solid, the extent of the extraction, the extent of the pressing, and the particle diameter leaving the mill.

As the duplication in series in a given operation affects the upstream and downstream operations in the process, structural alternatives for the plant were generated in the model to tackle this situation. Depending on the alternative, different expressions for the size and time factors of the same operation were obtained. This is the first attempt to model more realistic plants where time and size factors can depend on the plant structure, besides the use of process variables previously cited.

The proposed model was formulated as a LGDP model. This approach is very useful taking into account the nested decisions involved. The representation of alternatives corresponding to different structural options of the plant was greatly simplified using this approach. The convex hull reformulation was used to transform it into a MILP model. To obtain a linear model, the process variables were restricted to take values from a set of meaningful values proposed by the designer. Moreover, the sizes of units are considered available in discrete sizes which correspond to the real procurement of equipment. Although this approach is less accurate than the continuous ones, it enables the simultaneous assessment of several decision levels in preliminary plant design. Otherwise, several models should be solved to represent all the possible alternatives.

Table 8. Comparison of the Performance and Characteristics of the Optimal Solutions of the MILP and MINLP[23] Models

Results	MILP	MINLP[23]
Total cost, CT ($)	1,818,411	1,748,080
CPU time (s)	27.61	1.745
Constraints	18,872	128
Continuous variables	12,565	54
Binary variables	3120	22

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Notation

Subscripts

a = structural alternative of the plant
b = semi-continuous subtrain
h = units in series
i = product
j = batch stage
k = semi-continuous operation
l = process variable
m = units in parallel
p = batch operation
r = discrete value of the process variable
s = discrete size for the batch units
u = discrete size for the semi-continuous units

Superscripts

d = downstream
L = lower bound
u = upstream
U = upper bound

Parameters

c_{solv} = recovery cost per kg of solvent
cp_{o} = specific heat capacity of the oleoresin
cp_{sol} = specific heat capacity of the solvent (2.51 kJ kg^{-1} K^{-1})
da = solid particle diameter fed into the mill
H = time horizon
K = distribution ratio of the solute
K_{R} = Rittinger's constant
k_{a} = mass ratio of additives and oleoresin (0.2)
ke = consolidation coefficient (3.744 h^{-1})
L = set of process variables with the highest impact on the process
M_p^{U} = maximum number of units that can be added in parallel in the operation p
N = rotational speed of the impeller (1 s^{-1})
q_i = production requirement of product i
t_{d} = fixed feeding and/or discharging time (0.25 h in the extractor and press, and 0.1 h in the mixer)
U_{esp} = overall heat transfer coefficient in the thickener (116.30 W m^{-2} K^{-1})
U_{eva} = overall heat transfer coefficient in the evaporator (290.75 W m^{-2} K^{-1})
ve_{a} = specific volume of the additives (1.095 m^3 kg^{-1})
ve_{mp} = specific volume of the raw material that enters in the extractor
ve_{o} = specific volume of the oleoresin
ve_{sol} = specific volume of the solvent (1.2531 L kg^{-1})
ve_{t} = specific volume of the cake in the press
x = mass fraction of oleoresin in the solid
y = mass fraction of oleoresin in the solvent (extract)
α_p = cost coefficient for the batch operation p
β_p = cost exponent for the batch operation p
γ_k = cost coefficient for the semi-continuous operation p
δ_k = cost exponent for the semi-continuous operation p
κ_i = price for the raw material of product i
λ_{sol} = heat of vaporization of the solvent (904.35 kJ kg^{-1})
τ_{b} = normal boiling point of the solvent (351.65 K)
τ_{in} = inlet solvent temperature (298.15 K)
τ_{out} = outlet solvent temperature in the thickener (358.15 K)
$\Delta\tau_{\text{esp}}$ = logarithmic mean temperature difference in the thickener (288.89 K)
$\Delta\tau_{\text{eva}}$ = logarithmic mean temperature difference in the evaporator (293.60 K)
ϖ = consolidation behavior index (1.4)
Γ = diffusivity of the solute in the solid

Boolean variables

$O_{air_1,r_2,\ldots,r_L}$ = true if the discrete value r_l is selected for the process variable l for product i with a plant structure a
W_{jpsa} = true if the unit at stage j in operation p has size s with a plant structure a
Y_{jpma} = true if the stage j in operation p has m units in parallel working out-of-phase
Z_a = true if the structural alternative a is selected for the batch plant

Continuous variables

B_i = batch size of product i
C_p = investment cost of operation p
db_i = solid particle diameter for product i
D_{ika} = duty factor of product i for semi-continuous unit k
n_i = number of batches of product i
e_{il} = process decision variable l for product i
E_i = mass ratio of solvent to solid for product i
R_k = size of semi-continuous unit k
RM_i = raw material for product i
S_{ijpa} = size factor of product i at stage j for operation p in alternative a
t_{ijpa} = processing time of product i at stage j for operation p in alternative a
T_i = cycle time for producing product i
TL_i = limiting cycle time of product i
V_p = size of a batch unit in operation p
ε_i = grade of advance in the press for product i
η_i = grade of advance in the extractor for product i
θ_{ik} = processing time of product i for semi-continuous unit k
ϕ_{ib} = operating time of a semi-continuous subtrain b for product i

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Appendix A: Size and Time Factors

In this section, the size and time factor expressions as functions of process decision variables for each operation of the vegetable extraction process are presented.

Grinding

$$D_{\text{gri}} = \frac{K_R}{(1+k_a)y_{\text{ext}}^{\text{out}}\left[1+E+(0.2\varepsilon-1.2)\frac{(1-x_{\text{ext}}^{\text{in}})}{(1-x_{\text{ext}}^{\text{out}})}\right]}\left(\frac{1}{db}-\frac{1}{da}\right) \tag{A1}$$

Extraction

$$S_{\text{ext}} = \frac{1.25(E\,ve_{\text{sol}}+ve_{\text{mp}})}{(1+k_a)y_{\text{ext}}^{\text{out}}\left[1+E+(0.2\varepsilon-1.2)\frac{(1-x_{\text{ext}}^{\text{in}})}{(1-x_{\text{ext}}^{\text{out}})}\right]} \tag{A2}$$

$$t_{\text{ext}} = t_d + \frac{db^2(2KE+1)^2}{\Gamma(KE+1)^2\pi^2} \times \ln\left\{\frac{2KE(2KE+1)^2}{\left[(2KE+1)^2+(KE+1)(KE)^2\pi^2\right](1-\eta)}\right\} \tag{A3}$$

$$x_{\text{ext}}^{n+1}[1+KE(1-\eta)] = x_{\text{ext}}^{n}(1+KE-\eta)+\eta x_{\text{ext}}^{1}. \tag{A4}$$

This last expression allows to obtain the mass fractions leaving every unit in the series of n extractors with a countercurrent arrangement. Here, x_{ext}^{n+1} is the solute concentration that enters into the extractor, that is, $x_{\text{ext}}^{\text{in}}$ and x_{ext}^{1} is the final concentration. In other words, there is a system of equations that relates mass fractions in the series. In this way, when there are different numbers of units in series in the extraction operation, Eq. A4 takes different forms and thus, the size and time factors of each operation where $x_{\text{ext}}^{\text{out}}$ is involved, take different expressions.

Then, the mass fraction of solute (oleoresin) in the solution (liquid extract) is obtained from a solute mass balance, considering that only the solute is soluble in the solvent and that all the solvent entering the extractor, leaves it in the extract stream. Thus, the solute mass fraction in the solution is given by:

$$y_{\text{ext}}^{\text{out}} = \frac{x_{\text{ext}}^{\text{in}} - x_{\text{ext}}^{\text{out}}\frac{(1-x_{\text{ext}}^{\text{in}})}{(1-x_{\text{ext}}^{\text{out}})}}{E + x_{\text{ext}}^{\text{in}} - x_{\text{ext}}^{\text{out}}\frac{(1-x_{\text{ext}}^{\text{in}})}{(1-x_{\text{ext}}^{\text{out}})}}. \tag{A5}$$

In the following discussion, the final expression of the size factor for the extraction operation is shown, eliminating intermediate variables $x_{\text{ext}}^{\text{out}}$ and $y_{\text{ext}}^{\text{out}}$. Thus, it is solely expressed in terms of the process variables. Therefore, the changes in the size factor expression are shown for each structural alternative in terms of units in series in this operation.

Considering the first configuration, that is, the extraction operation is carried out by a single extractor as is shown in Figure A1. In this way, in Eq. A4, the superscript represents the number of stages in series, that is, $n = 1$.

$$x_{\text{ext}}^{2}[1+KE(1-\eta)] = x_{\text{ext}}^{1}(1+KE-\eta)+\eta x_{\text{ext}}^{1} \tag{A6}$$

$$x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)] = x_{\text{ext}}^{\text{out}}(1+KE) \tag{A7}$$

$$x_{\text{ext}}^{\text{out}} = \frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}. \tag{A8}$$

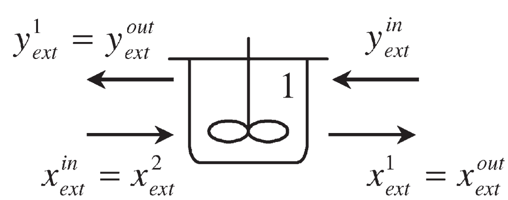

Figure A1. A single extractor.

Equation A8 is replaced in Eq. A5 giving the following expression of $y_{\text{ext}}^{\text{out}}$ in terms of process variables E and η:

$$y_{\text{ext}}^{\text{out}} = \frac{x_{\text{ext}}^{\text{in}} - \left(\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)\frac{(1-x_{\text{ext}}^{\text{in}})}{\left(1-\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)}}{E + x_{\text{ext}}^{\text{in}} - \left(\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)\frac{(1-x_{\text{ext}}^{\text{in}})}{\left(1-\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)}}. \tag{A9}$$

Finally, if the intermediate variables $x_{\text{ext}}^{\text{out}}$ and $y_{\text{ext}}^{\text{out}}$ in Eq. A2 are substituted for their expressions in terms of the process variables (Eqs. A8 and A9), the equation for determining the size factor of the extraction operation as a function of process variables is given by:

$$S_{\text{ext}} = \frac{1.25(E\,ve_{\text{sol}} + ve_{\text{mp}})}{(1+k_a)\left(\frac{x_{\text{ext}}^{\text{in}} - \left(\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)\frac{(1-x_{\text{ext}}^{\text{in}})}{\left(1-\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)}}{E+x_{\text{ext}}^{\text{in}} - \left(\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)\frac{(1-x_{\text{ext}}^{\text{in}})}{\left(1-\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)}}\right)} \times \frac{1}{\left[1+E+(0.2\varepsilon-1.2)\frac{(1-x_{\text{ext}}^{\text{in}})}{\left(1-\frac{x_{\text{ext}}^{\text{in}}[1+KE(1-\eta)]}{(1+KE)}\right)}\right]}. \tag{A10}$$

Following the same procedure, the size factors for different number of units in series in the extraction operation can be found.

Pressing

$$S_{\text{pre}} = \frac{1.5(1-x_{\text{ext}}^{\text{in}})ve_{\text{t}}}{(1-x_{\text{ext}}^{\text{out}})(1+k_a)y_{\text{ext}}^{\text{out}}\left[1+E+(0.2\varepsilon-1.2)\frac{(1-x_{\text{ext}}^{\text{in}})}{(1-x_{\text{ext}}^{\text{out}})}\right]} \tag{A11}$$

$$t_{\text{pre}} = t_d + \frac{\varepsilon^2}{ke(1-\varepsilon^{2\varpi})^{1/\varpi}} \tag{A12}$$

Evaporation

$$D_{\text{eva}} = \frac{\lambda_{\text{sol}} + (\tau_{\text{b}} - \tau_{\text{in}})\left[cp_{\text{sol}} + cp_{\text{o}}\left(\frac{y_{\text{ext}}^{\text{out}}}{1-y_{\text{ext}}^{\text{out}}}\right)\right]}{U_{\text{eva}}\Delta\tau_{\text{eva}}(1+k_a)y_{\text{ext}}^{\text{out}}}\left(1-\frac{y_{\text{ext}}^{\text{out}}}{y_{\text{eva}}^{\text{out}}}\right) \tag{A13}$$

Thickening

$$D_{\text{thi}} = \frac{\lambda_{\text{sol}} + (\tau_{\text{out}} - \tau_{\text{b}})\left[cp_{\text{sol}} + cp_{\text{o}}\left(\frac{y_{\text{eva}}^{\text{out}}}{1-y_{\text{eva}}^{\text{out}}}\right)\right]}{U_{\text{esp}}\Delta\tau_{\text{esp}}(1+k_a)}\left(\frac{y_{\text{esp}}^{\text{out}}}{y_{\text{eva}}^{\text{out}}}-1\right) \tag{A14}$$

Table A1. Values of Parameters Used in Size and Time Factor Expressions

Parameter	Product	
	Sweet Bay	Rosemary
cp_{o} (kJ kg^{-1} K^{-1})	1.13	1.17
da (cm)	2.5	1.5
K	1.15	1.22
K_{R} (kW h cm kg^{-1})	5.34×10^{-4}	1.95×10^{-4}
ve_{mp} (m^3 kg^{-1})	4	3.2
ve_{o} (dm^3 kg^{-1})	0.85	0.89
ve_{t} (dm^3 kg^{-1})	0.95	0.92
x_i^{in}	0.1	0.05
y_i^{in}	0	0
$y_{i,\text{eva}}^{\text{out}}$	0.85	0.8
Γ (cm^2 h^{-1})	8.5×10^{-6}	7.2×10^{-6}

Blending

$$S_{\text{ble}} = \frac{1.25(ve_{\text{o}} + k_{\text{a}}ve_{\text{a}})}{(1+k_{\text{a}})} \tag{A15}$$

$$t_{\text{ble}} = t_d + 58.058\frac{1}{N}. \tag{A16}$$

Table A1 summarizes the data for the products elaborated in the numerical example presented in numerical results and discussion section of this work. The information of the solvent and the values that are independent from the product are given in the notation section.

Appendix B: Convex Hull Reformulation of the Model

The convex hull relaxation of the presented disjunctive model for the example of oleoresins production is posed as follows:

$$\sum_a z_a = 1 \tag{B1}$$

$$\sum_c\sum_b\sum_f\sum_d O_{aicbfd} = z_a \quad \forall i, a \tag{B2}$$

$$D_{i,\text{Mol}} = \sum_a\sum_c\sum_b\sum_f\sum_d f_a^D \times (R_{ic}, \varepsilon_{if}, db_{id}, x_{icba}^{\text{out}}, y_{icba}^{\text{out}})O_{aicbfd} \quad \forall i \tag{B3}$$

$$S_{i,\text{Ext}} = \sum_a\sum_c\sum_b\sum_f\sum_d f_a^S(R_{ic}, \varepsilon_{if}, x_{icba}^{\text{out}}, y_{icba}^{\text{out}})O_{aicbfd} \quad \forall i \tag{B4}$$

$$S_{i,\text{Pre}} = \sum_a\sum_c\sum_b\sum_f\sum_d f_a^S(R_{ic}, \varepsilon_{if}, x_{icba}^{\text{out}}, y_{icba}^{\text{out}})O_{aicbfd} \quad \forall i \tag{B5}$$

$$D_{i,\text{Eavp}} = \sum_a\sum_c\sum_b\sum_f\sum_d f_a^D(y_{icba}^{\text{out}})O_{aicbfd} \quad \forall i \tag{B6}$$

$$\sigma b_{icbfda,\text{Pre}} = f_a^t(\varepsilon_{if}) nb_{icbfda,\text{Pre}} \quad \forall i,c,b,f,d,a \tag{B7}$$

$$\sigma b_{icbfda,\text{Ext}} = f_a^t(db_{id}, R_{ic}, \eta_{ib}) nb_{icbfda,\text{Ext}} \quad \forall i,c,b,f,d,a \tag{B8}$$

$$\sigma_{i,p} = \sum_a \sum_c \sum_b \sum_f \sum_d \sigma b_{icbfdap} \quad \forall i, p = \text{pre, ext} \tag{B9}$$

$$\sigma b_{icbfdap} \leq \sigma_{ip}^U o_{aicbfd} \quad \forall i,c,b,f,d,a,p = pre, ext \tag{B10}$$

$$n_i = \sum_a \sum_c \sum_b \sum_f \sum_d nb_{icbfdap} \quad \forall i, p = \text{pre, ext} \tag{B11}$$

$$nb_{icbfdap} \leq n_i^U o_{aicbfd} \quad \forall i,c,b,f,d,a,p = \text{pre, ext} \tag{B12}$$

$$CM_i = \sum_a \sum_c \sum_b \sum_f \sum_d f_a(x_{icba}^{\text{out}}) o_{aicbfd} \quad \forall i \tag{B13}$$

$$CS_i = \sum_a \sum_c \sum_b \sum_f \sum_d f_a(R_{ic}, x_{icba}^{\text{out}}) o_{aicbfd} \quad \forall i \tag{B14}$$

$$\sum_s w_{ps} = 1 \quad \forall p \tag{B15}$$

$$\left(\frac{Sb_{ips}}{v_{ps}}\right) q_i \leq nc_{ips} \quad \forall i,p,s \tag{B16}$$

$$S_{ip} = \sum_s Sb_{ips} \quad \forall i,p \tag{B17}$$

$$Sb_{ips} \leq S_{ip}^U w_{ps} \quad \forall i,p,s \tag{B18}$$

$$n_i = \sum_s nc_{ips} \quad \forall i,p \tag{B19}$$

$$nc_{ips} \leq n_i^U w_{ps} \quad \forall i,p,s \tag{B20}$$

$$\sum_u g_{ku} = 1 \quad \forall u \tag{B21}$$

$$\left(\frac{Db_{iku}}{\omega_{ku}}\right) q_i \leq \xi b_{iku} \quad \forall i,k,u \tag{B22}$$

$$D_{ik} = \sum_u Db_{iku} \quad \forall i,k \tag{B23}$$

$$Db_{iku} \leq D_{ik}^U g_{ku} \quad \forall i,k,u \tag{B24}$$

$$\xi_{ib} \geq \sum_u \xi b_{iku} \quad \forall i,b,k, \in b \tag{B25}$$

$$\xi b_{iku} \leq \xi_{ib}^{\text{U}} g_{ku} \quad \forall i,b,k, \in b, u \tag{B26}$$

$$CR_k = \sum_u \gamma_k \omega_{ku}^{\delta_k} g_{ku} \quad \forall k \tag{B27}$$

$$\sum_m y_{pm} = 1 \quad \forall p \tag{B28}$$

$$Tc_{ipm} \geq \frac{\xi c_{ib^u pm} + \sigma c_{ipm} + \xi c_{ib^d pm}}{m} \quad \forall i,p,m \tag{B29}$$

$$T_i = \sum_m Tc_{ipm} \quad \forall i,p \tag{B30}$$

$$Tc_{ipm} \leq T_i^U y_{pm} \quad \forall i,p,m \tag{B31}$$

$$\xi_{ib} = \sum_m \xi c_{ibpm} \quad \forall i,b,p \tag{B32}$$

$$\xi c_{ibpm} \leq \xi_{ib}^U y_{pm} \quad \forall i,b,p,m \tag{B33}$$

$$\sigma_{ip} = \sum_m \sigma c_{ipm} \quad \forall i,p \tag{B34}$$

$$\sigma c_{ipm} \leq \sigma_{ip}^U y_{pm} \quad \forall i,p,m \tag{B35}$$

$$\text{CO}_p = \sum_s \alpha_p v_{ps}^{\beta_p} w_{ps} \quad \forall p \tag{B36}$$

$$m\text{CO}b_{pm} \leq \text{CB}b_{pm} \quad \forall p,m \tag{B37}$$

$$\text{CO}b_{pm} \leq \text{CO}_p^{\text{U}} y_{pm} \quad \forall p,m \tag{B38}$$

$$\text{CO}_p = \sum_m \text{CO}b_{pm} \quad \forall p \tag{B39}$$

$$\text{CB}b_{pm} \leq \text{CB}_p^{\text{U}} y_{pm} \quad \forall p,m \tag{B40}$$

$$\text{CB}_p = \sum_m \text{CB}b_{pm} \quad \forall p \tag{B41}$$

$$\text{CB}_p = \sum_a \text{CB}c_{pa} \quad \forall p \tag{B42}$$

$$\text{CB}c_{pa} \leq \text{CB}_p^{\text{U}} z_a \quad \forall p,a \tag{B43}$$

$$C_p = \sum_a N_{pa} \text{CB}c_{pa} \quad \forall p. \tag{B44}$$

In summary, the MILP problem obtained by applying the convex hull relaxation to the original model involves the minimization of the objective function represented by Eq. 40 subject to the constraints in Eqs. 16, 35, and B1–B44.

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