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Design of Multiproduct Batch Plants with Units in Series Including Process Performance Models

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This work deals with the simultaneous optimization of process decision variables and the structure of multiproduct batch plants considering the duplication of units in series to perform a given unit operation. Performance process models allow expressing the size and time factors of the posynomial formulation as a function of the process variables with the highest impact on costs. They are added into the design problem and handled as extra constraints. Structural alternatives for the plant were defined in order to include the duplication of units in series. Thus, the problem is formulated as an optimization problem, using mixed integer nonlinear programming to minimize the total cost of the process, subjected to design specifications. The model application is illustrated with a process for the production of oleoresins. The convenience of including the duplication in series together with process variables in process optimization is tested through the resolution of various problem cases.

1. Introduction

The design of batch plants has been extensively addressed in the literature over the past decades. A comprehensive review of this area has been recently provided by Barbosa-Póvoa.[1] Most of the work was restricted to batch plant design models described by constant time and size factors.[2−6] To compute these fixed factors for each product, the process variables that characterize each unit operation must be fixed at a constant figure obtained from either pilot plant or laboratory data. Also, these fixed factors only depend on the product under consideration and no interactions with other products are taken into account.

Thus, in these models, the use of constant size and time factors and their independency of the process decision variables is a strong restriction which avoids finding superior solutions in the design problem. Moreover, these process variables may trade-off several elements in the process which can be reasonably taken into account through their inclusion into the optimization model. To overcome these limitations, optimization approaches including process performance models into the design of multiproduct batch plants have been the subject of several reports.[7−10] These performance models describe size and time factors as a function of the process decision variables selected for the optimization. In this way, process variables with the highest economic impact on the process performance are included into the formulation. A first level of detail proposed by Salomone and Iribarren[7] for process performance models are additional algebraic equations obtained from mass balances and simplified kinetic equations that describe every unit operation in the process. In general, they are kept as simple as possible but retaining the influence of the process decision variables selected to optimize the plant. Other authors have resorted to more complex performance models, for example, dynamic models,[11] dynamic simulations,[8,12] or discrete-event simulations.[13] To sum up, all those variables with economic interest for multiproduct batch plants are optimized through these models. The incorporation of information about the production process in the plant design through performance models introduces complex equations, generally nonlinear and nonconvex, which increase the level of detail of individual process unit operations. Thus, the whole model is more detailed and can yield better solutions.

As regards the design problem, besides the traditional duplication of units in parallel working out of phase, duplication of units in series has been included as a new structural decision in multiproduct batch plants in previous works.[14,15] In these articles, several assumptions had to be made in order to address this decision maintaining the posynomial formulations with fixed size and time factors. For example, yields were fixed for all the configurations in series so as not to affect the size and time factors of the up- and downstream operations of the operation that is being duplicated in series. Duplication of units in series has not been studied in depth in the literature of batch processes. This structural decision considers that a unit operation can be performed by more than one unit, so that the number of stages is a variable in the model.

There are several batch processes that involve unit operations which can be carried out with different numbers of units in series. An important application of this structural alternative is the multistage countercurrent extraction operation. Series of identical units is an engineering resource used to overcome disadvantages of single-stage extraction such as low extraction yields, long extraction times, and high solvent consumption. Another sound application is in fermentation batch processes where, depending on the inoculum cost and the equipment cost, the optimal solution can vary the number of fermentors in series to be used. Besides, adopting a different number of units in series may change the cycle time of the operation, and so the plant cycle time if this operation was the limiting one. Unlike duplication in parallel that is a valid option for any stage, duplication of units in series can be only applied in specific operations.

In the aforementioned context, the present work proposes a general nonconvex MINLP (mixed integer nonlinear programming) model that includes process information into the design

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of a multiproduct batch plant, taking into account both structural decisions of duplicating units in series and in parallel. Thus, the complete approach considers the design model for multiproduct batch plants including process performance models for the unit operations in the process. Specifically, the proposed model simultaneously considers the plant structure (duplication of units in parallel and in series), the decision variables of the batch plant (unit sizes, number of batches, processing times), and the process decision variables (e.g., for the extraction operation, the mass ratio of solvent to solid and the extent of the extraction). Since the duplication in series in a given operation affects the up- and downstream operations in the plant, structural alternatives were generated in the model to tackle this situation.

Furthermore, the most significant contribution of this work is the introduction of process variables to overcome the assumption of fixed size and time factors used in previous works[14,15] where the structural option of duplicating units in series was introduced. Size and time factors are then functions of the process variables of the same operation and of the other up- and downstream operations. Also, these factors are different functions depending on the configuration in series adopted in each operation. Here, by taking into account important process variables that affect all process operations and possible configurations in series in each of them, times and yields of all process operations can be directly optimized when a particular configuration in series is selected for a given operation. Thus, the design is optimized taking into account all the trade-offs involved in the process. It should be pointed out that the proposed model is nonlinear and nonconvex. Therefore, global optimality of its solution cannot be guaranteed, as it could be done when keeping the posynomial formulation.[2]

As an example, the presented model is applied to the production of vegetable extracts, particularly the production of oleoresins. For instance, in the extraction operation, decision variables include the mass ratio of solvent to solid and the extent of the extraction. These variables establish trade-offs among different cost components embracing several operations of the production process.

2. Problem Definition

The problem addressed in this article deals with a multiproduct batch plant which processes $i = 1, 2,..., I$ products through $p = 1, 2,..., P$ batch operations. Each operation p can be carried out by different configurations of units in series h. Let H_p be the set of possible configurations h to perform the operation p. Moreover, every configuration h determines a number of stages j. Let J_{ph} be the set of stages j included in the configuration h for the operation p.

In addition, each stage j in the configuration in series h selected 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.

Let L be the selected set of process decision variables which have the largest impact on the economics of the process. Each of these variables can affect either just the operation that introduces it or other operations of the process. Because of this, a set of variables L_p is defined which includes the process variables that impact on operation p.

Taking into account that the plant produces several products i, the variable e_{il} represents the process variable l for the product i. In this way, size and time factors of every product for each operation in the process are expressed as a function of these process decision variables.

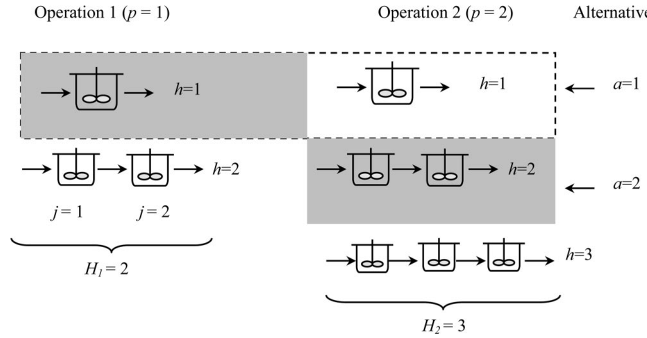

Figure 1. Structural alternatives a in the plant.

One key feature of this approach is that the duplication of units in series selected in every operation not only affect itself but also the rest of the operations. In this way, this approach overcomes the restrictions of previous works[14,15] where several assumptions had to be introduced to ensure the model factors could be assessed without considering the remaining operations. Therefore, the constraints that determine unit dimensions and times of every operation, which in this case are expressed depending on the process variables through the size and time factors, are affected by the combination of configurations in series selected in each operation of the plant.

In order to tackle this situation, a new concept, the structural alternative a of the plant, is introduced. Let A be the total number of structural alternatives of the plant, which is determined by all the possible combinations among every configuration in series h in each operation p of the plant that can be written as:

$$A = \prod_{p=1}^{P} H_p \tag{1}$$

For example, Figure 1 shows 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 ($H_2 = 3$). Thereby, the number of structural alternatives of this plant is $A = 6$.

To illustrate this concept, in Figure 1 two of the six possible structural alternatives in this plant are highlighted. The first structural alternative of the plant ($a = 1$) corresponds to one unit in the first operation ($p = 1$, $h = 1$) and one unit in the second operation ($p = 2$, $h = 1$), corresponding to the structure closed by the dotted line in Figure 1. The second alternative ($a = 2$) corresponds to one unit in the first operation ($p = 1$, $h = 1$) and two units in series in the second one ($p = 2$, $h = 2$), i.e., the structure in gray in Figure 1.

Thus, each of these structural alternatives 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 affected by the process variables e_{il} that belong to the set L_p. Note that these expressions can be different in every operation for each product in every stage and also in each alternative of duplication in series. Besides, each product manufactured in this plant must satisfy an a priori known demand q_i in a time horizon H.

In summary, the resulting nonlinear model simultaneously optimizes the process decision variables, e_{il}, and the plant design to meet the required demand q_i in the time horizon H with a minimum total investment cost.

3. Model Formulation

In this section, the mixed-integer nonlinear programming (MINLP) formulation for the optimal design and operation of the aforementioned problem is presented.

Different configurations of units in series h exist in every operation p and one option must be selected. In order to deal with this situation a binary variable z_{ph} is defined. The value of this binary variable is 1 if in operation p the configuration of units in series h is adopted; otherwise, z_{ph} is zero. This condition is expressed mathematically by the following constraint:

$$\sum_{h} z_{ph} = 1 \quad \forall p \tag{2}$$

Furthermore, each one of the structural alternatives a that can appear in the plant depends on the configuration in series h selected in every operation p of the plant. For this reason, the binary variable r_a is introduced whose value is 1 if the structural alternative a has been adopted in the plant; otherwise it is zero.

In this way, both binary variables z_{ph} and r_a are related by the following expression, where the alternatives h forming the structural alternative a are included:

$$r_a \geq \sum_{p=1}^{P} \sum_{h \in a} z_{ph} - (P - 1) \quad \forall a \tag{3}$$

Therefore, the variable r_a will take the value 1 only when all variables z_{ph} corresponding to that alternative are equal to 1.

In this context, the sizing equation of the unit at stage j for operation p, which is applied to each product i can be expressed in the following form:

$$V_{jp} \geq S_{ijpa}(e_{il})B_i - BM_{jp}(1 - r_a) \quad \forall i, j \in J_{ph}, l \in L_p, p, h \in a, a \tag{4}$$

in which V_{jp} is the size of the batch unit at stage j in operation p, B_i is the batch size and S_{ijpa} is the size factor of product i at stage j in operation p for alternative a.

Constraint (4) belongs to the big-M type, where BM_{jp} is a scalar whose value is large enough, so that if the alternative a is not selected as the structure of the plant (i.e., $r_a = 0$), it renders the inequality (4) redundant.

In the present study, the size factor of product i in operation p, S_{ijpa}, is a function, since it depends on the set of process decision variables L_p that are optimized in the model. These factors are introduced as additional constraints in the formulation for every operation, product, and alternative considered. They may be constant values, an equation, or even a system of equations in accordance with the selected level of detail. It should be noted that, with this approach, the model has a particular formulation, which depends on the operations and products involved.

The limiting cycle time of product i, TL_i, considering M_{jp} units in parallel working out-of-phase at stage j in the operation p, is given by the following constraint:

$$TL_i \geq \frac{t_{ijpa}(e_{il})}{M_{jp}} - BM_i(1 - r_a) \quad \forall i, j \in J_{hp}, l \in L_p, p, h \in a, a \tag{5}$$

This expression, like eq 4, is considered in the formulation when the structural alternative a is selected for the plant ($r_a = 1$).

Similarly, the processing time in operation p, t_{ijpa}, is expressed as a function of the set of process variables e_{il} that affect this operation and its expression depends on the structural alternative selected in the plant.

To attain an integer number for M_{jp}, a binary variable y_{jpm} is defined. This variable is equal to 1 if the stage j in the operation p has m identical units in parallel; otherwise, the variable is equal to zero. Then, the following constraints are posed:

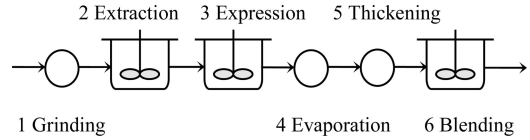

Figure 2. Operations in the batch plant for the production of oleoresins.

$$M_{jp} = \sum_{m=1}^{M_p^U} m y_{jpm} \quad \forall j, p \tag{6}$$

$$\sum_{m} y_{jpm} = 1 \quad \forall j, p \tag{7}$$

The following constraint establishes that the production targets of all products must be satisfied within the time horizon, H.

$$\sum_{i} \frac{TL_i q_i}{B_i} \leq H \tag{8}$$

The cost of the units at stage j in operation p, C_{jp}, is determined through the following constraints:

$$C_{jp} \leq \alpha_p V_{jp}^{\beta_p} + BM_{jp}(1 - z_{ph}) \quad \forall j \in J_{hp}, p, h \in H_p \tag{9}$$

$$C_{jp} \geq \alpha_p V_{jp}^{\beta_p} - BM_{jp}(1 - z_{ph}) \quad \forall j \in J_{hp}, p, h \in H_p \tag{10}$$

where the parameters α_p and β_p are specific cost coefficients for each batch operation p.

The previous expressions, again big-M type, are considered when the configuration of units in series h is selected in operation p, i.e., when z_{ph} takes the value 1.

The objective function of the model consists in minimizing the total investment cost due to purchases of the units employed at every stage j in each operation p of the plant.

$$\min \psi = \sum_{p} \sum_{j} M_{jp} C_{jp} \tag{11}$$

It is worth noting that some of the previous expressions can be convexified or even linearized. However, due to the high degree of detail incorporated by the algebraic equations that determine both size and time factors in the formulation, these performance models present highly nonconvex equations that cannot be satisfactorily convexified. To summarize, it is not possible to ensure global optimality in the solution of this model.

4. Motivating Example: Production of Oleoresins

4.1. Process Description. Figure 2 shows the flowsheet of a multiproduct batch plant for the production of oleoresins. This process is carried out through several operations, as described in the following subsections.

4.1.1. Grinding. This task is made to reduce the size of raw material that enters into the mill with a particle size da to db, (i.e., to increase the surface area). The final particle size must be sufficiently small to accelerate the solute (oleoresin) diffusion through the particle in the posterior operation of extraction. This process variable is selected as an optimization variable due to the trade-off between smaller sizes that allow to increase the extraction rate in the next operation and the greater power of the mill needed to produce such size reduction. Thus, the reduction of the particle sizes in the grinding operation influences the kinetics of the extraction operation.

4.1.2. Extraction. In this task the solute, in a solid phase (herbs or spices), is separated by contacting the solid with a liquid, the organic solvent (ethanol). A series of units or stages in a countercurrent arrangement is employed. In this case, a pure solvent enters to the first unit in the battery of extractors. This operation introduces the mass ratio of the solvent to solid, E, and the extent of the extraction, η, as optimization variables.

4.1.3. Expression. In this operation, hydraulic pressure is used for separating the solution (liquid extract) from the insoluble solid residue. The greater is the extent of the expression, ε, the higher is the time employed to carry out it. Hence, the extent of the expression is included in the set of process decision variables.

4.1.4. Evaporation. A heat exchanger (falling-film evaporator) is used to separate the solvent of the fluid final product. In this case, a specification of the maximum mass fraction of solvent in the product is given, $y_{\mathrm{eva}}^{\mathrm{out}}$. The higher the solvent to solid ratio employed in previous extraction operation, the greater is evaporation cost (i.e., larger amount of solvent to evaporate).

4.1.5. Thickening. This operation separates the residual solvent of final semisolid products using a special design heat exchanger (rotary drum evaporator). This is realized in some products in which the high viscosity of the final product needs a special unit equipment.

4.1.6. Blending. In this task, soluble agents, polysorbate 80, and/or fluid additives are added to fluidize the oleoresin, for example, propylene glycol or essential oils of the same spice to reinforce its aroma. The proportions are variables and obtained from product development, but in this case they are estimated in 20%.

The extraction, pressing, and blending operations use batch process units whereas the rest of the operations are performed by semicontinuous units.

4.2. Formulation. 4.2.1. Design Constraints. As is well-known, staged extraction is a common engineering practice used to overcome the limitations of single-stage extraction such as long extraction time, high solvent consumption, and low extraction efficiency. In this process, the extraction operation is carried out by units in series with identical size in a countercurrent arrangement. For that reason, the subscript j in eq 4 for sizing batch units can be eliminated, and the following expression is obtained:

$$V_p \geq S_{ipa}(e_{il})B_i - BM1_p(1 - r_a) \quad \forall i, l \in L_p, p, h \in a, a \quad (12)$$

As was previously mentioned, in this process some operations are performed by semicontinuous units. Thus, it is necessary to consider its sizing and add it to the general model proposed in the previous section. Taking into account that only the batch operations are duplicated in series and also that the expressions to obtain the capacity of the units in semicontinuous operations are different from the batch ones, the subscripts k will be used for the semicontinuous operations of grinding, evaporation and thickening included in this process.

In order to determine the size R_k and the operating time θ_k of the units used in semicontinuous operations the following general constraint is employed:[3]

$$\theta_{ik} \geq \frac{D_{ik}B_i}{R_k} \quad \forall i, k \quad (13)$$

A series of semicontinuous units with no batch unit among them is a semicontinuous subtrain b. All the units belonging to subtrain b must operate for the same length of time to avoid accumulation of material. Thus, the operating time of a semicontinuous subtrain is the maximum operating time of all semicontinuous units k that belong to that subtrain. Therefore, eq 13 can now be written as

$$\varphi_{ib} \geq \frac{D_{ika}(e_{il})B_i}{R_k} - BM2_{ib}(1 - r_a) \quad \forall i, b, k \in b, l \in L_p, a \quad (14)$$

where $D_{ika}(e_{il})$ is the duty factor of product i for semicontinuous unit k when the plant adopts the structural configuration a. Similarly to batch operations, it is a function of the process decision variables, e_{il}. Moreover, this equation is a big-M constraint which is considered when the value of the binary variable r_a takes the value 1; otherwise eq 14 is redundant due to the high value of the scalar $BM2_{ib}$.

4.2.2. Cycle Time Constraints. By including semicontinuous units in the model, the cycle time of product i in the batch operation p, T_{ip}, is composed of the processing time of product i in operation batch p, t_{ip}, and both the feeding time, $\varphi_{ib^{\mathrm{u}}}$, and the discharging time, $\varphi_{ib^{\mathrm{d}}}$, corresponding to the upstream and downstream semicontinuous subtrains, respectively. Thus,

$$T_{ip} = \varphi_{ib^{\mathrm{u}}} + t_{ip}(e_{il}) + \varphi_{ib^{\mathrm{d}}} \quad \forall i, p \quad (15)$$

It should be noted that when semicontinuous units are included in the process, the limiting cycle time, TL_i, is obtained considering the maximum time of all operations in the process, i.e., both batch and semicontinuous operations. Thus, the limiting cycle time is given by the following expressions:

$$TL_i \geq \frac{\varphi_{ib^{\mathrm{u}}} + t_{ipa}(e_{il}) + \varphi_{ib^{\mathrm{d}}}}{M_p} - BM3_i(1 - r_a) \quad \forall i, l \in L_p, p, h \in a, a \quad (16)$$

$$TL_i \geq \varphi_{ib} \quad \forall i, b \quad (17)$$

Equation 16 considers the existence of M_p units in parallel working out of phase in operation p. Note that, since the processing time of all units in series in the extraction operation is the same; if this operation is duplicated in parallel, then all the stages are duplicated simultaneously. Consequently, the subscript j can be eliminated in eqs 6 and 7 and the following constraints are posed:

$$M_p = \sum_{m=1}^{M_p^U} m y_{pm} \quad \forall p \quad (18)$$

$$\sum_m y_{pm} = 1 \quad \forall p \quad (19)$$

Because units in each stage in series have the same size, their cost in the operation p, C_p, can now be expressed in the following way:

$$C_p \leq h\alpha_p V_p^{\beta_p} + BM4_p(1 - z_{ph}) \quad \forall p, h \in H_p \quad (20)$$

$$C_p \geq h\alpha_p V_p^{\beta_p} - BM4_p(1 - z_{ph}) \quad \forall p, h \in H_p \quad (21)$$

4.2.3. Process Performance Models. In the following paragraphs, the decision variables are selected and their effect on this process is analyzed.

The particle size of each product i leaving the mill, db_i, is a process decision variable for the optimization. On the one hand,

Table 1. Product Data for the Example

product	name	production (kg/year)	initial concn x_i^{in}	raw material cost ($/kg)
A	Sweet bay	12000	0.10	1.00
B	Rosemary	14000	0.05	0.80

Table 2. Bounds on the Process Decision Variables

product	E_i	η_i	ε_i	db_i (cm)
A	1.00−5.00	0.370−0.990	0.40−0.995	0.01−2.50
B	1.00−5.00	0.380−0.995	0.40−0.995	0.01−1.50

Table 3. Cost of Equipment

operation	size	cost
grinding	R_k (kW)	$5700R^{0.45}$
extraction	V_p (L)	$6920V^{0.6}$
expression	V_p (L)	$6820V^{0.6}$
evaporation	R_k (m^2)	$5500R^{0.5}$
thickening	R_k (m^2)	$5100R^{0.55}$
blending	V_p (L)	$5570V^{0.6}$

smaller particle size increases the extraction rate in the following extraction operation in the process, but on the other hand, it requires a larger power of the mill.

Furthermore, both the mass ratio of the solvent to solid for each product, E_i, and the extent of the extraction, η_i, have an economic impact not only on the extraction operation but also on other operations. For instance, larger ratios of solvent to solid increase the yield of the extracted solute per kilogram of raw material. However, the cost of recovery of spent solvent is increased. Larger contact times also increase the yield, but require larger sizes of the extraction units to maintain the same production rate.

By increasing the extent of the expression, ε_i, increases the amount of recovered extract is enlarged (i.e., a larger amount of the desired product). However, the pressing time is also increased so as to maintain the production rate. Thus, the unit must handle a larger batch size resulting in a larger unit size. On the contrary, if the extent is small both desired product and solvent are lost with the solid residues of the plant.

Summarizing, the decision variables db_i, E_i, η_i, and ε_i have a large impact on the process and establish trade-offs between different cost elements of the process. So a model with higher level of detail was generated to include the most important process variables to determine both size and time factors.

In the Appendix, the algebraic equations that describe the size and time factors for each unit operations of this process are presented. These factors depend on the previously mentioned process variables. In this section, only general expressions of each size and time factor as function of the involved process variables are presented:

$$S_{i,\text{ext}} = f(E_i, \varepsilon_i, \eta_i) \tag{22}$$

$$S_{i,\text{pre}} = f(E_i, \varepsilon_i, \eta_i) \tag{23}$$

$$D_{i,\text{mil}} = f(E_i, \varepsilon_i, \eta_i, db_i) \tag{24}$$

$$D_{i,\text{eva}} = f(E_i, \eta_i) \tag{25}$$

$$t_{i,\text{ext}} = f(E_i, \eta_i, db_i) \tag{26}$$

$$t_{i,\text{pre}} = f(\varepsilon_i) \tag{27}$$

In order to avoid complexity in the presentation and taking into account that each size and time factor may depend on different process variables, a general function of the process decision variables e_{il} will be used in the formulation.

Table 4. Optimal Values of Process Variables

product	E_i	η_i	ε_i	db_i (cm)
A	1.0000	0.3763	0.7017	0.0100
B	1.0000	0.3838	0.7327	0.0100

Besides the equipment investment cost, other factors will be considered in the objective function. First, 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 calculated through the following expression:

$$RM_i = \frac{q_i}{(x_{i,\text{ext}}^{\text{in}} - x_{i,\text{ext}}^{\text{out}})} \quad \forall i \tag{28}$$

where $x_{i,\text{ext}}^{\text{in}}$ and $x_{i,\text{ext}}^{\text{out}}$ are the mass fractions of product i at the entry and the exit of the extractor, respectively. The variable $x_{i,\text{ext}}^{\text{out}}$ is a function of the process decision variables e_{il} and is kept as intermediate process variable of the extraction operation in the formulation. As is detailed in the Appendix, this variable is expressed by different functions $f_h(e_{il})$ depending on the configuration of units in series h that is selected in the extraction operation (p = ext). Hence, the following expressions must be added to the formulation:

$$x_{i,\text{ext}}^{\text{out}} \le f_h(e_{il}) + BM5_i(1 - z_{\text{ext},h}) \quad \forall i, l \in L_p, h \in H_{\text{ext}} \tag{29}$$

$$x_{i,\text{ext}}^{\text{out}} \ge f_h(e_{il}) - BM5_i(1 - z_{\text{ext},h}) \quad \forall i, l \in L_p, h \in H_{\text{ext}} \tag{30}$$

As was described in previous paragraphs, E_i is a process variable which relates the amount of solvent $Solv$ (kg) to the amount of solid raw material RM_i by means of the expression:

$$Solv = E_i RM_i(e_{il}) \tag{31}$$

Actually, larger values of E_i (i.e., larger amount of solvent) increase the efficiency in the extraction operation, whereas larger unit sizes are required. For this reason, both the amount of raw material and the amount of solvent fed to the extractor affect the total costs. Because of this, they must be included in the objective function together with the investment cost. Thereby, the trade-offs between process decision variables, unit sizes, and the resources used in the process are considered simultaneously.

4.2.4. Objective Function. The final objective function for the presented process consists of minimizing the total cost of the process CT in the time horizon H.

$$\min CT = \sum_p M_p C_p + \sum_k \gamma_k R_k^{\delta_k} + \sum_i \kappa_i RM_i(e_{il}) + \sum_i c_{\text{solv}} E_i RM_i(e_{il}) \tag{32}$$

In this expression, γ_k and δ_k are cost coefficients and cost exponents for semicontinuous operations, κ_i is the purchase price per kg of raw material used to elaborate oleoresin i, and c_{solv} is the recovery cost per kg of solvent. In this case, ethanol was used as the solvent for the extraction of all products. The last two terms in the objective function correspond to the total cost of raw material and total cost of solvent, respectively, used in the process to manufacture the required quantity q_i of the product i in the production time horizon.

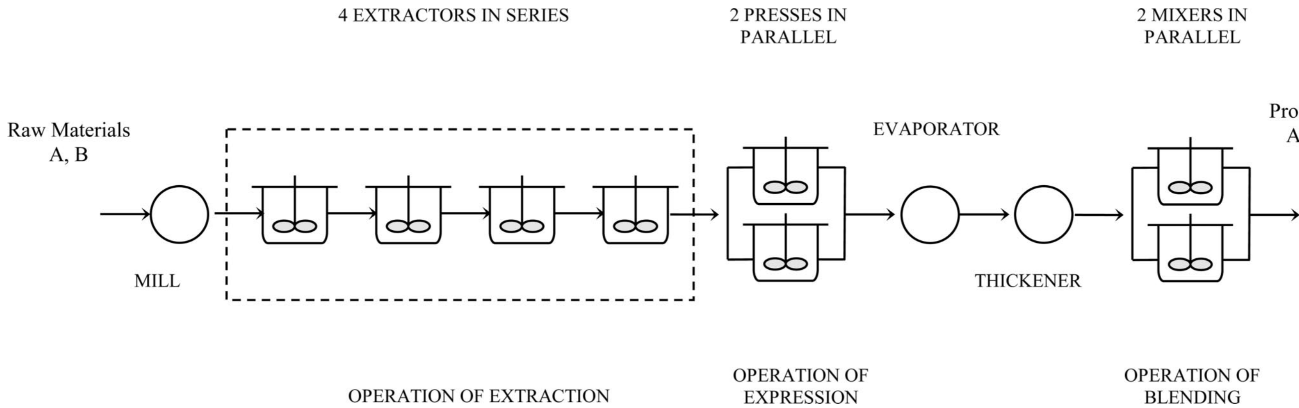

Figure 3. Optimal plant structure for the production of oleoresins.

The following expressions allow to obtain the values for the big-M scalars used in the previous constraints.

$$BM1_p = V_p^U \quad \forall p \tag{33}$$

$$BM2_{ib} = \max_{a,k}\left(\frac{D^U_{ika}(e^U_{il})B^U_i}{R^L_k}\right) \quad \forall i, b \tag{34}$$

$$BM3_i = \max_{a,p}(\varphi^U_{ib^u} + t^U_{ipa}(e^U_{il}) + \varphi^U_{ib^d}) \quad \forall i \tag{35}$$

$$BM4_p = H_p \alpha_p V_p^{U\,\beta_p} \quad \forall p \tag{36}$$

The values of parameters $BM5$ for each product depend on the expression $f_h(e_{il})$ that is obtained with the expression of $x^{out}_{i,ext}$ using the upper bound of the process variables involved.

4.2.5. Summary. The final model minimizes the objective function (32) subject to the constraints in eqs 2, 3, 8, 12, 14, 16−21, and 28−30 plus variable bounds that may apply. In these constraints the expressions for the size and time factors are presented as functions of the process variables.

The resulting mathematical model is a mixed integer nonlinear program (MINLP) because the problem has nonlinear objective function and constraints as well as binary variables. The code DICOPT, which is included in the GAMS optimization modeling software, was employed for solving the MINLP problem. The program is based on the extensions of the outer-approximation algorithm for the equality relaxation strategy. The algorithm solution method consists of the decomposition of the original MINLP problem into a series of subproblems: a nonlinear programming (NLP) subproblem and a mixed-integer programming (MIP) subproblem. These subproblems can be solved using any NLP or MIP solver that runs under GAMS.

5. Numerical Example

This example and the treated cases were implemented and solved in the software GAMS 21.6 on a Pentium (R) IV CPU, 3.00 GHz.

In order to illustrate the use of the proposed MINLP model, a batch plant that elaborates two oleoresins, sweet bay (A) and rosemary (B), is considered. The mass fractions of the solute in each raw material and product demands are shown in Table 1. The information corresponding to the values of the parameters used in the calculation of the size and time factors of the performance model are detailed in the Appendix; these factors only depend on the process decision variables. In Table 2, lower and upper bounds on the process variables are reported.

Table 3 presents the costs coefficients α_p and β_p for batch operations, and γ_k and δ_k for semicontinuous operations. The recovery cost c_{solv} of ethanol (solvent used in this process) is assumed to be 0.05$/kg. This cost accounts for the distillation needed to concentrate spent solvent due to the slowly incorporation of water to the solvent during its contact with the raw material. Also, it is assumed that a maximum number of six stages may be assigned in the extraction operation. Because of this, there are six possible configurations of units in series to carry out this operation ($H_2 = 6$). All batch operations can be duplicated in parallel up to four units ($M_p^U = 4$) working out of phase. In this case, a global time horizon of 6000 h (1 year) has been considered.

The model involved 54 continuous variables, 22 binary variables, and 128 constraints. DICOPT solved this problem in 1.745 CPU s and gave a total cost (CT) of $1,748,080.00.

The optimal plant structure to meet the production demands given in Table 1 is shown in Figure 3. As can be observed, it consist of four units in series in the batch operation of extraction and two units in parallel working out of phase in the batch operations of pressing and blending.

The values of process variables obtained in the optimal solution are presented in Table 4. Table 5 reports in detail the optimal unit sizes in each operation. It also indicates the number of units operating in series and the number of out-of-phase duplicated units obtained in the solution.

Table 6 lists the operating times in every operation and the limiting cycle time for the production of oleoresins. The cycle time of batch operations is obtained adding to its processing time the operating time of the semicontinuous unit that fills and/or empties it. In this case, for example, the cycle time of the extraction operation is obtained by adding its processing time to the operating time of the grinding operation that fills it.

Table 5. Optimal Sizes and Duplication of Units in Each Operation

	operations					
	1	2	3	4	5	6
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 6. Operating Times Per Product in Each Operation (h)

	operations						
i	1	2	3	4	5	6	TL_i
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

Table 7. Comparison of Original Problem with Four Units in Parallel in Extraction Operation

description	optimal values	
	original problem	4 extractors in parallel
units in series in extraction	4	1
units in parallel in extraction	1	4
volume of extractor (L)	280.068	1345.993
volume of press (L)	69.735	335.330
volume of mixer (L)	5.000	14.594
limiting cycle time (h)	A: 0.411 B: 0.461	A: 1.968 B: 2.326
cost of extractors ($)	813,812.72	2,087,332.83
CT ($)	1,748,080.00	3,332,345.03

It is interesting to note that, for each product, the optimal solution adopts almost equal cycle times in all the batch operations, which avoids idle times and allows to reduce unit sizes used to carry out them. In this way, the limiting cycle time is 0.4112 h for product A and 0.4612 h for product B. Also, note that very short idle times exist in the operation of blending (6).

As the number of stages in series increases in the extraction operation, the extent of the extraction of each one of them decreases. Thus, the time used to achieve a satisfactory extraction, i.e., a good yield, decreases. Because of this, the extent of the extraction η_i adopts the values summarized in Table 4. Similarly, the extent of the expression ε_i adopts values that allow to obtain a cycle time similar to the rest of the batch operations in order to eliminate idle times in the plant.

As can be seen in Table 4, the optimal values of the process variables E_i and db_i are in the lower bounds imposed for these variables. For the particle size that leaves the mill, a lower bound of 0.01 cm was imposed to avoid compaction and difficult separation of the solvent from the solid bed in the expression operation. A small size facilitates the solute (oleoresin) diffusion in the solid particle toward the solvent in the extraction operation decreasing its operating time.

The mass ratio E_i determines the amount of solvent that must enter with the solid to the extraction operation. If a one-to-one relation is attained, the necessary unit size is the double the amount of solid fed; whereas if the relation is bigger, the unit size increases proportionally. Additionally, though an increase in E_i improves the extraction efficiency, this causes an increment in the total costs (see eq 32) due to the larger recovery cost of the solvent. For this reason, the mass ratio of the solvent to solid is in the lower bound.

In the extraction operation, the selection of four units in series allows to reduce the limiting cycle time of both products elaborated in the plant. If there were four units in parallel working out of phase and duplication in series was not allowed in this operation, the limiting cycle times for products A and B would be 1.968 and 2.326 h, respectively (see Table 7).

In this way, it can be seen that the use of units in series in the operation of extraction reduces considerably the limiting cycle time for both products in comparison with the use of four units in parallel operating out of phase (maintaining the same duplication in the other batch operations). Such a decrease in the cycle time allows to handle a smaller batch size for both products in order to maintain the production rate. Thus, the unit sizes in the series and in the rest of the batch operations are smaller, reducing the total investment cost versus the cost of using units in parallel ($1,748,080.00 vs $3,332,345.03).

Table 8. Case a: Values of the Process Variables Obtained for Each Product

product	E_i	η_i	ε_i	db_i (cm)
A	1.0000	0.4890	0.6885	0.0100
B	1.0000	0.5161	0.9542	0.0100

5.1. Study of Different Alternatives. In this section, different cases are solved for the posed problem in order to analyze and compare results with the ones obtained in the optimal solution of the original problem. First, the problem is applied for a single-product plant. Second, two structural options in the batch plant are posed. Finally, a model with constant size and time factors is analyzed.

5.1.1. Case a. In this case, the optimization of the process is considered for each product separately, i.e., considering a single-product plant. Then, the decision variables obtained in its solution are used as input data for the subsequent optimization of the multiproduct batch plant with fixed factors.

Table 8 gives details of the values of the process variables obtained for every single-product plant, i.e., producing only product A (sweet bay) and only product B (rosemary).

As can be seen in Table 8, the extents of both extraction and expression operations obtained in each single-product plant differ from those obtained in the optimal solution of the original multiproduct plant. In multiproduct plants, thus, it is important to include all the products in order to consider simultaneously all the interactions between them during the process optimization. For example, when fixed size factors are used, if a product needs a larger unit size to meet its production requirements, the other product underutilizes the equipment capacity. Otherwise, if process variables are included, they adjust themselves at the optimum to better use the available capacity for both products.

If the process variables obtained in Table 8 are now fixed in the multiproduct plant, and they are replaced in the equations presented in Appendix, fixed size and time factors are obtained.

In the optimal solution, the total cost is $2,143,970.44 which is a 23% higher than that of the original solution. Table 9 presents optimal unit sizes in every operation and the plant configuration for this case.

It is interesting to note the impact of considering the decision variables in a model that simultaneously optimizes the plant structure for all the products. This case shows that very significant improvement can be obtained compared with the values obtained when the optimization is made for each single-product separately.

5.1.2. Case b. Regarding the structural options in the plant (i.e., duplication of units in series and in parallel), in this case the original problem is considered without the option of duplicating units in series in the batch operations. Particularly, in the extraction operation which, in this process, is the only one that admits such duplication. Hence, the only structural option available is the traditional duplication of units in parallel. The solution obtained consists in duplicating out of phase all the batch operations in the process. In other words, there are two units in the operations of extraction, expression and blending. Optimal sizes and number of units in parallel for each operation are shown in Table 10. Also, the optimal values of process decision variables are presented in Table 11.

Table 9. Case a: Optimal Structure with Data of Monoproduct Plants

	operations					
	1	2	3	4	5	6
sizes	22.371 (kW)	736.663 (L)	183.184 (L)	4.774 (m^2)	0.200 (m^2)	7.824 (L)
units in parallel	–	1	2	–	–	2
units in series	–	3	1	–	–	1

Table 10. Case b: Optimal Plant Structure without Considering Duplication in Series

	operations					
	1	2	3	4	5	6
sizes	22.371 (kW)	2758.506(L)	687.208(L)	5.000 (m^2)	0.200 (m^2)	29.913(L)
units in parallel	–	2	2	–	–	2
units in series	–	1	1	–	–	1

Table 11. Case b: Optimal Values of Process Variables without Considering Duplication in Series

product	E_i	η_i	ε_i	db_i (cm)
A	1.0000	0.9486	0.9914	0.0100
B	1.0000	0.9546	0.9933	0.0100

Table 12. Case b: Operating Times without Considering Duplication in Series (h)

	operations						
i	1	2	3	4	5	6	TL_i
A	0.7448	7.3456	4.0452	4.0452	2.8840	0.4225	4.0452
B	0.3200	9.2383	4.7791	4.7791	2.3990	0.4225	4.7791

Table 13. Case c: Optimal Plant Structure without Considering Duplication in Parallel

	operations					
	1	2	3	4	5	6
sizes	22.371 (kW)	2035.142(L)	505.054(L)	5.000 (m^2)	0.200 (m^2)	23.385(L)
units in parallel	–	1	1	–	–	1
units in series	–	2	1	–	–	1

Table 14. Case c: Optimal Values of Process Variables without Considering Duplication in Parallel

product	E_i	η_i	ε_i	db_i (cm)
A	1.0000	0.7308	0.6885	0.0100
B	1.0000	0.7523	0.6885	0.0100

The total cost of the design in this case is \$3,120,765.54, i.e., approximately 78% higher than the one from the original problem (\$1,748,080). As can be observed in Table 12, the limiting cycle time is 4.0452 h for product A and 4.7791 h for product B which is determined by the operations of extraction and expression. Consequently, the blending operation with a cycle time of 2.234 and 2.601 h for product A and B, respectively, presents significant idle times.

Although the number of units in parallel in the extraction operation is larger than the one in the optimal solution of the original problem (2 vs 1), it is not enough to reduce the limiting cycle times to the values obtained in the original problem. As a result of this larger cycle time, operations handle a larger batch size to maintain the production rate. Therefore, the unit sizes are bigger and their cost increases.

Furthermore, in order to fulfill product demands and obtain a good yield with the unique stage in the extraction operation, the extent of the extraction increases compared with the original solution. To achieve such extent, a significant increase in the time employed to carry out this operation is required. On the other hand, the extent of the expression increases in order to avoid idle times, which increase its operating time up to its cycle time equals the cycle time of the extraction operation.

This example allows to obtain the solution for a formulation with the traditional structural options in the literature. Overall, it is clear from the previous discussion that the incorporation of the duplication in series allows to obtain a noteworthy improvement as can be seen in the solution of the original problem.

5.1.3. Case c. In this case, the model is solved without the structural option of duplicating units in parallel and, thus, only the duplication in series is allowed in the extraction operation. The optimal configuration found for that operation consists of two stages in series. The unit sizes are shown in Table 13, whereas in Table 14 the values of the design variables for this case are reported.

The objective function for this problem has a value of \$2,317,769.39, a 32% higher than the value obtained for the original problem. Table 15 shows that the limiting cycle time is reduced to 3.2442 h for product A and 3.7437 h for product B with respect to the original solution (see Table 12).

The selection of two units in series in the extraction operation reduces the limiting cycle time for both products, so that small batch size is processed to maintain the production rate. Hence, smaller equipment size is employed. In addition, because duplication in parallel was not allowed the optimal solution did not add more units in series in the extraction operation, because downstream operations are those that determine the limiting

Table 15. Case c: Operating Times without Considering Duplication in Parallel (h)

	operations						
i	1	2	3	4	5	6	TL_i
A	0.5495	2.6947	0.4225	2.8216	2.2549	0.4225	3.2442
B	0.2361	3.5076	0.4225	3.3211	1.9005	0.4225	3.7437

Table 16. Case d: Estimated Values of the Process Variables

product	E_i	η_i	ε_i	db_i (cm)
A	1.0000	0.7000	0.8000	0.0100
B	1.0000	0.7000	0.8000	0.0100

Table 17. Case d: Optimal Structure Considering Fixed Time and Size Factors

	operations					
	1	2	3	4	5	6
sizes	22.371 (kW)	1452.075(L)	358.945(L)	4.875 (m^2)	0.200 (m^2)	19.479(L)
units in parallel	–	1	1	–	–	1
units in series	–	3	1	–	–	1

Table 18. Case d: Operating Times Considering Fixed Time and Size Factors (h)

	operations						
i	1	2	3	4	5	6	TL_i
A	0.3921	2.3909	0.5455	2.1074	1.8782	0.4225	2.7830
B	0.1684	2.8607	0.4225	2.4836	1.5586	0.4225	3.0292

Table 19. Summary of Costs Associated with Each Solved Case

	optimal values				
description	original problem	case a	case b	case c	case d
investment cost for batch units	1,017,207.45	1,439,532.92	2,378,001.90	1,660,032.48	1,904,187.91
investment cost for semicontinuous units	40,740.61	40,460.06	40,740.61	40,740.61	40,585.49
raw material cost	652,281.10	627,600.84	663,509.92	583,170.01	512,800.40
solvent cost	37,850.84	36,376.62	38,513.10	33,826.29	29,776.57
CT ($)	1,748,080.00	2,143,970.44	3,120,765.54	2,317,769.39	2,487,350.37

Table 20. Size factor, Processing Time and the Extent of the Extraction Operation

		obtained values				
description		original problem	case a	case b	case c	case d
size factor (L/kg)	A	106.960	104.839	102.690	96.908	83.009
	B	178.510	163.327	172.868	160.999	140.073
processing time (h)	A	0.3356	0.8952	2.6947	7.3456	2.3909
	B	0.4287	1.2456	3.5076	9.2383	2.8607
extent of the extraction	A	0.3763	0.4889	0.9486	0.7307	0.7000
	B	0.3838	0.5161	0.9545	0.7520	0.7000

cycle time. Thus, a greater number of units in series in the extraction would not reduce the total cost of the process in this case.

5.1.4. Case d. In order to compare the design problem with performance models to those with the fixed size and time factors, in this section the model of batch plant is solved assigning reasonable estimates for the process variables as is shown in Table 16.

The equipment unit sizes, obtained in the optimal solution of this problem, are given in Table 17.

It is important to point out that fixed values of the process decision variables do not allow the size and time factors to take values that avoid idle times and the underutilization of the units capacities in the plant.

The operating times of each operation and the limiting cycle time per product in the process are displayed in Table 18. This case presents limiting cycle times of 2.7830 and 3.0292 h for product A and product B, respectively, which is determined by the extraction operation. As mentioned previously, time factors cannot be optimized since the values for process variables are fixed, so that blending operation presents idle times of 0.2531 h for product A and 0.1231 h for product B whereas in the expression operation smaller idle times are presented for both products.

The optimal solution considering fixed factors yields a total cost of $2,487,350.37. This cost is approximately 42% higher than the one found including process performance models. It can be seen that performance models provide an additional cost savings in plant with respect to fixed factors, which are obtained from a better utilization of the plant capacity and the available time.

In Table 19 each component of the objective function is summarized for all the cases presented previously.

Comparing the results obtained in each case solved, it can be seen that the proposed approach yields a plant design with the lowest total cost. In other words, the simultaneous optimization of the process variables and the plant design, considering the new structural option of duplicating stages in series, allows a reduced total cost. Similarly, it can be seen that the major cost reduction corresponds to the investment cost for batch units for the original problem. This result shows that the inclusion of performance models allows an additional reduction of idle times by adjusting size and time factors and, consequently, a reduction in the unit capacities.

Finally, size factor, processing time, and extent of the extraction obtained in the extraction operation for each product in the optimal solution are presented in Table 20. As can be seen, the values are significantly different for each case solved. In contrast with our previous works,[14,15] where the duplication in series was introduced using fixed size and time factors, the approach presented here shows that these values change greatly depending on several problem elements. This effect can be only assessed when process variables are included, and, the production recipe and the design of the plant are simultaneously optimized.

6. Concluding Remarks

A general MINLP model that incorporates the information of the process in the design of multiproduct batch plants considering the structural option of duplicating units in series has been developed.

This model increases the level of detail with respect to the models with fixed size and time factors, since process performance models are included into the plant design. These models add to the formulation the optimization of the process decision variables in order to overcome the assumption of constant yields needed to obtain fixed size and time factors in previous models[14,15] where the new design decision of duplicating units in series was introduced.

The performance models in this work are algebraic equations that were added to the design problem to obtain the size and time factors as a function of the decision variables with the greatest economic impact in the process. Here, the size and time factors take different expressions according to the selected structural alternative in the plant due to their dependence with the configuration in series adopted in each operation.

The model was formulated using mixed integer nonlinear programming (MINLP). All the structural alternatives for the plant were defined according to the combinations of possible configurations of units in series in each operation. The optimization problem consisted of minimizing the total capital cost in the batch plant. Thereby, the model determines the plant structure selecting the configuration of units in series in each operation as well as the duplication of units in parallel out-of-phase at each stage in the series of every operation. Moreover, the optimal values of the process decision variables are determined in this approach.

A real plant for the production of oleoresins was used to illustrate this approach, in which the extraction operation is the only one that admits the duplication of units in series. Several cases considering different structural options as well as constant size and time factors were analyzed and the results were compared with the presented approach.

The incorporation of the process decision variables in the model allows to obtain more economic designs with significant reductions in idle times and a better utilization of the unit capacity in each operation. In this way, the results obtained show that the performance model provides a better solution due to the extra degrees of freedom introduced in this approach.

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Appendix: Size and Time Factors

Here, the size and time factor expressions (i.e., the coefficients of the posynomial model) for each operation of the vegetable extraction process are presented. These equations are obtained from balances and kinetic equations that describe the process. They are expressed as a function of the process decision variables and experimental constants. The following expressions of each operation in the process of extraction of oleoresins are the same for every product elaborated.

Mill. In order to determine the final particle size of raw material leaving the mill and its power consumption, a behavior according to Rittinger's law was considered. This assumes that the energy required is proportional to the generated area and that the ratio area/volume of the particles is inversely proportional to the particle size.

$$D_{\mathrm{Mill}} = \frac{K_{\mathrm{R}}}{(1 + k_{\mathrm{a}})y_{\mathrm{ext}}^{\mathrm{out}}\left[1 + E + (0.2\varepsilon - 1.2)\dfrac{(1 - x_{\mathrm{ext}}^{\mathrm{in}})}{(1 - x_{\mathrm{ext}}^{\mathrm{out}})}\right]} \times \left(\frac{1}{db} - \frac{1}{da}\right) \quad \text{(A1)}$$

Extractor.

$$S_{\mathrm{ext}} = \frac{1.25(Eve_{\mathrm{sol}} + ve_{mp})}{(1 + k_{\mathrm{a}})y_{\mathrm{ext}}^{\mathrm{out}}\left[1 + E + (0.2\varepsilon - 1.2)\dfrac{(1 - x_{\mathrm{ext}}^{\mathrm{in}})}{(1 - x_{\mathrm{ext}}^{\mathrm{out}})}\right]} \quad \text{(A2)}$$

The prediction of the operating times as a function of process variables is obtained by modeling the diffusion of the solute from the solid particle to the solvent.[16]

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

The expression A10 found in Moreno et al.[17] relates the feed solute concentration $x_{\mathrm{ext}}^{\mathrm{in}}$ with the final concentration in the solid residue $x_{\mathrm{ext}}^{\mathrm{out}}$ as follows:

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

This 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 $x_{\mathrm{ext}}^{\mathrm{in}}$ and x_{ext}^{1} is the final concentration. In other words, there is a system of equations that relate mass fractions in the series. In this way, when there are different number of units in series in the extraction operation, eq A4 take different form and thus, the size and time factors of each operation where $x_{\mathrm{ext}}^{\mathrm{out}}$ is involved takes 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 that enters exits in the extract stream. Thus, the solute mass fraction in the solution is given by

$$y_{ext}^{out} = \frac{x_{ext}^{in} - x_{ext}^{out}\dfrac{(1 - x_{ext}^{in})}{(1 - x_{ext}^{out})}}{E + x_{ext}^{in} - x_{ext}^{out}\dfrac{(1 - x_{ext}^{in})}{(1 - x_{ext}^{out})}} \quad (A5)$$

Press. It is assumed that the quantity of liquid retained in the extracted solid is 20% of the dry weight of the solid residue to the exit of the extractor, and that it has the same composition of the extract.

$$S_{Pre} = \frac{1.5(1 - x_{ext}^{in})ve_t}{(1 - x_{ext}^{out})(1 + k_a)y_{ext}^{out}\left[1 + E + (0.2\varepsilon - 1.2)\dfrac{(1 - x_{ext}^{in})}{(1 - x_{ext}^{out})}\right]} \quad (A6)$$

$$t_{Pre} = t_d + \frac{\varepsilon^2}{ke(1 - \varepsilon^{2\varpi})^{1/\varpi}} \quad (A7)$$

Evaporator.

$$D_{Eva} = \frac{\lambda_{sol} + (\tau_b - \tau_{in})\left[cp_{sol} + cp_o\left(\dfrac{y_{ext}^{out}}{1 - y_{ext}^{out}}\right)\right]}{U_{eva}\Delta\tau_{eva}(1 + k_a)y_{ext}^{out}}\left(1 - \frac{y_{ext}^{out}}{y_{eva}^{out}}\right) \quad (A8)$$

Thickener.

$$D_{Thi} = \frac{\lambda_{sol} + (\tau_{out} - \tau_b)\left[cp_{sol} + cp_o\left(\dfrac{y_{eva}^{out}}{1 - y_{eva}^{out}}\right)\right]}{U_{esp}\Delta\tau_{esp}(1 + k_a)}\left(\frac{y_{esp}^{out}}{y_{eva}^{out}} - 1\right) \quad (A9)$$

Mixer.

$$S_{Mix} = \frac{1.25(ve_o + k_a ve_a)}{(1 + k_a)} \quad (A10)$$

$$t_{Mix} = t_d + 58.058\frac{1}{N} \quad (A11)$$

Table 21 summarizes the information for the products elaborated in the numerical examples presented in section 5 of this work. The information of the solvent and the values that are independent from the product are given in the nomenclature section.

Table 21. Values of Parameters Used in Size and Time Factors Expressions

parameter	product	
	Sweet Bay	Rosemary
cp_o (kJ/(kg K))	1.13	1.17
da (cm)	2.5	1.5
K	1.15	1.22
K_R (kW h cm/kg)	5.34×10^{-4}	1.95×10^{-4}
ve_{mp} (m^3/kg)	4	3.2
ve_o (L/kg)	0.85	0.89
ve_t (L/kg)	0.95	0.92
x^{in}	0.1	0.05
y^{in}	0	0
y_{eva}^{out}	0.85	0.8
Γ (cm^2/h)	8.5×10^{-6}	7.2×10^{-6}

Nomenclature

Subscripts

a = structural alternative
b = semicontinuous subtrain
h = units in series
i = product
j = batch stage
k = semicontinuous stage
l = process variable
m = units in parallel
p = operation

Superscripts

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

Parameters

A = total number of structural alternatives of the plant
BM = big-M parameter
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 K)
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_p = set of process variables that impact on the operation p
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)
U_{eva} = overall heat transfer coefficient in the evaporator (290.75 W/m^2 K)
ve_a = specific volume of the additives (1.095 m^3/kg)
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)
ve_t = specific volume of the cake in press
x = mass fraction of oleoresin in the solid
y = mass fraction of oleoresin in the solvent
α_p = cost coefficient for the batch operation p
β_p = cost exponent for the batch operation p
γ_k = cost coefficient for the semicontinuous operation p
δ_k = cost exponent for the semicontinuous operation p
κ_i = price for the raw material of product i
λ_{sol} = heat of vaporization of the solvent (904.35 kJ/kg)
τ_b = normal boiling point of the solvent (351.65 K)
τ_{in} = inlet solvent temperature (298.15 K)
τ_{out} = oultlet solvent temperature in the thickener (358.15 K)
$\Delta\tau_{esp}$ = logarithmic mean temperature difference in the thickener (288.89 K)
$\Delta\tau_{eva}$ = logarithmic mean temperature difference in the evaporator (293.60 K)
ϖ = consolidation behavior index (1.4)

Γ = diffusivity of the solute in the solid

Binary Variables

y_{pm} = 1 if operation p has m units in parallel working out of phase
r_a = 1 if the structural alternative a is selected for the batch plant
z_{ph} = 1 if the configuration of units in series h is selected in operation p

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 semicontinuous unit k
n_i = number of batches of product i
e_{il} = process decision variables for product i that belong to set L_p
E_i = mass ratio of the solvent to solid for product i
R_k = size of semicontinuous unit k
RM_i = raw material for product i
S_{ipa} = size factor of product i for operation p in alternative a
t_{ipa} = processing time of product i 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 press for product i
η_i = grade of advance in the extractor for product i
θ_{ik} = processing time of product i for semicontinuous unit k
ϕ_{ib} = operating time of a semicontinuous subtrain b for product i

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