1. The dispersed-phase holdup increases with increasing the dispersed-phase velocity and particle size and with decreasing the continuous-phase velocity in a three-phase (liquid–liquid) fluidized bed. A similar trend was observed in the two-phase (liquid–liquid) system.

2. The presence of solid particles leads to an increase in the volumetric mass-transfer coefficient and a decrease in mixing intensity.

3. The bed with larger particles (0.00436 m) is characterized by drop breakup and that with smaller particles (0.00227 m) is characterized by drop coalescence.

4. The volumetric mass-transfer coefficient increases with increasing the dispersed-phase velocity and particle size and slightly decreasing the continuous-phase velocity.

5. The dispersion coefficient in the bed with smaller particles initially decreases, passes a minimum value, and then increases as the dispersed-phase velocity is progressively increased. However, in the bed with larger particles, the dispersion coefficient initially decreases and then levels off. In the two-phase system, the Peclet number based on the column diameter is constant with a value of 0.1152 ± 0.005.

Nomenclature

a = interfacial area per unit volume, 1/m
C_A = concentration of NaOH in the continuous phase, kmol/m^3
C_0 = concentration of acetic acid in the dispersed phase, kmol/m^3
$\bar{C}_0 = C_0/(C_0)_{in}$
C_0^* = equilibrium concentration of acetic acid in the continuous phase, kmol/m^3
E_d = dispersion coefficient of the dispersed phase, m^2/s
H = bed height, m
K_0 = overall mass-transfer coefficient, m/s
N_{od} = number of transfer units
Pe_{dD} = Peclet number based on column diameter, $(u_0D)/(E_d\epsilon_0)$
Pe_{dH} = column Peclet number, $(u_0H)/(E_d\epsilon_0)$
Pe_{dp} = particle Peclet number, $(u_0d_p)/(E_d\epsilon_0)$
u_A = continuous-phase superficial velocity, m/s
u_0 = dispersed-phase superficial velocity, m/s
V_{CD} = drift flux, m/s
Z = axial length, m
$\bar{Z} = Z/H$

Greek Symbols

ϵ_0 = the dispersed-phase holdup

Literature Cited

Acharjee, D. K.; Mitra, A. K.; Roy, A. N. *Indian J. Technol.* **1978**, *16*, 262.
Bailes, P. J.; Huges, M. A. *Chem. Eng.* **1976**, 86.
Baird, M. H. I. *Can. J. Chem. Eng.* **1974**, *33*, 341.
Chang, S. S. Master Thesis, National Taiwan Institute of Technology, Taipei, Taiwan, R.O.C., 1984.
Chiu, T. M. Ph.D. Thesis, Polytechnic Institute of New York, Brooklyn, 1982.
Dakshinamurty, P.; Krishnamurty, R.; Prasad, M. S. S. S.; Rajasekhar, P. B. *Indian J. Technol.* **1983**, *21*, 20.
Dakshinamurty, P.; Subrahmanyam, V.; Rao, R. V. P.; Vijayaaradhi, P.; *Ind. Eng. Chem. Process Des. Dev.* **1984**, *23*, 132.
Dakshinamurty, P.; Subrahmanyam, V.; Seshagirirao, V. V. B.; Prasad, M. S. S. S. *Indian J. Technol.* **1980**, *18*, 501.
Epstein, N. *Can. J. Chem. Eng.* **1981**, *59*, 649.
Godfrey, J. C.; Slater, M. J. *Chem. Ind.* **1978**, 745.
Husung, G.; Marr, R.; Wolschner, B. *Proc. World Congr. Chem. Eng., 2nd* **1981**, *4*, 439.
Jancic, S. J.; Zuiderweg, F. J.; Streiff, F. *AIChE Symp.* **1984**, *80*(238), 139.
Kim, B. K.; Kim, K.; Ryu, M. S. *Proc. Pac. Chem. Eng. Congr., 3rd* **1983**, *1*, 124.
Komasawa, I.; Ingham, J. *Chem. Eng. Sci.* **1978**, *33*, 341.
Losev, B. D.; Zheleznyak, A. S. *J. Appl. Chem. USSR (Engl. Transl.)* **1976**, *49*, 1593.
Noh, S. H.; Baird, M. H. I. *AIChE J.* **1984**, *30*, 120.
Roszak, J.; Gawronski, R. *Chem. Eng. J.* **1979**, *17*, 101.
Schugerl, K. *Proc. Int. Symp. Fluid.* **1967**, *9.4*, 782.
Takahashi, K.; Kamiha, H.; Uchida, S.; Takeuchi, H. *Solvent Extr. Ion Exch.* **1983**, *1*, 311.
Wallis, G. B. *One-dimensional Two Phase Flow*; McGraw-Hill, New York, 1969; Chapter 6.

Received for review November 20, 1985
Revised manuscript received October 21, 1986
Accepted December 6, 1986

Optimal Retrofit Design of Multiproduct Batch Plants

Jane A. Vaselenak,† Ignacio E. Grossmann,* and Arthur W. Westerberg
Department of Chemical Engineering, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213

The problem of retrofit design of multiproduct batch plants is considered in which the optimal addition of equipment to an existing plant must be determined in view of changes in the product demands. In order to circumvent the combinatorial problem requiring the analysis of many alternatives, the problem is formulated as a mixed-integer nonlinear program (MINLP) and solved with the outer-approximation algorithm of Duran and Grossmann. It is shown that by using suitable variable transformations and approximations, the global optimum solution is guaranteed. Two numerical examples are presented.

This paper will address the problem of optimal retrofit design of multiproduct batch plants. In this problem, the sizes and types of equipment for an existing multiproduct batch plant are given. Due to the changing market conditions, it is assumed that new production targets and selling prices are specified for a given set of products. The problem then consists in finding those design modifications that involve purchase of new equipment for the existing plant to maximize the profit.

The production targets that are given for the retrofit problem could be fixed or be given as upper limits. In this work the production levels are treated as upper limits to account for the following possibility. If the cost of the new equipment to operate at these new production levels is more than the revenue from the increased production, then either no new equipment should be purchased or else limited additions of equipment should be made at lower production levels. Therefore, the production levels must be optimized as part of the retrofit design problem.

* Author to whom correspondence should be addressed.
† Current address: Shell Development Co., Houston, TX 77001.

0888-5885/87/2626-0718$01.50/0

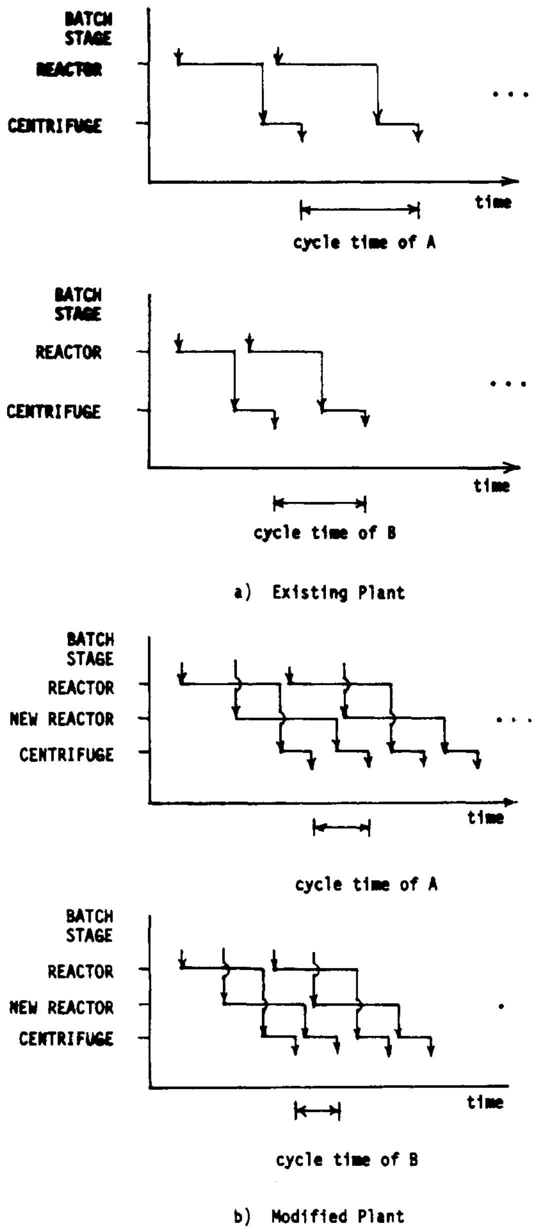

Figure 1. Option C: decrease cycle time.

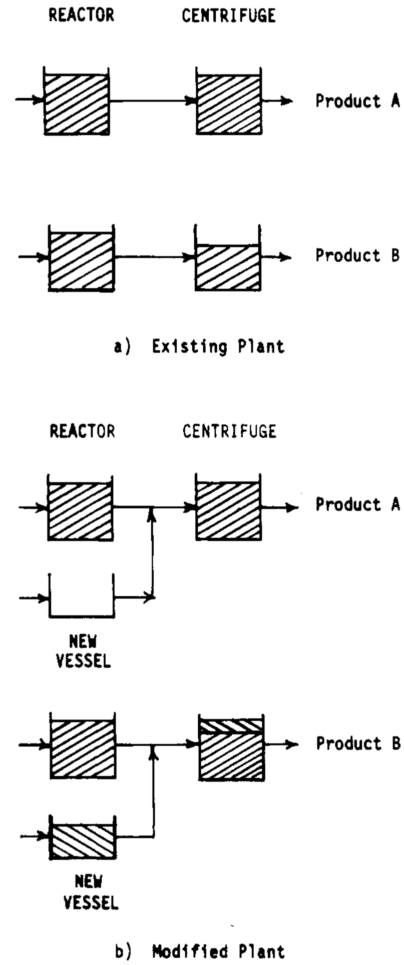

Figure 2. Option B: expand batch size.

Other assumptions that will be used in the retrofit design problem of this paper correspond to the ones that are commonly used in the optimal design of multiproduct batch plants (e.g., Sparrow et al., 1975; Grossmann and Sargent, 1979). These assumptions include the following: The recipes for all the products are given, while fixed processing times are specified for each of the products in each type of equipment. The products are manufactured sequentially by using an overlapping production schedule. Also, it is assumed that material can be held in its processing unit until the next stage is ready. That is, the processing vessels can act as their own storage tanks. In addition, a continuous range of equipment sizes is assumed to be available, and the number of batches is permitted to be noninteger since this is usually a large number. Finally, no semicontinuous equipment is considered for the plant design, although in principle this aspect could be included in the problem formulation (see Knopf et al., 1982).

As will be shown in this paper, the optimal retrofit design problem for multiproduct batch plants can be formulated as a mixed-integer nonlinear programming (MINLP) problem in which two possibilities for adding new equipment in each batch stage are included. The added equipment can be used to decrease cycle times or to increase the batch sizes of the different products. By use of exponential transformations and piecewise linear approximations, it is shown that the outer-approximation method of Duran and Grossmann (1986) will converge to the global optimum solution of the MINLP problem. Two examples are presented to show that with the suggested approach the combinatorial problem in the retrofit design can be handled rigorously and that only few alternatives need to be analyzed with modest computational effort.

Options for New Equipment

The design modifications that are considered in the retrofit design of a multiproduct batch plant will involve the addition of new equipment to the existing plant. Any new equipment can be utilized in two ways: (1) to ease bottleneck stages by operating in parallel but sequentially (option C) or (2) to increase the size of the present batches by operating in parallel and in phase with the current equipment (option B). Option *C* increases production by decreasing the *cycle* time of a product, the time needed to make one batch of a product. The new equipment used in this way operates out of phase with the existing equipment. The Gantt charts of Figure 1 demonstrate how production is increased with this design alternative. As can be seen, option C decreases the idle time of a unit, thus allowing for more efficient utilization of the equipment. Option *B*, on the other hand, increases production by augmenting the *batch* size of a product. New equipment utilized in this fashion operates in parallel and in phase with the existing equipment, as shown in Figure 2. This option takes advantage of the excess volume of a unit,

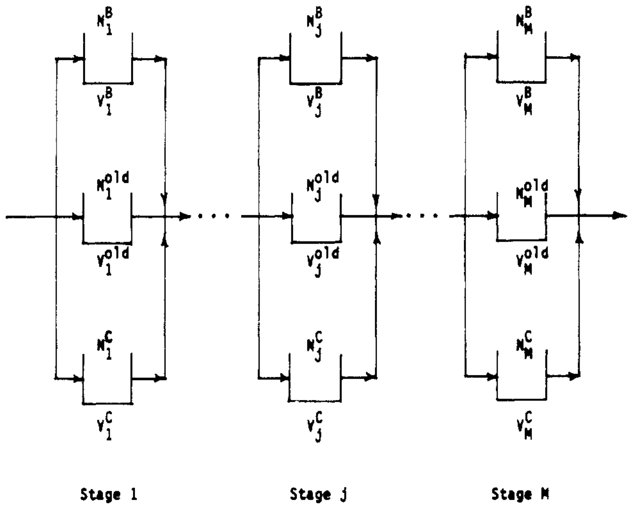

Figure 3. Superstructure for retrofit design of a multiproduct plant.

allowing for better utilization of the capacity of the unit. Appendix I presents a very simple example to illustrate that in general either of the two options can lead to an optimal retrofit design.

Since the two options cited above can be applied to each of the batch stages, all the alternatives for equipment addition in the retrofit of a multiproduct batch plant can be embedded within a superstructure as shown in Figure 3. Although just one potential new unit per stage is shown in this figure, it is clearly possible to specify multiple units for each option at each stage. By use of this superstructure representation, the retrofit problem can be formulated as a mixed-integer nonlinear program to determine the optimal design modification without having to examine all the possible alternatives.

Formulation

The goal of the retrofit design problem is to maximize the profit of the batch processing plant, given new product demand and prices. Profit is defined here as the net income from selling the products minus the annualized investment cost. The expected net profit per unit of product P_i will be denoted as p_i. To account for the economies of scale, the cost of the equipment will be approximated by a fixed-charge cost model, where K_j is the annualized fixed charge of equipment type j, which includes the costs of piping, instrumentation, and some installation expenses, and c_j is the annualized proportionality constant of equipment type j, which accounts for the linear increase of cost with the size of the vessel.

The objective function for the retrofit problem can then be formulated as

$$\max \sum_{i=1}^{N} p_i n_i B_i - \sum_{j=1}^{M}\{\sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} c_j (V_{jk}^B)_m + \sum_{k=1}^{Z_j^C} c_j V_{jk}^C\} - \sum_{j=1}^{M}\{\sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} K_j (y_{jk}^B)_m + \sum_{k=1}^{Z_j^C} K_j y_{jk}^C\} \quad (1)$$

where n_i = number of batches of product i, B_i = batch size of product i, $(y_{jk}^B)_m$ = binary variable for the kth new unit used to expand the batch size of the mth old unit of stage j, y_{jk}^C = binary variable for the decrease cycle time option for the kth unit of stage j, $(V_{jk}^B)_m$ = volume of the kth new unit of stage j used for option B (increase batch size) of existing unit m stage j, V_{jk}^C = volume of the kth unit of stage j used for option C (decrease cycle time), i = index for products (i = 1, 2, ..., N), j = index for stages (j = 1, 2, ..., M), k = index for number of possible new units for stage j (k = 1, 2, ..., Z_j^B for option B, k = 1, 2, ..., Z_j^C for option C), and m = index for existing parallel units of stage j (m = 1, 2, ..., N_j^{old}). Note that new vessels used for option C are denoted by y_{jk}^C (binary variable for the existence of a unit) and V_{jk}^C (volume); new items used for option B are symbolized by y_{jk}^B (binary variable for the existence of a unit) and V_{jk}^B (volume). The binary variables, y_{jk}^C and y_{jk}^B represent the existence of a particular unit (y_{jk} = 1) or the absence of a particular unit (y_{jk} = 0) in the superstructure. Also, this definition of variables allows different equipment items to have unequal sizes; for example, stage s can have the volumes V_s^{old}, V_{s1}^C, and V_{s2}^C.

Upper bounds on the production of each product, as given by the predicted demand, are expressed in the way

$$n_i B_i \leq Q_i \qquad i = 1, 2, ..., N \quad (2)$$

where Q_i = the upper limit on production of product P_i. The total number of units (N_j) used in determining the cycle time for each stage j is the sum of the number of old and new units, omitting the "expand batch size" (option B) type units since they operate in phase with the old, existing units. That is,

$$N_j = N_j^{old} + \sum_{k=1}^{Z_j^C} y_{jk}^C \qquad j = 1, 2, ..., M \quad (3)$$

The limiting cycle time of product P_i is given by

$$T_{Li} \geq t_{ij}/N_j \qquad i = 1, 2, ..., N \qquad j = 1, 2, ..., M \quad (4)$$

where t_{ij} is the processing time of product i in stage j.

Combining constraints 3 and 4 leads then to the inequality

$$N_j^{old} + \sum_{k=1}^{Z_j^C} y_{jk}^C \geq t_{ij}/T_{Li} \quad (5)$$
$$i = 1, 2, ..., N \qquad j = 1, 2, ..., M$$

The cycle time (T_{Li}) and the number of batches (n_i, i = 1, 2, ..., N), define the total processing time that is required for each product. These processing times must not exceed the total time available, H, as stated by the constraint

$$\sum_{i=1}^{N} n_i T_{Li} \leq H \quad (6)$$

The total number of new units for each stage must lie between a lower bound, 0, and a specified upper bound, N_j^U:

$$0 \leq \sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} (y_{jk}^B)_m + \sum_{k=1}^{Z_j^C} y_{jk}^C \leq N_j^U \quad (7)$$
$$j = 1, 2, ..., M$$

Also, to ensure that the equipment can accommodate the required production levels, constraints are written such that the size of the equipment must be greater than the batch volume needed by each product using that stage. For the case of expanding the batch size (option B), the constraint is given by

$$\sum_{k=1}^{Z_j^B} (V_{jk}^B)_m + (V_j^{old})_m \geq S_{ij} B_i \qquad i = 1, 2, ..., N \quad (8)$$
$$j = 1, 2, ..., M \qquad m = 1, 2, ..., N_j^{old}$$

where S_{ij} is the size factor for product P_i in stage j and V_j^{old} is the size of the existing piece of equipment.

For the case of the option for reducing the cycle time (option C), the capacity constraint is

$$U[1 - y_{jk}^C] + V_{jk}^C \geq S_{ij} B_i \qquad i = 1, 2, ..., N \quad (9)$$
$$j = 1, 2, ..., M \qquad k = 1, 2, ..., Z_j^C$$

Table I. Data for Example 1

product	stage 1	stage 2
(a) Size Factors, S_{ij}, L/kg of product		
A	2.0	1.0
B	1.5	2.25
(b) Processing Times, t_{ij}, h		
A	4.0	6.0
B	5.0	3.0

where U is a large number that makes this constraint redundant when this option is not selected (i.e., $y_{jk}{}^{C} = 0$).

Additional bounds and integrality constraints for the above cases are

$$0 \le (V_{jk}{}^{B})_m \le (V_j{}^{B})^{U} \quad j = 1, 2, ..., M \quad k = 1, 2, ..., Z_j{}^{B} \quad m = 1, 2, ..., N_j{}^{old} \tag{10}$$

$$0 \le V_{jk}{}^{C} \le (V_j{}^{C})^{U} \quad j = 1, 2, ..., M \quad k = 1, 2, ..., Z_j{}^{C} \tag{11}$$

$$(V_{jk}{}^{B})_m \le U(y_{jk}{}^{B})_m \quad j = 1, 2, ..., M \quad k = 1, 2, ..., Z_j{}^{B} \quad m = 1, 2, ..., N_j{}^{old} \tag{12}$$

$$V_{jk}{}^{C} \le U y_{jk}{}^{C} \quad j = 1, 2, ..., M \quad k = 1, 2, ..., Z_j{}^{C} \tag{13}$$

where $(V_j{}^{B})^{U}$ is the maximum size of a new unit for stage j, option B, and $(V_j{}^{C})^{U}$ is the maximum size of a new unit for stage j, option C. Finally, constraints that assign a priority selection for the postulated units in each stage are included to eliminate redundant combinations of the binary variables.

$$(y_{jk}{}^{B})_m \ge (y_{j,k+1}{}^{B})_m \quad j = 1, 2, ..., M \quad k = 1, 2, ..., (Z_j{}^{B} - 1) \quad m = 1, 2, ..., N_j{}^{old} \tag{14}$$

$$y_{jk}{}^{C} \ge y_{j,k+1}{}^{C} \quad j = 1, 2, ..., M \quad k = 1, 2, ..., (Z_j{}^{C} - 1) \tag{15}$$

The problem defined by eq 1, 2, and 5–15 corresponds to a mixed-integer nonlinear program (MINLP). In this MINLP formulation, the goals for retrofit design of multiproduct batch facilities are mathematically expressed, and all of the alternatives that are postulated for the new addition of equipment are embedded in this formulation.

In order to appreciate the combinatorial nature of this formulation, it will be useful to consider first a small example problem.

Example

To illustrate the use of the MINLP formulation presented in the previous section, consider the case of two products, A and B, that are currently manufactured in a multiproduct plant consisting of two stages. Each stage has one unit with volumes $V_1 = 4000$ and $V_2 = 3000$ L. The size factors and processing times are given in Table I.

The existing equipment is used to produce 1×10^6 kg/year of product A and 8×10^5 kg/year of product B. From market research data, it is established that production can be increased to 1.2×10^6 kg/year for product A and to 1×10^6 kg/year for product B. These goals represent upper limits on production. The net profit is \$1/kg for A and \$2/kg for B. Thus, if product A and product B are manufactured at the upper limits, the maximum revenue is 3200(10^3 \$/year). The cost of installing a new unit in the plant is given by the correlation 32.54(V/1000) + 30.56(10^3 \$/year). On the basis of this information, it is desired to determine what new equipment, if any, should be purchased to maximize profit for a given horizon of 1 year (6000 working h).

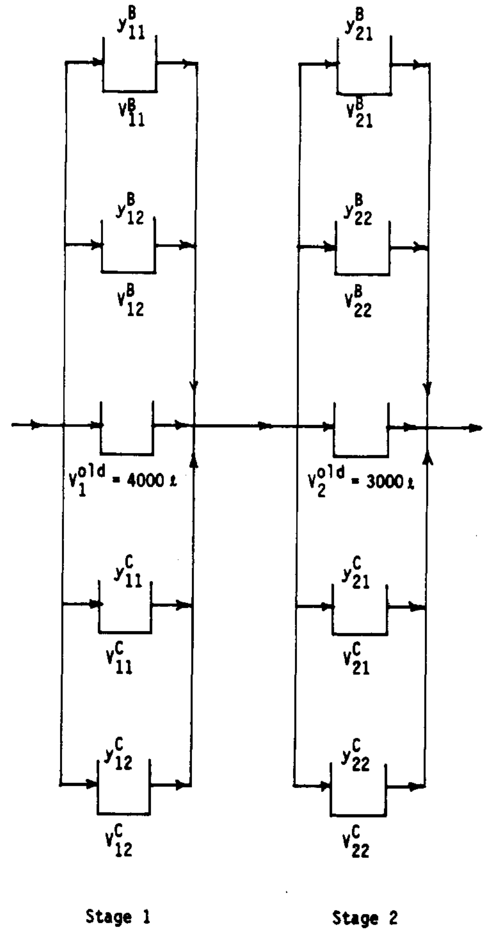

Figure 4. Superstructure for example problem 1.

Table II. Options for the Addition of Equipment for Example 1

case	$N_1{}^{c}$	$N_2{}^{c}$	$N_1{}^{B}$	$N_2{}^{B}$	goals met?	production profit (× 10^3 \$)
1	0	0	0	0	no	2750
2	1	0	0	0	yes	3044
3	0	1	0	0	no	2997
4	0	0	1	0	no	3029
5	0	0	0	1	yes	3115
6	1	0	0	1	yes	3014
7	1	0	1	0	yes	3014
8	1	1	0	0	yes	3000
9	0	1	0	1	yes	3033
10	0	1	1	0	yes	3033
11	0	0	1	1	yes	3090
12	2	0	0	0	yes	2889
13	0	2	0	0	yes	2869
14	0	0	2	0	no	2998
15	0	0	0	2	yes	3084

Figure 4 shows the superstructure for this problem, where up to two possible additions for the two options are considered in each stage. The corresponding MINLP formulation, which can be found in Vaselenak (1985), involves 8 binary variables, 6 continuous nonlinear variables (number batches, cycle times, and batch sizes), 8 continuous linear variables (volumes new vessels), and 31 inequality constraints.

One simple method to solve this MINLP is to enumerate all of the possible alternative plant configurations by solving the corresponding NLP problems that result from fixing different combinations for the binary variables. As shown in Appendix II, these NLP subproblems have a unique optimum solution provided the production amounts for each product are strictly greater than zero.

Fifteen different alternatives can be considered for the purchase of two or fewer pieces of equipment, as shown in Table II. For each alternative, MINOS/Augmented (Murtagh and Saunders, 1980) was used to solve the resulting NLP, requiring about 2.5 CPU s on a DEC-20 computer for each case. Thus, the total CPU time required to analyze the 15 cases was about 38 CPU s.

In Table II the production levels for the existing plant are optimized first to obtain a lower bound on the profit, as seen in case 1. The next four cases show the maximum profit that is obtained when one new piece of equipment is added in the plant. The remaining cases show the profit for the addition of two units. The optimal solution is case 5, the use of one unit to expand the capacity of stage 2 which leads to a profit of 3115(10^3 \$/year). This represents a 13% increase of the profit with respect to the case when no new equipment is added to the existing plant.

The following reasoning allows the search in this example to be terminated at two units for each stage. The maximum profit that can be attained from using three units or more is the difference between the maximum revenue and the fixed-charge cost of three units, 3200 − 3(30.56) = 3108(10^3 \$/year). Since this maximum profit is less than the profit of case 5, combinations involving three or more units can be eliminated.

This small example problem examined 15 different plant configurations and solved 15 NLP problems. Since larger and more realistic problems would require analyzing a much larger number of alternatives, an efficient solution procedure for solving the MINLP is required.

Solution Procedure

The primary methods used to solve general MINLP problems include generalized Benders decomposition (Geoffrion, 1972), the alternative dual approach (Balas, 1971), and branch and bound search with solution of a NLP subproblem at each node of the enumeration tree (e.g., Garfinkel and Nemhauser, 1972). The solution approach used here is the outer-approximation algorithm (Duran and Grossmann, 1986), which has been developed for solving the class of mixed-integer nonlinear programs that are linear in the binary variables and nonlinear in the continuous variables. This is precisely the structure of the MINLP formulation of this paper.

The outer-approximation method consists of solving an alternating sequence of NLP and MILP master problems to optimize the continuous and the binary variables, respectively. Specifically, this method involves first fixing the binary variables and then finding an optimal solution of the resulting NLP subproblem. For the case of minimization of the objective function, this solution provides an upper bound. The original MINLP is then approximated with a master problem by linearizing the nonlinear functions at the solution of the NLP. For nonlinear convex functions, these linearizations will underestimate the objective function and overestimate the feasible region. By including an integer cut to exclude the binary combination that was analyzed, the resulting MILP master problem is solved to obtain a new set of binary variables and a lower bound on the objective function (minimization case).

The new binary values are then substituted in the NLP subproblem, and the alternating sequence is repeated by accumulating in the MILP master problem all the successive linear approximations, as well as integer cuts to exclude alternatives previously analyzed. In this way, as iterations proceed in the sequence, the lower bounds predicted by the MILP master problem will increase monotonically since an increasingly tighter approximation of the original MINLP is obtained. The upper bounds predicted by the NLP subproblems will not necessarily decrease monotonically. The search procedure is stopped when the MILP master problem has no feasible solution because it cannot locate a new binary combination whose lower bound lies below the best upper bound obtained from the NLP subproblems. The global optimal solution will then correspond to the combination of binary variables that produced the best upper bound. This method can be shown to require fewer iterations than generalized Benders decomposition (Duran and Grossmann, 1984), and details of this algorithm are given in Duran and Grossmann (1986).

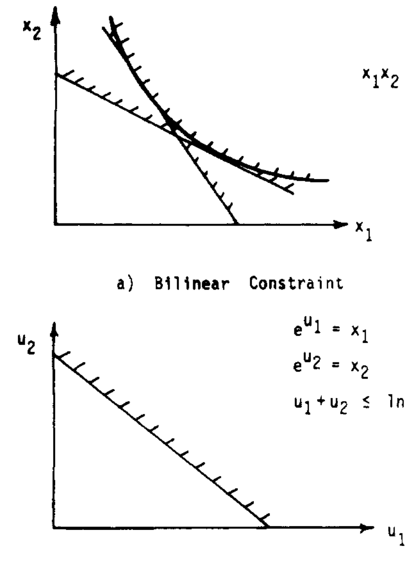

Figure 5. Bilinear constraint example.

In order to guarantee a global optimum solution in the outer-approximation algorithm of Duran and Grossmann, the MINLP formulation for the retrofit problem must be transformed to a convex form to rigorously ensure that feasible solutions that might correspond to the global optimum are not excluded by the master problem. For example, Figure 5a shows a bilinear constraint that is typical of this formulation. Linearization of this constraint excludes the shaded regions from analysis. To avoid elimination of potential solutions, an exponential transformation of the variables results in a convex constraint. In the two-variable example, the constraint becomes linear as shown in Figure 5b. The required transformations for the retrofit design problem are detailed in the following section.

Exponential Transformation of Variables

From the section on problem formulation, the objective function in terms of minimization can be expressed as

$$\min \Big(-\sum_{i=1}^{N} p_i n_i B_i + \sum_{j=1}^{M}\Big\{\sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} c_j (V_{jk}{}^B)_m + \sum_{k=1}^{Z_j^C} c_j V_{jk}{}^C\Big\} + \sum_{j=1}^{M}\Big\{\sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} K_j (y_{jk}{}^B)_m + \sum_{k=1}^{Z_j^C} K_j y_{jk}{}^C\Big\}\Big) \quad (1')$$

Since bilinear terms are involved in the first summation term, the following variables are defined and substituted into the objective function:

$$n_i = \exp(u_{1i}) \qquad i = 1, 2, ..., N \tag{16}$$

$$B_i = \exp(u_{2i}) \qquad i = 1, 2, ..., N \tag{17}$$

$$\min \left(-\sum_{i=1}^{N} p_i \exp(u_{1i} + u_{2i}) + \sum_{j=1}^{M}\{\sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} c_j(V_{jk}^B)_m + \sum_{k=1}^{Z_j^C} c_j V_{jk}^C\} + \sum_{j=1}^{M}\{\sum_{k=1}^{Z_j^B}\sum_{m=1}^{N_j^{old}} K_j(y_{jk}^B)_m + \sum_{k=1}^{Z_j^C} K_j y_{jk}^C\}\right) \tag{18}$$

If eq 16 and 17 are used, the production goals

$$n_i B_i \le Q_i \qquad i = 1, 2, ..., N \tag{2}$$

become the following linear constraints:

$$u_{1i} + u_{2i} \le \ln Q_i \qquad i = 1, 2, ..., N \tag{19}$$

Constraint 5 defining cycle times can be rearranged as

$$-\sum_{k=1}^{Z_j^C} y_{jk}^C + \frac{t_{ij}}{T_{Li}} \le N_j^{old} \tag{20}$$

Note that the term t_{ij}/T_{Li} is convex. However, T_{Li} appears in the horizon constraint 6 in the bilinear term $n_i T_{Li}$, which is nonconvex along some directions. Therefore, it is convenient to define

$$T_{Li} = \exp(u_{3i}) \qquad i = 1, 2, ..., N \tag{21}$$

with which (20) becomes

$$-\sum_{k=1}^{Z_j^C} y_{jk}^C + t_{ij}\exp(-u_{3i}) \le N_j^{old} \tag{22}$$

which is also a convex constraint.

Finally, if eq 16 and 21 are used, the horizon constraint in (6) can be expressed as a convex constraint:

$$\sum_{i=1}^{N} \exp(u_{1i} + u_{3i}) \le H \tag{23}$$

The constraints defining the volumes of the new vessels are shown below.

$$\sum_{k=1}^{Z_j^B} (V_{jk}^B)_m + (V_j^{old})_m \ge S_{ij}B_i \qquad i = 1, 2, ..., N \qquad j = 1, 2, ..., M \qquad m = 1, 2, ..., N_j^{old} \tag{24}$$

$$U[1 - y_{jk}^C] + V_{jk}^C \ge S_{ij}B_i \qquad i = 1, 2, ..., N \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., Z_j^C \tag{25}$$

$$0 \le (V_{jk}^B)_m \le (V_j^B)^U \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., Z_j^B \qquad m = 1, 2, ..., N_j^{old} \tag{26}$$

$$0 \le V_{jk}^C \le (V_j^C)^U \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., Z_j^C \tag{27}$$

$$(V_{jk}^B)_m \le U(y_{jk}^B)_m \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., Z_j^B \qquad m = 1, 2, ..., N_j^{old} \tag{28}$$

$$V_{jk}^C \le U y_{jk}^C \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., Z_j^C \tag{29}$$

If B_i is transformed as in (17), the above linear constraints for capacity become nonlinear. Since the number of nonlinear constraints should be kept at a minimum to facilitate the solution procedure, it is convenient to keep the variable B_i for constraints 24 and 25. The following convex inequalities can be used for this purpose:

$$\exp(u_{2i}) - B_i \le 0 \qquad i = 1, 2, ..., N \tag{30}$$

Because u_{2i} is maximized in objective function 18, this variable will take its largest possible value. However, since B_i will be limited by at least one constraint in (24) or (25), and increasing B_i increases the required volumes, constraint 30 will actually hold as an equality. Finally, the constraints used previously to eliminate redundant combinations of binary variables are included here also.

$$(y_{jk}^B)_m \ge (y_{j,k+1}^B)_m \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., (Z_j^B - 1) \qquad m = 1, 2, ..., N_j^{old} \tag{31}$$

$$y_{jk}^C \ge y_{jk+1}^C \qquad j = 1, 2, ..., M \qquad k = 1, 2, ..., (Z_j^C - 1) \tag{32}$$

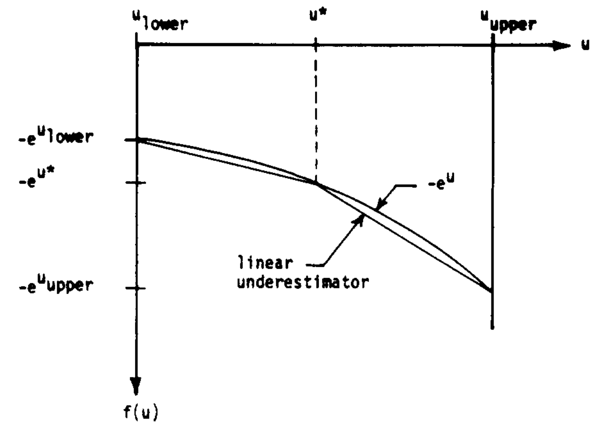

Figure 6. Piecewise linear approximation of objective function.

Piecewise Linear Approximation of Objective Function

All the nonlinear terms in the transformed MINLP defined by eq 18–20 and 22–32 are convex except for the negative exponentials of the income term in the objective function. Despite the fact that these terms are concave, for fixed values of the binary variables, the corresponding NLP has a unique optimum solution as shown in Appendix II. However, since the linearization of the negative exponential terms in (18) will overestimate the objective function, the MILP master problem may eliminate some valid solutions, possibly the global optimum. To remedy this situation, a piecewise, linear underestimator must be constructed to approximate the negative exponentials in the objective function as shown in Figure 6.

In this work the base points for the piecewise linear approximation are those solutions that result from the successive NLP subproblems. Lower and upper bounds of the function are selected for the initial iteration. The following constraints can then be written for the selected points of the piecewise linear approximation (see Garfinkel and Nemhauser, 1972):

$$x = \sum_{i=1}^{N} \lambda_i s_i \qquad y^* = \sum_{i=1}^{N} \lambda_i f_i \tag{33}$$

$$\sum_{i=1}^{N} \lambda_i = 1 \qquad \lambda_i \ge 0 \qquad i = 1, 2, ..., N \tag{34}$$

$$\lambda_1 \le \delta_1 \tag{35}$$

$$\lambda_i \le \delta_i + \delta_{i-1} \qquad i = 2, 3, ..., (N-1) \tag{36}$$

$$\lambda_N \le \delta_{N-1} \tag{37}$$

$$\sum_{i=1}^{N-1} \delta_i = 1 \tag{38}$$

where s_i and f_i are given variable and function values, x and λ_i are continuous variables, y^* is the approximation

Table III. Progress of Lower and Upper Bounds for Example 1

iteration	lower bound (NLP subproblem)	upper bound (MILP master)
1 (all y_{jk} = 0)	2750	3142
2 (y_{21}^B = 1; other y_{jk} = 0)	3115	(no solution)

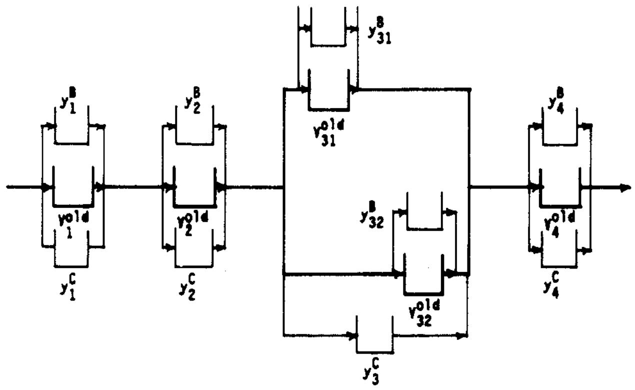

Figure 7. Superstructure for example 2.

of the function, and δ_i are 0–1 binary variables.

Each binary variable (δ_i) is associated to a line segment. A value of δ_i equal to one indicates that x lies within the interval (s_i, s_{i+1}), whose function is approximated by the line segment containing function values f_i and f_{i+1}. Constraint 38 forces only one δ_i to be non-zero. If inequalities 35–37 are used, at most two consecutive λ_i can be non-zero. Equation 33 defines the point at which the approximation y^* is obtained as a linear combination of two adjacent function values.

The underestimation of the negative exponential terms of the objective function assures the global solution of the MINLP because valid linearizations preserve the bounding properties in the MILP master problem. Note also that the solution of the NLP subproblems is unique.

Example 1

The example problem presented previously in the paper will be solved with the outer-approximation method of Duran and Grossmann (1986) by using the suggested exponential transformations and the piecewise linear approximations for the master problem. The existing plant (all integer variables set equal to zero) was selected as the initial point. MINOS/Augmented was used to solve the NLP, and the MILP was solved by using LINDO (Schrage, 1981). Two iterations were necessary to find the optimal solution, 3115(10^3 \$/year), as listed in Table III. It should be noted that since maximization of the objective function has been used, the NLP provides for this case a lower bound, while the MILP provides an upper bound. Each iteration (MILP and NLP solutions) required about 6 CPU s on a DEC-20 computer. Thus, this method only required 12 CPU s vs. the 38 CPU s of the enumeration of the 15 cases in Table II. For larger problems, greater savings with the outer-approximation method can be expected as will be shown with the next example.

Example 2

Table IV presents the data for example 2, a multiproduct facility involving four products and four stages for which the total operating time considered is 6000 h/year. The superstructures embedding all of the alternatives for new equipment are shown in Figure 7. The thick lines represent the existing structure. The use of one item for each option (cycle or batch) has been considered in each

Table IV. Data for Example 2

product	stage 1	stage 2	stage 3	stage 4
(a) Processing Times, t_{ij}, h/batch				
A	6.3822	4.7393	8.3353	3.9443
B	6.7938	6.4175	6.4750	4.4382
D	1.0135	6.2699	5.3713	11.9213
E	3.1977	3.0415	3.4609	3.3047
(b) Size Factors, S_{ij}, L/kg/batch				
A	7.9130	2.0815	5.2268	4.9523
B	0.7891	0.2871	0.2744	3.3951
D	0.7122	2.5889	1.6425	3.5903
E	4.6730	2.3586	1.6087	2.7879

stage j	V_j, L	N_j	K_j	c_j
(c) Existing Equipment and Cost of New Equipment				
1	4000	1	15.28	0.1627
2	4000	1	38.20	0.4068
3	3000	2	45.84	0.4881
4	3000	1	10.18	0.1084

product i	p_i	Q_i
(d) Forecast of Prices (\$/kg) and Demands (kg)		
A	1.114	268 200
B	0.535	156 000
D	0.774	189 700
E	0.224	166 100

Table V. Results of Example 2

iteration	non-zero binary variables	lower bound (NLP subproblem)	upper bound (MILP master problem)
(a) Progress of Lower and Upper Bounds			
1	none	460 900	532 700
2	$y_4^B = 1$	513 300	523 600
3	$y_1^B = 1$	461 900	

product i	n_i	B_i, kg	T_{Li}, h
(b) Optimal Solution, V_4^B = 2547 L			
A	530.6	505.5	6.382
B	95.48	1634.0	6.794
D	122.8	1545.0	11.92
E	151.7	856.0	3.305

stage. The resulting MINLP formulation requires 9 binary variables to represent the potential new units, 25 continuous variables, 26 nonlinear constraints, and 52 linear constraints. The cost coefficients (in 10^3 \$/year) for this model are shown in Table IV.c.

If the outer-approximation algorithm is used, the three iterations (one NLP and one MILP per iteration) shown in Table V.a require 1.7 min of CPU time on a DEC-20 computer. As seen in Table V.b, the optimal solution is to buy one unit (V_4^B = 2547 L) to expand the capacity of stage 4. This solution was found at the second iteration and has a profit of \$513 300/year, compared to the profit of \$460 900/year when no additional equipment is purchased for the existing plant. Thus, an 11% increase in the profit is achieved with the optimal retrofit design. The production levels of the products were at their upper bounds in the optimal solution.

This example problem has 2^9 or 512 possible different combinations for additions of new equipment. Since the NLP for each iteration requires an average of 6.5 CPU s, 55 CPU min would have been required to enumerate all of the possibilities. Since the outer-approximation method only required 1.7 CPU min, it is clear that significant computational savings have been achieved.

Discussion

The optimal retrofit design of multiproduct batch plants has been formulated as an MINLP problem which provides a systematic approach for solving this problem. As has been shown, by use of exponential transformations and piecewise linear approximations, the global optimum solution is rigorously guaranteed with the outer-approximation method. Furthermore, this method circumvents the combinatorial problem of requiring the analysis of all possible alternatives for the addition of equipment. In the two examples, only two or three alternatives had to be analyzed, respectively, using modest computer time to determine the global optimum solution.

It is interesting to note that in the solution of the two examples the production limits were chosen at the upper bounds and that the equipment was selected to increase the batch sizes. In general, the former result is expected to hold when the investment cost for additional equipment is offset by the increased revenue with the new production targets. The option of increasing batch sizes cannot always be expected to be optimal as shown in Appendix I. However, this option will tend to hold when the bottleneck stage is different for each product and when fixed values are assumed for the processing times as was done in this work. If processing times increase monotonically with the batch sizes, the option of adding equipment to reduce cycle time will become more attractive, as then smaller batch sizes will lead to greater reductions in the cycle times. The treatment of variable processing times that are expressed as power functions of the batch sizes can be readily incorporated in the proposed method by using the suggested variable transformations.

Finally, it should be noted that the proposed MINLP model can be extended to account for multiperiod forecasts of prices and demands (see Vaselenak, 1985). This model, which can also be convexified by using the transformations in (16), (17), and (21), allows the determination of the optimal expansion policy of a multiproduct batch plant over several time periods.

Acknowledgment

We gratefully acknowledge financial support from the National Science Foundation under Grants CPE-8210971 and CPE-8351237.

Appendix I

Example of Batch Size vs. Cycle Time Option. Consider an existing two-stage plant that manufactures 100 000 kg/year of product A. The plant data are as follows: $S_1 = 4$ L/kg, $S_2 = 2$ L/kg, $t_1 = 1$ h, $t_2 = 3$ h, $V_1^{\text{old}} = 200$ L, $V_2^{\text{old}} = 100$ L, one unit per stage. If the new production requirement increases to 150 000 kg/year, it is easy to show from (5), (6), (8), and (9) that option C for reducing the cycle time requires less additional volume and modification in only one stage; that is, for 6000 h/year,

option B

$$V_1^{\text{B}} = 100 \text{ L} \qquad V_2^{\text{B}} = 50 \text{ L}$$

option C

$$V_2^{\text{C}} = 75 \text{ L}$$

If the existing volume of stage 1 had been 300 L, then clearly option B would have been superior, as then only an additional volume of 50 L in stage 2 is required.

Appendix II

On the Uniqueness of the Solution of the NLP Subproblems. For fixed values of the binary variables, the MINLP defined by eq 1, 2, and 5–15 can be written in compact form as

$$\max \sum_{i=1}^{N} p_i n_i B_i - \Phi(V_1, V_2, ..., V_M) \tag{A1}$$

s.t.

$$n_i B_i \le Q_i \qquad i = 1, 2, ..., N \tag{A2}$$

$$T_{\text{L}i} \ge t_{ij}/N_j \qquad i = 1, 2, ..., N \qquad j = 1, 2, ..., M \tag{A3}$$

$$V_j \ge S_{ij} B_i - a_j \qquad i = 1, 2, ..., N \quad j = 1, 2, ..., M \tag{A4}$$

$$\sum_{i=1}^{N} n_i T_{\text{L}i} \le H \tag{A5}$$

where the cycle and batch volumes have been merged in the vector variables $V_1, V_2, ..., V_M$, which have zero components for the volumes not selected by the binary variables; Φ is the linear investment cost function. In constraint A3, the number of units N_j is a constant for fixed binary variables as implied by eq 3; constraint A4 represents constraints 8 and 9, with a_j being the corresponding nonnegative constant terms. Finally, (A5) is identical with eq 6.

Since the variables (N_j) are constant, as well as the processing times (t_{ij}), the cycle times ($T_{\text{L}i}$) in (A3) can be set to

$$T_{\text{L}i} = \max_{j=1,2,...,M} \{t_{ij}/N_j\} \qquad i = 1, 2, ..., N \tag{A6}$$

Furthermore, if the actual production amounts q_i are defined as

$$q_i \le n_i B_i \qquad i = 1, 2, ..., N \tag{A7}$$

the formulation given by (A1)–(A5) can be written as

$$\max \sum_{i=1}^{N} p_i q_i - \Phi(V_1, V_2, ..., V_M)$$

s.t.

$$\begin{aligned} q_i &\le n_i B_i \qquad i = 1, 2, ..., N \\ q_i &\le Q_i \qquad i = 1, 2, ..., N \\ V_j &\ge S_{ij} B_i - a_j \qquad i = 1, 2, ..., N \quad j = 1, 2, ..., M \\ \sum_{i=1}^{N} n_i T_{\text{L}i} &\le H \end{aligned} \tag{A8}$$

since n_i and B_i, are bounded by the last two constraints and q_i has a positive incremental profit in the objective function. Note that the variables for the optimization are q_i, V_j, B_i, and n_i. Also, the objective function and all the constraints are linear, except the first one which can be rewritten as

$$q_i/n_i B_i \le 1 \qquad i = 1, 2, ..., N \tag{A9}$$

If $n_i B_i > 0$, this constraint is quasi-convex since in general the ratio function $f(x)/g(x)$, where $f(x)$ is convex and $g(x) > 0$, can be shown to be quasi-convex (see Greenberg and Pierskalla, 1971). Therefore, formulation A8 with the constraint in (A9) corresponds to a nonlinear program that involves a linear objective function, linear inequalities, and quasi-convex inequalities. It then follows that if a Kuhn–Tucker point exists in this nonlinear program, it will correspond to the global optimum solution (see Avriel, 1976). Hence, the NLP subproblems that arise from fixing the binary variables in the MINLP given by eq 1, 2, and 5–15 have a unique local optimum solution provided the production amounts for each product are strictly greater than zero.

Literature Cited

Avriel, M. *Nonlinear* Programming: *Analysis and Methods*; Prentice Hall: Englewoods Clifs, NJ, 1976.
Balas, E. *Lin. Alg. Its Appl.* **1971**, *4*, 341-352.
Duran, M. A.; Grossmann, I. E. Technical Report DRC 06-68-84, 1984; Design Research Center, Carnegie-Mellon University, Pittsburgh, PA.
Duran, M. A.; Grossmann, I. E. *AIChE J.* **1986**, *32*, 592-606.
Garfinkel, R. S.; Nemhauser, G. L. *Integer Programming*; Wiley: New York, 1972.
Geoffrion, A. M. *J. Opt. Theory Appl.* **1972**, *10*, 237-260.
Greenberg, H. J.; Pierskalla, W. P. *Opns. Res.* **1971**, *19*, 1553-1570.
Grossmann, I. E.; Sargent, R. W. H. *Ind. Eng. Chem. Process Des. Dev.* **1979**, *18*(2), 343-348.
Knopf, F. C.; Okos, M. R.; Reklaitis, G. V. *Ind. Eng. Chem. Process Des. Dev.* **1982**, *21*(1), 79-86.
Murtagh, B. A.; Saunders, M. A. Technical Report SOL 80-14, June 1980; Stanford University Systems Optimization Laboratory, Palo Alto, CA.
Schrage, L. *User's Manual for LINDO*; The Scientific: Palo Alto, CA, 1981.
Sparrow, R. E.; Forder, G. J.; Rippin, D. W. T. *Ind. Eng. Chem. Process Des. Dev.* **1975**, *14*(3), 197-203.
Vaselenak, J. A. Ph.D. Dissertation, Carnegie-Mellon University, Pittsburgh, PA, 1985.

Received for review December 2, 1985
Revised manuscript received September 29, 1986
Accepted December 6, 1986

Performance of a Continuous Solid-Liquid Two-Impinging-Streams (TIS) Reactor: Dissolution of Solids, Hydrodynamics, Mean Residence Time, and Holdup of the Particles

Abraham Tamir* and Moshe Grinholtz
Department of Chemical Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel

The two-impinging-streams (TIS) reactor, already employed for many gas-solid and gas-liquid operations, was successfully implemented here for liquid-solid systems. The following performance parameters of the reactor were investigated: mean residence time and holdup of the particles as well as the dissolution of urea in water, while both phases are in a continuous flow. It was found that the TIS reactor is a very effective device that provides the highest mass-transfer coefficients among the reactors designed for continuous operation.

Dissolution of solids is a very important operation in chemical engineering. It may be carried out in a batch device such as the agitated vessel (Hixon and Wilkens, 1933; Hixon and Baum, 1941; Johnson and Huang, 1956; Barker and Treybal, 1960) and the rotating dissolution cell (Bennet and Lewis, 1958) and in a semibatch apparatus such as a packed bed reactor (Ranz, 1952) or a trickle bed reactor (Hirose et al., 1976; Satterfield et al., 1978). Since the impinging-streams reactor, applied so far for gas-solids and gas-liquids systems, has proven to be a very efficient device for effecting various processes in chemical engineering (Elperin, 1972; Tamir et al., 1984; Luzzatto et al., 1984; Tamir and Hershkovitz, 1985; Tamir, 1986; Tamir and Luzzatto, 1985; Tamir and Luzzatto, 1985a,b; Tamir and Sobhi, 1985, Tamir et al., 1985), an attempt has been made to apply this reactor also for solid-liquid systems. Therefore, the major aims of the present work were (a) to develop and to test the two-impinging-streams reactor for dissolving solids in liquids, while both phases are in a steady continous flow; (b) to study the hydrodynamical behavior of the reactor and to find out the mechanical energy needed to transfer the solid-liquid suspension through the reactor; (c) to measure important properties needed for reactor design, such as the mean residence time of the particles in the reactor and their holdup; and (d) to measure mass-transfer coefficients in the dissolution process of urea in water in order to be able to evaluate the effectiveness of the reactor as compared to other commonly used devices.

The above aims were completely achieved, indicating that the TIS reactor is a very useful tool for dissolving solids in liquids.

* To whom correspondence should be addressed.

Liquid-Solid TIS Reactor Properties

The reactor is shown schematically in Figure 1, and it comprises the following main elements: (1) two inlet pipes, 9, for the solid-liquid suspension; (2) reactor, 4, with an inner pipe, 5, which directs the streams toward the active zone for the dissolution process where the streams collide; (3) particles feeding system, 6, which separates the flow into two streams. The particles enter the shown hopper from another hopper, whose exit diameter could be varied to obtain the desired particles flow rates; (4) conical exit, 7.

The device operates as follows: two streams of a solid-liquid suspension are fed tangentially into the annular space between the inner pipe 5 and the external cylinder 4. Consequently, the two streams are allowed to impinge at a predetermined location in the upper portion of the reactor. Oscillation of the solid particles is obtained at impinging zone 11, at high flow velocities of the suspension in the inlet pipes, due to the centrifugal and inertia forces acting on the particles. Thus, a particle penetrating into the opposed water stream may acquire a relative velocity $U = U_p - (-U_w) = U_p + U_w$. If under extreme conditions $U_p = U_w$ at the entrance of the reactor (point 2 in Figure 1), and assuming that this velocity is maintained up to the impingement zone, then $U = 2U_w$. Under practical conditions, the above value of U is probably not achieved. However, the relative velocity is increased with respect to U_p to such an extent that a significant reduction in the external resistance to the dissolution process occurs as compared to a configuration where countercurrent flow between particles and water does not exist. Thus, an enhancement in the dissolution mass-transfer rate may be expected. Another advantage of the configuration of impinging streams is the possible increase in the mean