

Price-Targeting Through Iterative Flowsheet Syntheses in Developing Novel Processing Equipment: Pervaporation

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Novel processing equipment, i.e., an operating unit, such as any of various separators, is continually under development for commercialization. An innovative strategy has been proposed to establish the economically viable target price of such an operating unit through iterative flowsheet syntheses by parametrically reducing its current price. The proposed strategy resorts to a P-graph- (process-graph-) based algorithmic method for process-network synthesis. The strategy has been demonstrated to be highly efficient by determining the target price of the pervaporation unit for downstream processing of biochemically manufactured butanol, ethanol, and acetone. It is worth noting that the proposed strategy for price targeting in developing a novel and immature operating unit, such as pervaporation, is fundamentally different from that involved in retrofitting, which involves only the mature operating units at their current costs.

1. Introduction

Novel processing equipment, i.e., an operating unit, such as a reactor or separator, that is deemed to be technically feasible is continually under development for commercialization. However, it is not always easy to establish the target or benchmark in terms of price to gauge whether the operating unit under development has become economically viable or cost-effective: The economic viability or cost effectiveness is invariably application-specific. For instance, pervaporation is technically one of the most promising separation methods developed in recent years for removing volatile organics from their dilute mixtures and solutions.^{1–5} Nevertheless, it might be cost-effective only for manufacturing pharmaceuticals having exorbitant prices but not for the large-tonnage production of an organic chemical or solvent of relatively low price at the current stage of its development.

An operating unit is seldom adopted in the stand-alone mode. More often than not, it is incorporated into a process network, schematically expressed as a flowsheet, comprising a multitude of operating units. The inclusion of a novel, immature operating unit or units in a flowsheet does not necessarily replace any of the existing mature operating units performing a similar or the same function. Rather, the two units might complement each other because of differences in their optimal operating conditions. This implies that price targeting in developing a novel operating unit should not be performed in isolation; instead, it should be carried out by visualizing this operating unit in the context of the flowsheet of the process in which it is to be deployed.

The current work proposes an innovative strategy for price targeting through iterative flowsheet syntheses to develop a novel operating unit. Specifically, it advocates that a series of

flowsheets be composed for comparison based on predicted future costs of the operating unit under development by parametrically reducing its current cost, thus entailing iterative syntheses of optimal flowsheets: Only the resultant minimum costs or maximum profits concomitant with the respective optimal flowsheets constitute the unique and rational basis for comparison.

Nevertheless, it would be daunting to confront the exponentially increasing combinatorial complexity involved in generating optimal flowsheets by any conventional algorithmic method;^{6–8} an inordinately robust and efficient algorithmic method is indeed needed. The rigorous graph-theoretic method based on process graphs (P-graphs) is one such method.^{9–11} This profoundly effective, axiomatic method is the consequence of the mass-conservation law and characteristics of process networks; it has been validated to be mathematically rigorous.^{9–14} The proposed price-targeting strategy engages this method whose effectiveness has been increasingly recognized.^{16–19} It is worth noting that the proposed strategy for price targeting in developing a novel operating unit is fundamentally different from that involved in retrofitting, which deals only with the mature operating units with known current costs.^{20,21}

As mentioned at the outset, pervaporation is one of the most, if not the most, touted operations for purifying or separating dilute mixtures and solutions of organics whose large-scale commercialization is slow to be realized.^{1–5} Dilute mixtures and solutions are ubiquitous in the biochemical production of various organic materials, one instance of which is the manufacture of butanol by fermentation. It, therefore, would be suitable to demonstrate the proposed price-targeting strategy by incorporating pervaporation into the flowsheeting of the biochemical production of butanol, ethanol, and acetone. Specifically, it involves the separation and purification of butanol (B), ethanol (E), acetone (A), water (W), and distillers dried grains (DDG) from the fermentation broth.^{20,21}

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Table 1. Summary of Novel Operating Units and Their Costs

Operating Units					Cost			
no.	no. of subunits	designation	type	function ^a	capital (10 ³ \$)	annualized capital ^e (10 ³ \$/yr)	operating (10 ³ \$/yr)	total (10 ³ \$/yr)
26		U1	ultrafilter ^b	removal of suspended solids from fermentation broth	2956	985	261	1246
27		P1	pervaporator ^c	separation of B, E, and A from liquid mixture of B, E, A, and W ^d	85050	28350	259	28609

^a B = butanol, E = ethanol, A = acetone, and W = water. ^b The insoluble and dissolved solids in the fermentation broth that do not permeate the ultrafiltration membrane are recycled to the fermentor. ^c The permeate from U1 is fed to one of the compartments of P1, where B, E, and A are adsorbed into the pervaporation membrane and subsequently evaporated into the remaining compartment under vacuum. ^d The pervaporation membrane's adsorption capacities for B, E, and A, are 85–90, <5, and 8–12 mg/g, respectively; the adsorption capacity is defined as the weight of solvent adsorbed per unit of pervaporation membrane. ^e Based on the 3-year payback period.

2. Process Description

The pervaporation unit needs to be preceded by the ultrafiltration unit to remove suspended or dissolved solids including cells in the fermentation broth, thus preventing them from fouling the pervaporation membrane.⁴ Ultrafiltration is a well-known membrane separation technology.²² It is based on differences in the molecular weights and sizes of components in a liquid mixture.^{22–24} The ultrafiltration unit is a hollow-fiber membrane with a nominal molecular weight cutoff of 500000.

The pervaporation unit consists of two compartments separated by a membrane. For the separation of B, E, and A from the cell-free fermentation broth, a plate of silicone–silicalite composite membrane, 306 μm thick, is employed.⁴ The pervaporation usually takes place at 78 °C. The temperature of the retentate, i.e., the cell-free fermentation broth from the ultrafilter containing mainly water, is controlled by circulating hot water through a shell and tube heat exchanger. The fermentation broth is circulated with a pump. The inlet and outlet pressures are 4.0 psig (27 580 Pa) and 1.0 psig (6895 Pa), respectively. The pressure on the permeate side ranges from 2 to 5 Torr (227–667 Pa), and the permeate, containing B, E, and A, is condensed in two liquid-nitrogen cooling tanks that are sealed.

In addition to the pervaporation and ultrafiltration units, a multitude of mature operating units are involved in constituting the flowsheets for the biochemical production of B, E, and A. These operating units comprise distillation, gas stripping, and extracting units, as well as adsorption and concomitant centrifugation units, for which the details are available elsewhere.^{20,21}

3. Methodology

The number of the aforementioned operating units, including the pervaporation unit and the concomitant ultrafiltration unit, totals 27, including 40 pieces of processing equipment; Table 1 contains the pertinent information on the pervaporation and ultrafiltration units, identified as P1 and U1, respectively. They are graphically represented in conventional diagrams as well as by P-graphs in Figure 1. Information on the other operating units is given elsewhere.^{20,21} The mass balances around the two units, P1 and U1, are based on the available data.⁴

It is worth noting that the proposed strategy of price targeting in our work is to guide the development of a novel operating unit in the context of the flowsheet of the process into which it is to be incorporated at its very early stage where the conceptual design is executed in parallel. At this stage, the synthesis of the entire process system is carried out by optimally linking

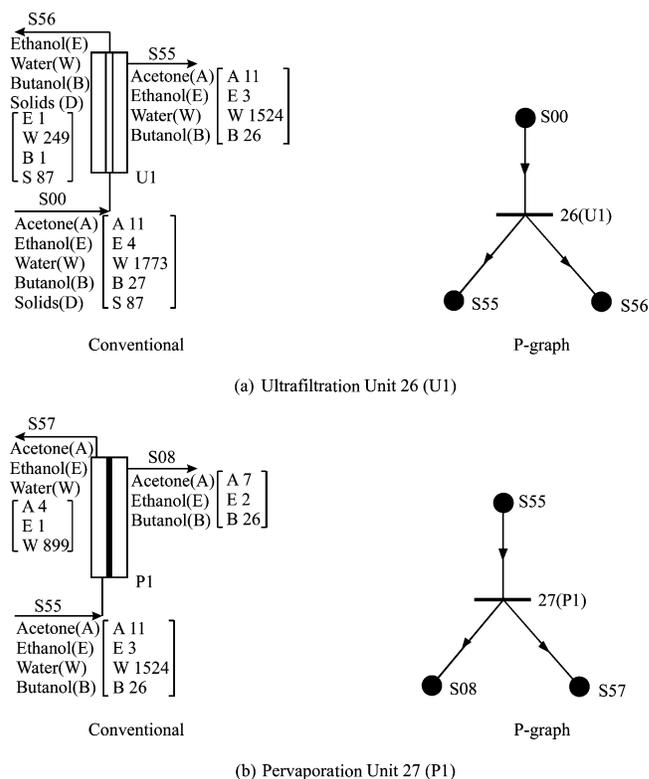


Figure 1. Conventional representation (with the component flow rate in 10³ lb/h) and process graph (P-graph) representation of novel operating units identified: (a) ultrafiltration unit 26 (U1), (b) pervaporation unit 27 (P1).

the subsystems, depicted as blocks in process flowsheets. All pieces of ancillary equipment, such as refrigeration systems, cooling systems, heat exchangers, pumps, and mixers, are not taken into account at the conceptual design stage.^{15,25,26} This gives rise to the simplified material balances and the approximate estimates of capital costs and operating costs. As stated by Douglas,²⁵ “In many cases the processing costs associated with the various process alternatives differ by an order of magnitude or more, so that we can use shortcut calculations to screen the alternatives.”

The current costs of the two units, P1 and U1, as indicated in Appendix 1 (Supporting Information), have been estimated as previously^{20,21} and are based on available information and data.^{4,15,20,27,28} The resultant costs are summarized in Table 1. Obviously, the current cost of P1, \$28 609 $\times 10^3$ /yr, is inordinately high; it needs to be substantially reduced to meet the requirement for commercialization. The objective function to be minimized is the flowsheet's cost. It is calculated as the

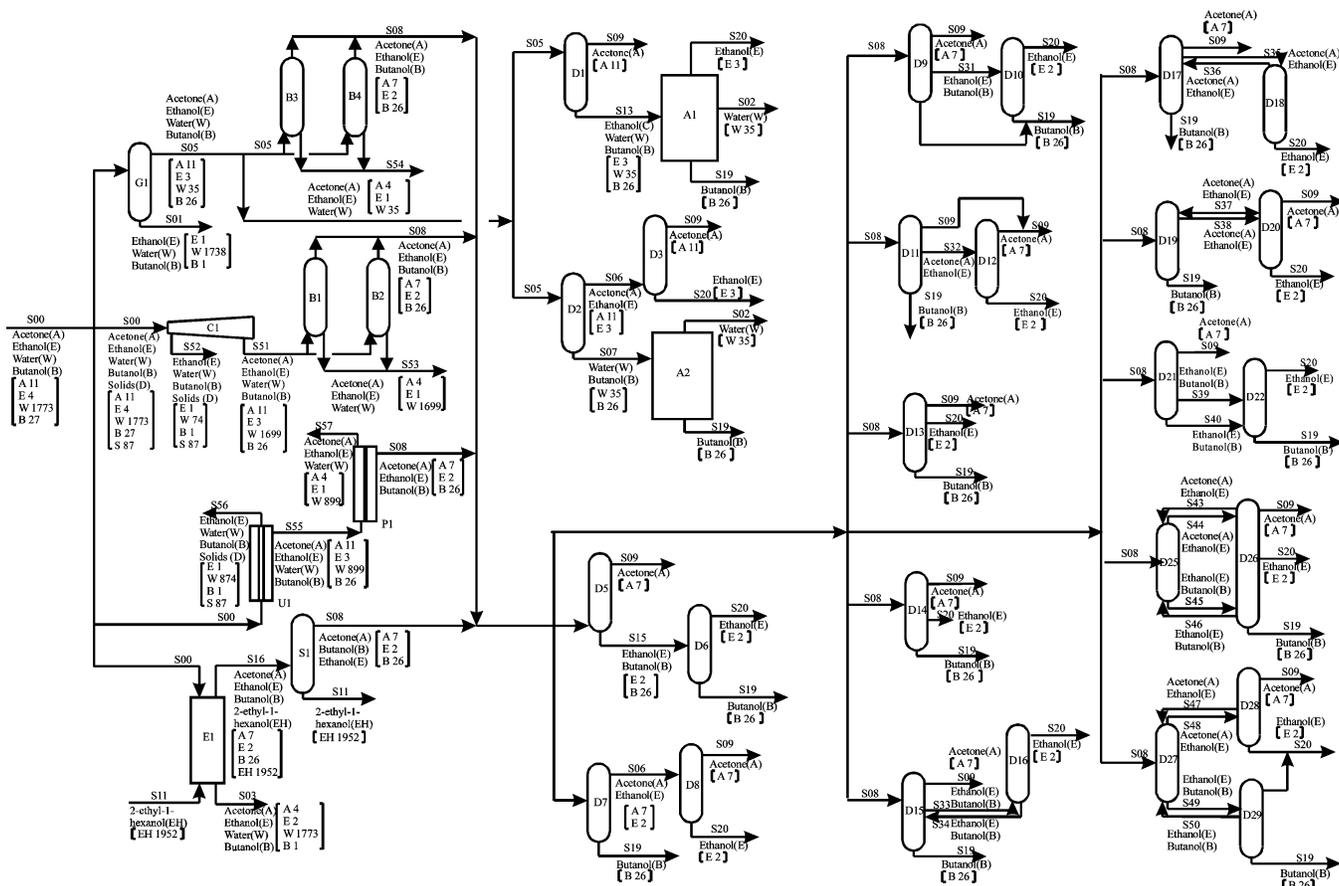


Figure 2. Comprehensive flowsheet corresponding to the maximal structure for the production of butanol, ethanol, and acetone with the inclusion of pervaporation: conventional representation with the component flow rate in 10^3 lb/h.

total sum of the annualized capital and operating costs in terms of their present values for all operating units in the flowsheet.

With the operating units identified, their current costs determined, and the objective function defined, the implementation of the methodology for the price-targeting strategy proceeds as follows:

Twenty-five operating units are taken into account in constructing the maximal structure. These operating units include Nos. 3–25 listed elsewhere,^{20,21} as well as Nos. 26 and 27 listed in Table 1, but exclude Nos. 1 and 2, the two reacting units that do not come into play in the current work. The raw material is the feed to the downstream processing, i.e., fermentation broth from these reacting units, and the products are pure B, E, A, and W. On the basis of the specifications of raw material and products as well as the P-graph representations of the operating units identified,^{20,21} algorithm MSG was used to construct the comprehensive flowsheet corresponding to the maximal structure has been constructed via algorithm MSG.

A series of optimal and near-optimal flowsheets in ranked order was generated directly from the comprehensive flowsheet using algorithm ABB (see Appendix 2, Supporting Information)¹⁵ and parametrically reducing the current cost of P1. The generation was terminated when the cost of the optimal flowsheet containing P1 became less than that of the optimal flowsheet containing only the mature operating units.

4. Results and Discussions

The comprehensive flowsheet corresponding to the maximal structure was constructed using algorithm MSG. The comprehensive flowsheet is presented in Figures 2 and 3 by the conventional and P-graph representations, respectively. It

includes the operating units comprising 1 gas stripper, 1 extractor, 27 simple distillation columns, 2 azeotropic distillation units, 1 centrifuge, 4 adsorption columns, 1 ultrafilter, and 1 pervaporator.

A series of optimal and near-optimal flowsheets was generated by parametrically reducing the current cost of P1 until the cost of the optimal flowsheet containing P1 became less than that of the optimal flowsheet containing only the mature operating units; this was accomplished using algorithm ABB (see Appendix 2, Supporting Information).¹⁵ For a given set of cost parameters, the algorithm generates a specific number, 10 in the current work, of optimal and near-optimal flowsheets of various structures directly from the comprehensive flowsheet in ranked order according to their objective-function values, which are their costs in the current work. Each of these optimal and near-optimal flowsheets contains some of the 25 operating units in the comprehensive flowsheet.

With the current cost of P1 at $\$28\,609 \times 10^3/\text{yr}$, all 10 of the best flowsheets listed in ranked order in Table 2 are identical to those generated previously;²¹ none of them includes P1 and U1. The cost of the best flowsheet is $\$5286 \times 10^3/\text{yr}$. This implies that, at present, pervaporation is not yet as cost-effective as the mature technologies, such as distillation and adsorption. Thus, its price needs to be reduced to be economically competitive.

Only when the cost of P1 is lowered by 84% to $\$4406 \times 10^3/\text{yr}$ does the 10th-best flowsheet generated contain P1 in conjunction with U1 and the conventional distillation unit, i.e., unit 21, comprising subunits 20-1 (D21) and 20-2 (D22) (see Table 3). The cost of this 10th-best flowsheet, with its conventional and P-graph representations shown in Figure 4, is

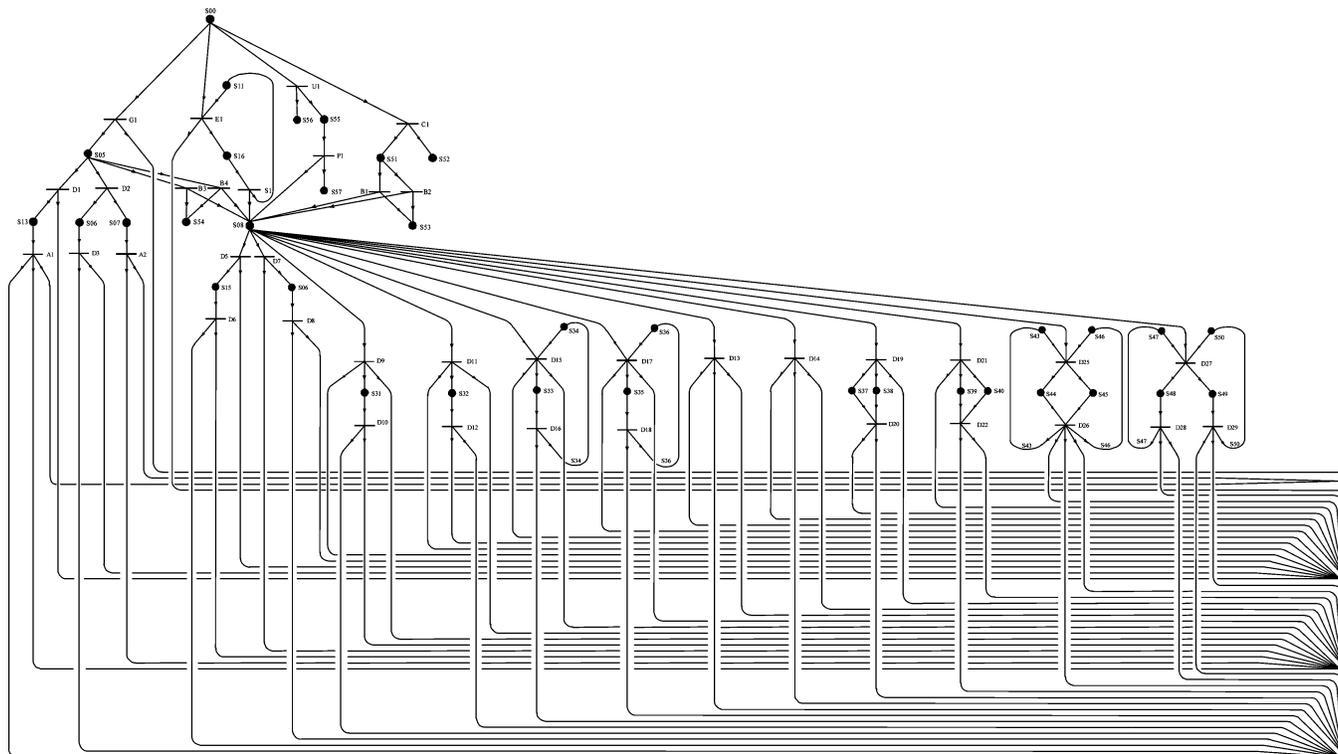


Figure 3. Comprehensive flowsheet corresponding to the maximal structure for the production of butanol, ethanol, and acetone with the inclusion of pervaporation: P-graph representation. A letter followed by a numeral adjacent to a bar designates an operating unit represented by the bar; a letter followed by a numeral adjacent to a small solid circle designates a stream of the material represented by the circle.

Table 2. Summary of the Optimal and Near-Optimal Flowsheets Generated by Algorithm ABB with the Current Cost of P1

rank	Number of Operating Units						total cost (10 ³ \$/yr)	
	gas strippers	extractors	centrifuges	adsorption columns	ultrafilters	pervaporators		distillation columns
1	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D21, D22)	5286
2	1 (G1)	0	0	2 (B3, B4)	0	0	3 (D27, D28, D29)	6042
3	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D7, D8)	6062
4	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D25, D26)	6081
5	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D5, D6)	6257
6	1 (G1)	0	0	2 (B3, B4)	0	0	1 (D13)	7450
7	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D11, D12)	7612
8	1 (G1)	0	0	2 (B3, B4)	0	0	1 (D14)	7694
9	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D9, D10)	7893
10	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D17, D18)	7939

Table 3. Summary of the Optimal and Near-Optimal Flowsheets Generated by Algorithm ABB with the Cost of P1 Lowered by 84%

rank	Number of Operating Units						total cost (10 ³ \$/yr)	
	gas strippers	extractors	centrifuges	adsorption columns	ultrafilters	pervaporators		distillation columns
1	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D21, D22)	5286
2	1 (G1)	0	0	2 (B3, B4)	0	0	3 (D27, D28, D29)	6042
3	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D7, D8)	6062
4	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D25, D26)	6081
5	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D5, D6)	6257
6	1 (G1)	0	0	2 (B3, B4)	0	0	1 (D13)	7450
7	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D11, D12)	7612
8	1 (G1)	0	0	2 (B3, B4)	0	0	1 (D14)	7694
9	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D9, D10)	7893
10	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D17, D18)	7939
10	0	0	0	0	1 (U1)	1 (P1)	2 (D21, D22)	7939

\$7939 × 10³/yr, whereas that of the optimal flowsheet is \$5286 × 10³/year (see Table 3).

When the cost of P1 is lowered by as much as 97% to \$782 × 10³/yr, the first through fifth optimal and near-optimal flowsheets generated contain P1 and U1. The corresponding costs of these flowsheets are \$4315 × 10³, \$5071 × 10³, \$5091 × 10³, \$5110 × 10³, and \$5286 × 10³ per year, respectively

(see Table 4). Note that the best flowsheet's configuration is identical to the 10th-best flowsheet with the cost of \$7939 × 10³/yr when P1's cost is lowered by 84% as mentioned in the preceding paragraph; nevertheless, the former's cost is reduced to \$4315 × 10³/yr.

When P1 is at the target cost of \$782 × 10³/yr, i.e., 3% of the current cost, the 11 flowsheets listed in Table 4, ranking

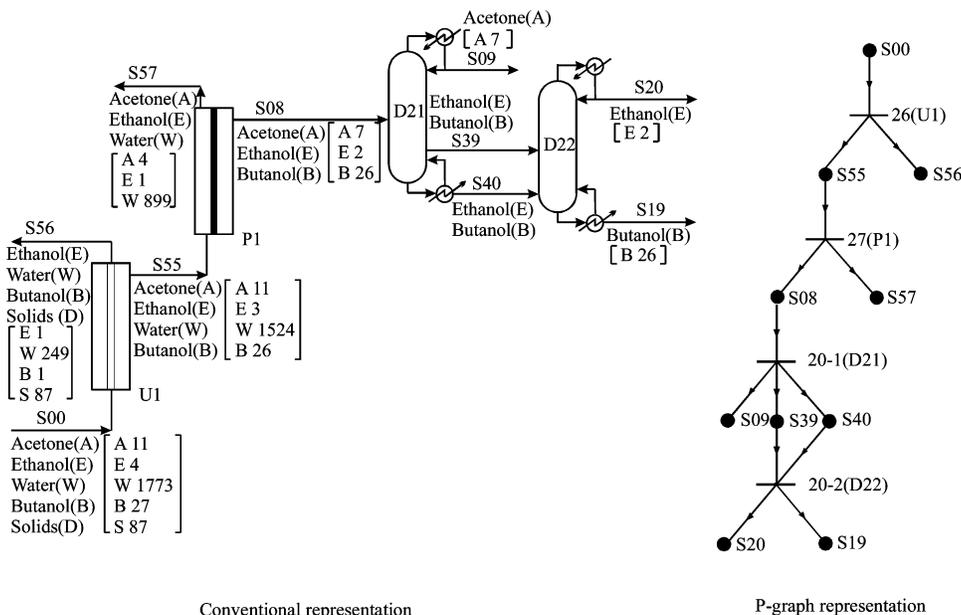


Figure 4. Tenth-best flowsheet with ultrafiltration and pervaporation units included with the cost of P1 lowered by 84%: conventional representation including the component flow rate in 10^3 lb/h. This is also the best flowsheet with the cost of P1 lowered by 97%.

Table 4. Summary of the Optimal and Near-Optimal Flowsheets Generated by Algorithm ABB with the Cost of P1 Lowered by 97%

rank	Number of Operating Units							total cost (10^3 \$/yr)
	gas strippers	extractors	centrifuges	adsorption columns	ultrafilters	pervaporators	distillation columns	
1	0	0	0	0	1 (U1)	1 (P1)	2 (D21, D22)	4315
2	0	0	0	0	1 (U1)	1 (P1)	3 (D27, D28, D29)	5071
3	0	0	0	0	1 (U1)	1 (P1)	2 (D7, D8)	5091
4	0	0	0	0	1 (U1)	1 (P1)	2 (D25, D26)	5110
5	0	0	0	0	1 (U1)	1 (P1)	2 (D5, D6)	5286
5	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D21, D22)	5286
6	1 (G1)	0	0	2 (B3, B4)	0	0	3 (D27, D28, D29)	6042
7	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D7, D8)	6062
8	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D25, D26)	6081
9	1 (G1)	0	0	2 (B3, B4)	0	0	2 (D5, D6)	6257
10	0	0	0	0	1 (U1)	1 (P1)	1 (D13)	6479

1st through 10th with two tied at the 5th, are markedly different in structure from those generated previously with only conventional operating units.²⁰ Moreover, the total cost of any of the flowsheets in the former is substantially less than those of the corresponding flowsheets in the latter. For instance, the total cost of the optimal flowsheet in the former is $\$4315 \times 10^3$ /yr, and that in the latter is $\$9416 \times 10^3$ /yr; obviously, the former is $\$5101 \times 10^3$ /yr (54%) less than the latter.

The total costs of all 10 best flowsheets, when P1 is at the target cost mentioned in the preceding paragraph, are only moderately less than the total costs of the corresponding flowsheets generated previously with the adsorbing units added to the conventional operating units.²¹ For instance, the total cost of the optimal, i.e., best, flowsheet in the former is $\$4315 \times 10^3$ /yr, whereas that in the latter is $\$5286 \times 10^3$ /yr; obviously, the former is only $\$971 \times 10^3$ /yr (18%) less than that of the latter.

As previously mentioned, P1's cost needs to be substantially lowered for its use to be economically viable. There is every indication that such a cost reduction is achievable through an increase in the selectivity and flux of its membrane, as well as through the fabrication of a membrane with substantially less expensive materials.^{4,27–32} Nevertheless, even when the flowsheet containing P1 and U1 becomes highly economically viable, it would be difficult to immediately deploy it commercially: Various concerns about pervaporation, such as its reliability,

stability, and operability, need to be fully resolved; in other words, it needs to attain sufficient maturity.

Note that cost effectiveness is always application-specific. Obviously, it is not yet economically viable to incorporate pervaporation in the biochemical production of butanol, ethanol, and acetone, which are low-cost commodity chemicals manufactured in large quantity. Nevertheless, it would be entirely conceivable that pervaporation, even at the current price, would be deployable for commercially manufacturing a relatively small quantity of extremely expensive fine chemical or biochemical from its dilute aqueous solutions. One such chemical might be Erythropoietin (Epogen), which is selling about $\$840\,000$ per gram.²³ This indicates that the price-targeting strategy for developing a novel operating unit should be performed in the context of the process in which it is to be deployed.

In the current work, the computing time in executing algorithm MSG to generate the comprehensive flowsheet was less than 2 s on a PC (266 MHz and 65 MB Pentium II; Windows 95). For a given set of cost parameters, the computing time for running algorithm ABB to generate the 10 best optimal and near-optimal flowsheets in ranked order was less than 4 s on the same PC. This slight increase of 2 s in the computing time over that required when P1 and U1 were absent in the flowsheet²¹ attests to the inordinate computational efficacy of the graph-theoretic method based on P-graphs.

5. Conclusion

An innovative strategy has been proposed to establish the economically viable target or benchmark price of a processing unit under development through repeated flowsheet resynthesis by parametrically reducing its current price. It uses the graph-theoretic algorithmic method for process-network synthesis based on P-graphs (process graphs). Price targeting through repeated flowsheet resynthesis is fundamentally different from process retrofitting through total flowsheet resynthesis: The former deals with novel and immature operating units with predicted future costs, whereas the latter involves newly developed but sufficiently mature operating units with their current costs. The efficacy of the proposed strategy has been ascertained by determining the target price of the pervaporation unit to be incorporated into the flowsheet for downstream processing of biochemically manufactured butanol.

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Supporting Information Available: Cost estimation for pervaporation and ultrafiltration units (Appendix 1) and Algorithm ABB (Appendix 2). This material is available free of charge via the Internet at <http://pubs.acs.org>.

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