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BATCH-DIST: A COMPREHENSIVE PACKAGE FOR SIMULATION, DESIGN, OPTIMIZATION AND OPTIMAL CONTROL OF MULTICOMPONENT, MULTIFRACTION BATCH DISTILLATION COLUMNS

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Abstract—BATCH-DIST is a general-purpose simulation package for the design, simulation and optimization of multicomponent, multifraction batch distillation columns operating under different modes (constant reflux, variable reflux and optimal reflux policy). The package includes simulation models of varying degrees of complexity and rigor; efficient but simplified models (based on short-cut methods) for preliminary design and rapid analysis of column behavior, and rigorous models (based on solution of transient heat and mass balance differential equations) for verification and detailed column design. Besides simulation and design, BATCH-DIST can also accomplish optimization and optimal control of columns. Coded in Fortran 77, the package is flexible and user-friendly. BATCH-DIST has been extensively tested with benchmark cases involving binary and multicomponent systems, with nonideal behavior and in columns with appreciable holdup effects. Such test cases have clearly demonstrated that predictions of the simplified models in the package compare well with those of the rigorous models. This powerful and comprehensive package is expected to be computationally more efficient than existing packages.

INTRODUCTION

Batch distillation is an important unit operation frequently used for small-scale production. Batch distillation is preferable to continuous distillation where small quantities of high-technology/high-value-added chemicals and biochemicals are to be separated. The batch unit requires less capital for separating relatively pure components. The most outstanding feature of batch distillation is its versatility. It is this flexibility and the inherent unsteady nature of the process which poses challenging design and operation problems. For a realistic simulation of batch distillation, the system has to accomodate several specifications and options.

The two well-known methods of operating batch columns are: variable reflux and constant product composition, and constant reflux and variable product composition.

The optimal reflux policy (optimal control policy) is essentially a trade-off between the two methods and is based on the ability to yield the most profitable operation.

The literature on batch distillation is sporadic and systematic design methods are not reported. Most of the available simulators like BATCHFRAC (Boston *et al.*, 1981), BASIS (Simulation Sciences Inc., 1989) etc. account for some of the above-mentioned specifications and in addition use the rigorous model to simulate the column. The rigorous theoretical treatment of batch distillation is computationally intensive.

BATCH-DIST can handle all types of options described above. It uses computationally efficient and reasonably accurate simplified models. Iterative design, optimization and optimal control can also be accomplished with BATCH-DIST.

The package is based on the Doctoral Dissertation of Diwekar (1988). The code has been developed in Fortran 77 and is user-friendly. It has been extensively tested for both binary and multicomponent systems; ideal as well as nonideal systems, and columns with and without holdup effects.

MAIN FEATURES

The use of rigorous models to simulate batch distillation involves the solution of a number of stiff differential equations. In addition, the dimensionality of the problem increases with an increase in the number of stages and components, which imposes limitations on the use of rigorous models. Finally, problems in design, optimization and control involve iterative procedures, and considerable computational effort would be required to solve them rigorously. As an efficient alternative, BATCH-DIST uses simplified models, and provides reasonably accurate solutions without much computational effort. The package is flexible and can handle all possible modes of operation, operating conditions and target specifications. The philosophy behind the development of the pack-

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age has been to provide for this versatility by making available to the user a variety of models and by developing suitable analysis and design algorithms based on these models. The simplified models used in BATCH-DIST include:

- A model based on the short-cut method
- A model based on the modified short-cut method
- A reduced-order dynamic model using the collocation method.

With these models as the basis, the package can accomplish numerous tasks which are:

- Rapid analysis of the column behavior
- Preliminary design
- Optimal design
- Control
- Evaluating different modes of operation
- Rapid simulation of large columns

The package can handle most cases of batch distillation including constant reflux, variable reflux or optimal reflux modes of operation for both ideal and nonideal systems. It has built in options of design, optimization and optimal control and a user-friendly input interface.

ORGANIZATIONAL STRUCTURE

The structure of the package is outlined in Fig. 1. The user can choose the task (simulation using various models, design, optimization or optimal control), the operating policy (constant reflux, variable reflux or optimal reflux/control) and the model. Thermodynamic options are also available with these packages. A brief description of each of the above options (task, operating policy, model and thermodynamic data) is furnished below:

Tasks

Simulation. This module is used for batch distillation column simulation. In BATCH-DIST different simulation models are incorporated, which makes the package computationally more efficient. The hierarchy of the models is given below in decreasing order of computational efficiency and increasing order of complexity (Fig. 2):

1. Model based on the short-cut method (Diwekar and Madhavan, 1991)—Based on the short-cut method for continuous columns and involves solution of algebraic equations. Applicable to nearly-ideal systems, and columns with constant molal overflow and negligible holdup effect.

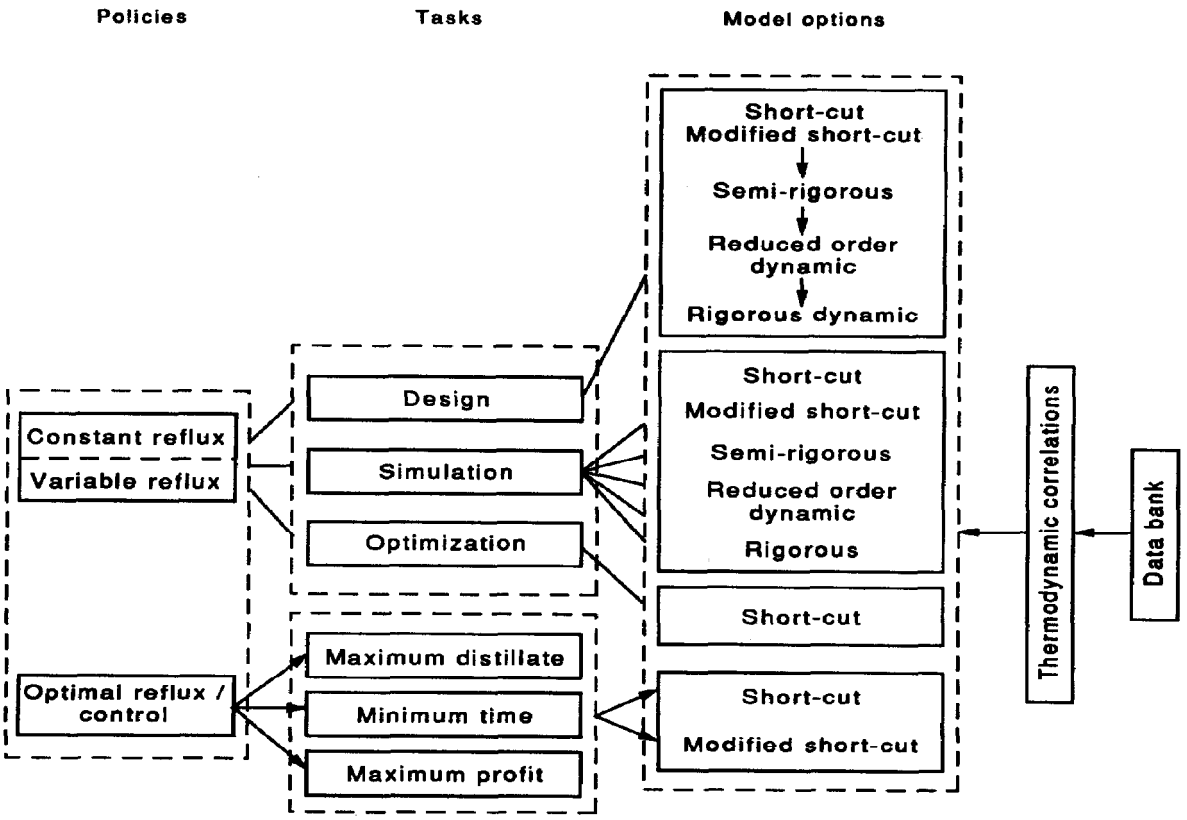

Fig. 1. Scope of BATCH-DIST.

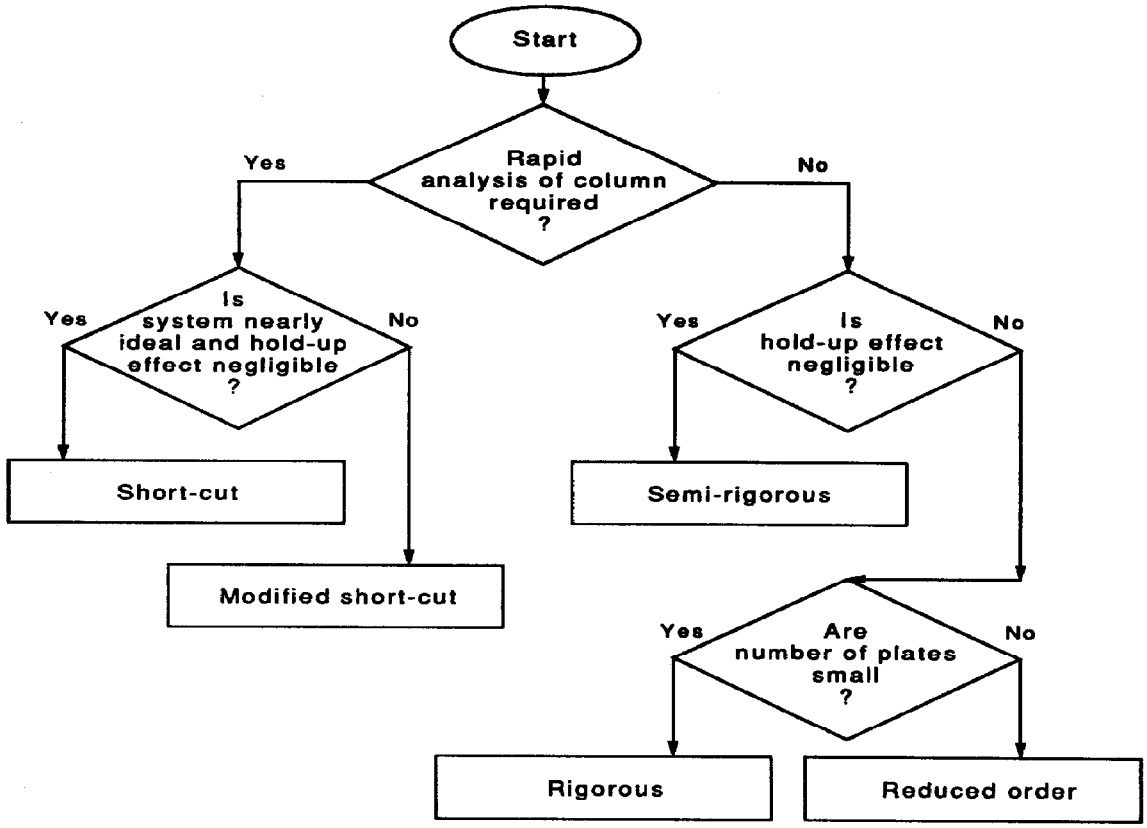

Fig. 2. Guidelines for the use of models.

2. Model based on the modified short-cut method (Diwekar and Madhavan, 1991)—A modification of the short-cut method for highly-nonideal systems and columns with significant holdup effects. The model includes the solution of a few differential equations along with the algebraic equations of the short-cut method. Approximates the performance of ideal/nonideal systems and columns with significant holdup effects. No heat effects are considered (constant molal overflow assumption).
3. Semi-rigorous model—Uses the plate-to-plate computation method of continuous distillation and involves solution of a few differential equations and algebraic equations for plate-to-plate calculations. Rigorous model for nonideal systems with negligible holdup effects. No heat effects are considered.
4. Reduced-order dynamic model—Employs the collocation method to reduce the order of the system of differential equations of the rigorous method. Reduced-order approximation for ideal/nonideal systems, columns with significant holdup effects. Heat effects are considered.
5. Rigorous dynamic model—Involves solution of stiff differential equations for the material and energy balances. Rigorous model for ideal/nonideal systems, columns with significant holdup effects. Heat effects are considered.

Design. This module is used for the iterative design of batch columns using the short-cut or the modified short-cut method. It yields preliminary estimates of the design parameters. The user has to supply minimum input information (components, thermodynamic model and design specifications). The design can be verified using rigorous models, the hierarchy of which is built into the design module as shown in Fig. 2.

Optimization. The short-cut method is used in this module to arrive at an optimal design for batch columns operating under constant or variable reflux conditions (Diwekar *et al.*, 1989). The problem analysis and solution methods are incorporated in the package. The choice of specifications as far as decision variables are concerned is left to the user. For example, in the variable reflux case for a single fraction, the decision variables are initial reflux, vapor rate and the termination criterion expressed in terms of time or final still composition. The user can select any of the three decision variables and specify the remainder.

Optimal control. In optimal control the column is operated with a reflux rate policy which optimizes a chosen performance index (Diwekar *et al.*, 1987). In BATCH-DIST the use of the short-cut method (with the time-implicit equations) and Pontryagin's maximum principle facilitates the development of an optimal control policy. The performance index can be either maximum distillate, or minimum time, or maximum profit.

Operating policies

Batch distillation, in practice, operates in one of the following modes:

1. Constant reflux and variable product composition.
2. Variable reflux and constant product composition.
3. Optimal control policy which is a combination of 1 and 2.

Thermodynamic options and data bank

BATCH-DIST could be easily linked to commercially-available or in-house data banks. A wide variety of thermodynamic models are included in the package for calculating enthalpies, liquid densities and vapor and liquid fugacities. The fugacity methods are based on the equations of state as well as the group contribution methods for both liquid- and vapor-phase nonidealities (Table 1).

Models

Model based on the short-cut method. The method is efficient and is based on the assumption that the batch distillation column can be considered as a continuous distillation column with changing feed. The Fenske–Underwood–Gilliland equations, which have been widely used for continuous columns, have been adapted to batch columns. The short-cut method can yield rapid and reasonably accurate results for nearly-ideal systems and columns in which holdup effects are not severe (currently used batch stills employ low holdup valve trays and bubble caps). Inherent advantages such as less computation time and low memory requirements makes this model an effective tool for the preliminary design and optimization of batch distillation columns. An additional advantage of this method is that the computation time and memory requirements are not affected by an increase in the number of plates.

Table 1. List of fugacity options

A. Vapor phase
1. Ideal
2. Virial equation
3. Redlich–Kwong
4. Soave–Redlich–Kwong
5. Peng–Robinson
6. Lee–Kesler–Plocker
B. Liquid phase
1. Ideal solution
2. Margules
3. Van-Laar
4. Wilson
5. Renon (NRTL)
6. Uniquac
7. Unifac
8. Redlich–Kwong
9. Soave–Redlich–Kwong
10. Peng–Robinson
11. Lee–Kesler–Plocker

Model based on the modified short-cut method. The short-cut method described above needs to be modified for highly-nonideal systems and for columns with large holdup effects. For nonideal systems a tuning parameter is introduced in the minimum reflux equation. The holdup effect is characterized by the parameter (τ = holdup/reflux/distillate rate). For large τ, the initial composition profiles predicted by the short-cut method depart from the rigorous model as the reflux is changed from total reflux to a very small value. This holdup effect is accounted for by partitioning the column into two sections: the top section, which is represented by a dynamic model and the remaining part of the column, which is assumed to be in a quasi-steady-state condition (the short-cut method is applied to this part of the column).

Semi-rigorous model. When holdup in the column is small, the differential equations of the rigorous model become stiff leading to computational difficulties. For small holdup, the quasi-steady-state approximation reduces the differential equations for plates to algebraic equations at any time step.

Reduced order dynamic model. Collocation methods have been used to reduce the model order of staged columns. This approach is based on approximating the column state variables using polynomials rather than a description in terms of discrete functions.

Rigorous dynamic model. The unsteady-state differential equations employed in this model are essentially mass and enthalpy balances. They are solved using an implicit method (GEAR) for stiff equations.

INPUT COMMANDS

The input to BATCH-DIST is user-friendly and is based on the concept of keywords. A typical input file is shown in Table 2.

Table 2. Sample input

```
C* SAMPLE KEYWORD INPUT
POLICY = CONSTANT REFLUX;
COMP-CODE = 1110, 1120, 1130, 1170;
THERMO-MODEL = PENG-ROB,PENG-ROB;
TASK = SHORT CUT;
FEED-COMP = 0.35, 0.10, 0.30, 0.25;
REFLUX-RATIO = 1.0;
LIGHT-KEY = 1110; HEAVY-KEY = 1170;
INITIAL-REFLUX = TOTAL;
NUMBER OF -INTERNAL-STAGES = 5;
PRESSURE OF -COLUMN (MM HG) = 760;
  REFERENCE-COMPONENT = 1110;
VAPOR-RATE = 100; FEED = 100;
  NUMBER-FRACTIONS = 1;
BATCH-TIME = 1.0;
END-TASK = 1;
END-POLICY = 1;
```

Table 3. Sample problems (variable reflux condition)

Case No	System	No. of plates	% Deviation $x_D^{(1)}$	% Deviation $x_B^{(1)}$	Fig(s)
1	*o*-nitrotoluene *m*-nitrotoluene *p*-nitrotoluene	8	0.98	2.1	3
2	*o*-nitrotoluene *m*-nitrotoluene *p*-nitrotoluene	10	0.98	5.7	4

The underlined boldface characters (first three letters) represent the ('keywords') which are recogized by the program. Parameters assigned to the keywords are separated by a comma (','). The commands are terminated by a semicolon (';').

The input must be given in the following order (with the exception of the comment commands):

- Policy commands.
- Thermodynamic option commands.
- Column specification commands.
- End commands.

Any number of commands can be included in a line. Spaces may also be introduced.

A special comment command (C*) can be used for user-specific documentation. This command can be inserted anywhere in the input and allows the user to make notes or remarks.

Any number of tasks can be performed within a policy and any number of policies within a run. Task starts with the word 'TAS = ' and policy with 'POL = ' and ends with 'END-TAS' and 'END-POL', respectively.

Dimensional units can be input with a parenthesis immediately after a keyword.

FILE STRUCTURE

The following four files which are either created or used by BATCH-DIST, are of interest to the user:

Data File:(input)—The data file is the user-input to the program.

History File:(output)—It stores the regression history if the modified short-cut method is used and the integration history if the reduced-order or rigorous method is used.

Error File:(output)—The error messages and warnings are stored in this file. These include errors in input specifications, convergence problems and termination criteria.

Results File:(output)—The results include column configuration, components, property options, and the terminal conditions of operation. It also tabulates the still and distillate composition profiles of all the components and displays the results in terms of alphanumeric plots. Instantaneous column profiles can also be depicted.

PERFORMANCE EVALUATION

The simplified models available in BATCH-DIST have been evaluated using several test cases. The results for a few representative cases are discussed below.

MODEL PREDICTIONS

Short-cut method verification

The validity of the short-cut method has been tested extensively for ideal as well as nonideal systems, with and without holdup. Table 3 shows the results for the variable reflux case and Table 4 for the constant reflux case (with and without holdup). Nonideal systems are addressed separately in the next section.

Variable reflux case. Table 3 summarizes the input conditions for the chosen sample problems and also shows deviations of the results from the rigorous method. Figures 3 and 4 (which include holdup effects) indicate that the predictions of short-cut method are good.

Constant reflux case. Table 4 lists the input conditions for the chosen sample problems and compares the results in terms of the maximum percentage deviation in key component compositions and the percentage deviation in the number of plates N. Figures 5 and 6 show the results for a ternary system. Again, the agreement is excellent.

Comparison with published data. Table 5 compares the predictions of the short-cut method with those of BATCHFRAC (Boston *et al.*, 1981) for the quaternary system consisting of propane, butane, pentane and hexane.

Figures 7 and 8 (Cases 3, 4) show a comparison of the model predictions with the experimental results for cyclohexane and toluene systems obtained by Domenech and Enjalbert (1978). The nonideality has been handled by using the UNIFAC equation.

Table 4. Sample problems (constant reflux condition)

Case No.	System	Reflux ratio	$x_D^{(1)}$	% Deviation x_D	% Deviation x_B	% Deviation N	Fig(s)
1	*o*-nitrotoluene *m*-nitrotoluene *p*-nitrotoluene	3	0.9412	< 1	< 1	2.25	5,6
2	Propene *Iso* butane N-butane	10	0.7400	< 1	< 1	3.2	

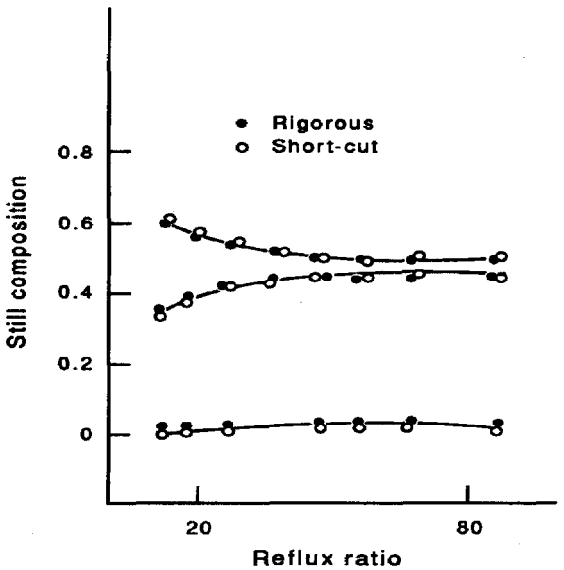

Fig. 3. Profiles (variable reflux) (Case 1, Table 3).

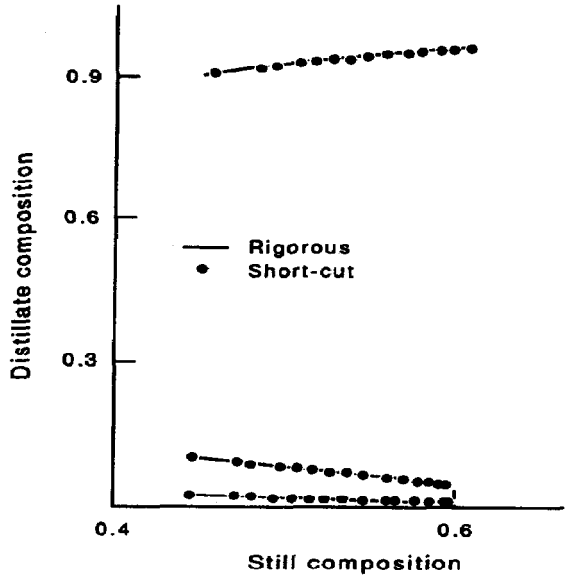

Fig. 5. Profiles (constant reflux) (Case 1, Table 4).

The experimental and theoretical results obtained by Stewart *et al.* (1973) are compared with the results obtained by the short-cut method in Figs 9 and 10 (for octane, nonane and decane). Figure 10 shows the profiles for different values of holdup.

Modified short-cut method verification

The results obtained by the modified short-cut method are compared with those obtained using rigorous dynamic models (Stewart *et al.*, 1973) for the ternary system comprising octane, nonane and decane (Fig. 11). As seen in the figures the inclusion of dynamic effect in the short-cut method results in closer correspondence with predictions of the rigorous model.

A comparsion of the results obtained by the modified short-cut method and the rigorous method, for a highly nonideal system (ethanol–water), is shown in Fig. 12.

Reduced-order dynamic model verification

Table 6 shows the input conditions for the selected sample problems and it also compares the results in

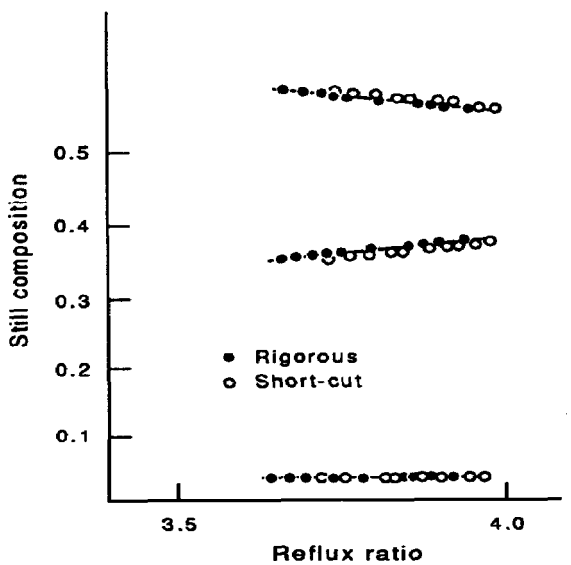

Fig. 4. Profiles (variable reflux) (Case 2, Table 3).

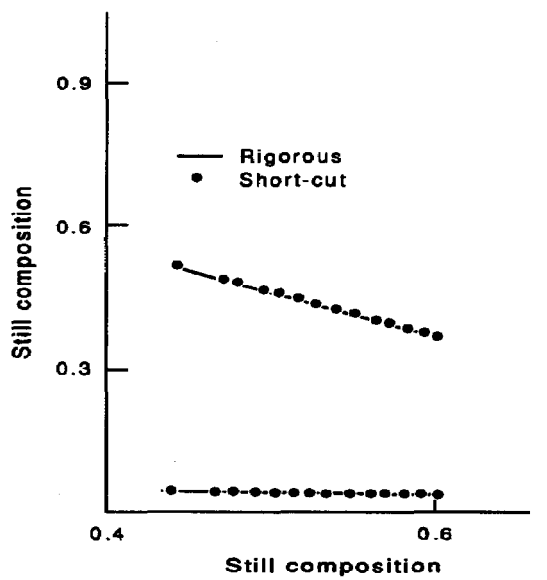

Fig. 6. Profiles (constant reflux) (Case 1, Table 4).

Table 5. Comparison with BATCHFRAC

Operational step purpose	Propane remove 1		Propane remove 2		Butane remove 3		Pentane remove 4		Pentane remove 5	
	BATCH-FRAC	BATCH-DIST	BATCH-FRAC	BATCH-DIST	BATCH-FRAC	BATCH-DIST	BATCH-FRAC	BATCH-DIST	BATCH-FRAC	BATCH-DIST
Reflux ratio	5	5	20	20	25	25	15	15	25	25
Distillate rate	2	2	2	2	2	2	2	2	2	2
Vapor rate	12	12	42	42	52	52	32	32	52	52
Batch time	4.07	4.07	1.81	1.81	18.27	18.27	4.31	4.31	1.78	1.78
Distillate composition (m.f.)										
Propane	0.8000	0.8173	0.0150	0.0190						
Butane	0.2000	0.1817	0.9850	0.9742	0.1644	0.1593				
Pentane				0.0063	0.8356	0.7521	0.8000	0.7638	0.0161	0.0168
Hexane				0.0005		0.0886	0.2000	0.2362	0.9839	0.9832
Average distillate composition at the end of each fraction (m.f.)										
Propane	0.9888	0.9853	0.5230	0.5220	0.0002					
Butane	0.0112	0.0145	0.4770	0.4750	0.9900	0.9915	0.0058	0.0050		
Pentane				0.0026	0.0098	0.0077	0.9845	0.9840	0.2994	0.3044
Hexane				0.0004		0.0008	0.0097	0.0110	0.7006	0.6956
	8.1321	8.1220	3.6130	3.6000	36.543	36.388	8.6020	8.6015	3.600	3.5390
Pot composition (m.f)										
Propane	0.0206	0.0217		0.0001						
Butane	0.3254	0.3252	0.3191	0.3193	0.0006	0.0006				
Pentane	0.1090	0.1088	0.1135	0.1134	0.1335	0.1335	0.0173	0.0174	0.0002	0.0002
Hexane	0.5450	0.5442	0.5674	0.5672	0.8658	0.8658	0.9872	0.9826	0.9998	0.9998
	91.735	91.878	88.124	88.136	71.600	71.736	62.998	62.999	59.398	59.458

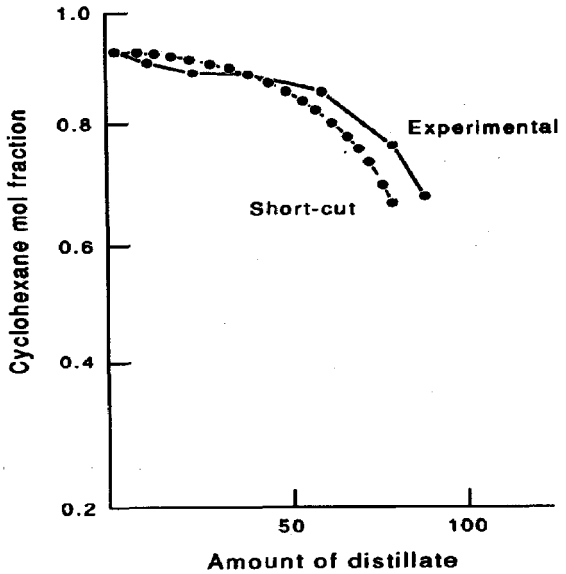

Fig. 7. Experimental and theoretical distillation curves for a nonideal system.

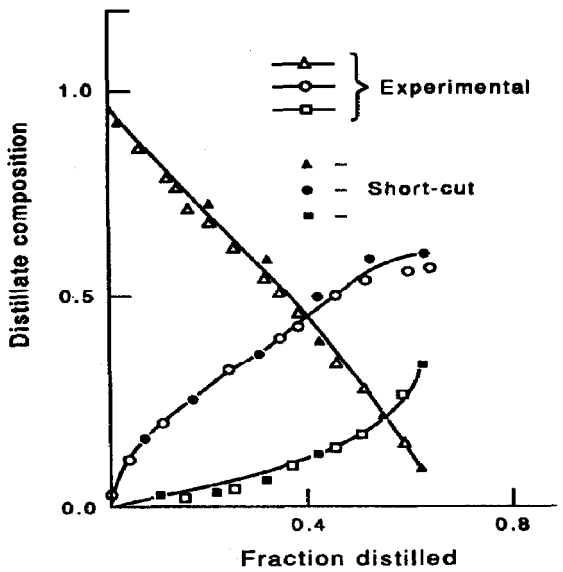

Fig. 9. Experimental and theoretical distillation curves (constant reflux).

terms of percentage deviation. Figure 13 shows the transient response of the ternary system. It is clear that the reduced-order model shows good agreement with the rigorous dynamic model and the accuracy increases with an increase in the number of collocation points. Figure 14 shows the composition profiles of the column after 0.6 s.

It can be concluded from the above benchmark examples that the different models used in BATCH-DIST provide accurate and reliable simulation of batch distillation for different kinds of systems.

CPU time comparsion

Table 6 [section (b)] lists the CPU time requirements of the different simulation models for a quaternary system described in section (a). Use of the appropriate simplified model in BATCH-DIST could lead to considerable savings in computation time over

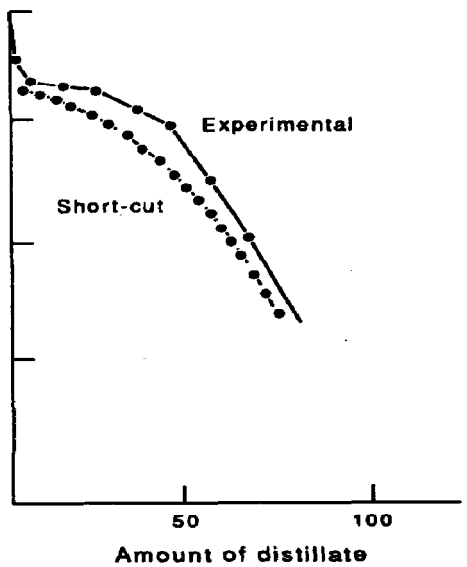

Fig. 8. Experimental and theoretical distillation curves for a nonideal system.

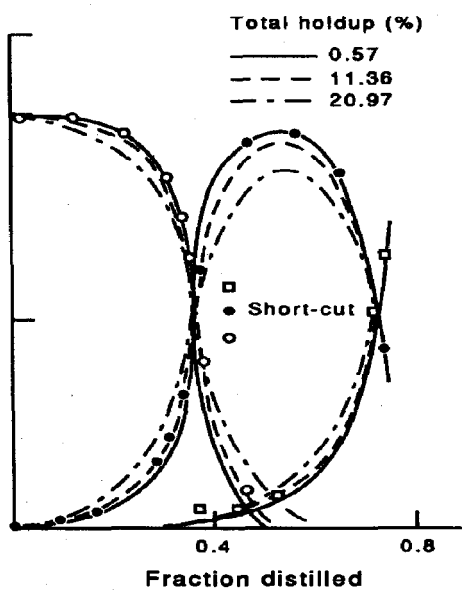

Fig. 10. Theoretical distillation curves.

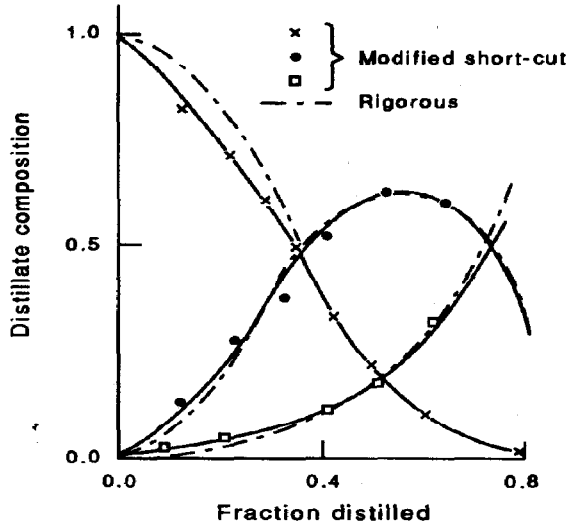

Fig. 11. Theoretical distillation curves (constant reflux).

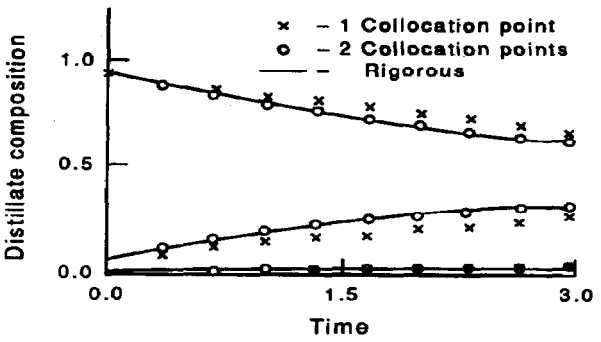

Fig. 13. Transient profiles (Case 1, Table 6).

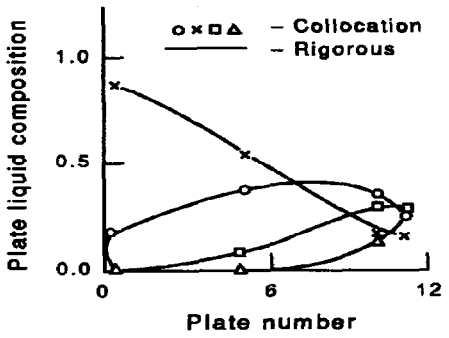

Fig. 14. Column profiles after time t = 0.6 (Case 2, Table 6).

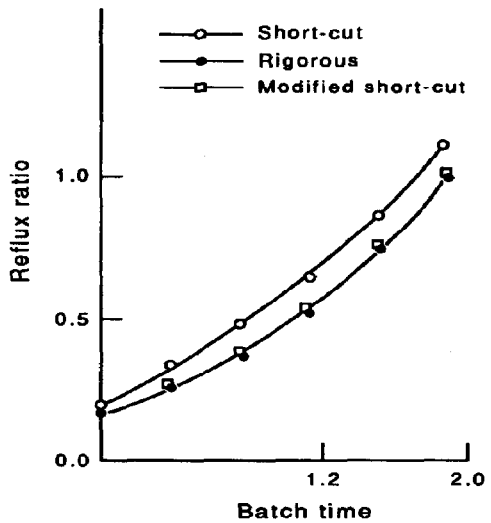

Fig. 12. Profiles for ethanol–water system (variable reflux).

the use of rigorous models in other batch distillation packages.

Our recent experience with the binary azeotropic systems (Diwekar, 1991) shows that for the problems considered in the study, the short-cut method is approx. 200–300 times faster than the semi-rigorous method.

CONCLUSIONS

We have discussed BATCH-DIST, a powerful and comprehensive package which can handle a variety of problems in multicomponent, multifraction batch distillation. The package has a great potential because of its inherent flexibility to all possible modes

Table 6. Sample problems (reduced order model)

System	Feed composition	N	R	No. of collation points	% deviation R	% deviation x_D	% deviation x_B	Fig(s)
Propene	0.4	10	3.0	1	0.9	8.0	0.3	13
Propane	0.3			2	0.9	0.1		
*Iso*butane	0.3							
Propene	0.25	10	3.0	1		0.2	0.4	14
Propane	0.25			2		0.6	0.8	
*Iso*butane	0.25							
Butane	0.25							
Propane	0.5	10	var.	1	4.5	0.47	5.9	
*Iso*butane	0.5							

Table 7. CPU time requirement for different models

(a) Problem definition (constant reflux condition)

Components	Relative volatility	Feed composition	N	R
Propane	4.0	0.1		
Butane	1.0	0.3	20	3.0
Pentane	0.25	0.1		
Hexane	0.05875	0.5		

Vapor rate = 12; feed = 100; holdup per plate = 0.2; batch time = 1

(b) Results

Model	CPU time[a](s)
Short-cut	0.480
Modified short-cut	1.080
Semi-rigorous	2.380
Reduced order	2.820
Rigorous	8.040

[a]ND-560 CPU time.

of operation, the use of new efficient algorithms leading to higher computional efficiency and its user-friendliness.

REFERENCES

Boston J. F., H. J. Britt, S. Jirponghan and V. B. Shah, *FOCAPD* **2,** 203 (1981).

Diwekar U. M., Simulation, design and optimization of multicomponent batch distillation columns. Ph.D. Thesis, Dept of Chemical Engineering, Indian Institute of Technology, Bombay (1988).

Diwekar U. M. An efficient design method for binary azeotropic batch distillation column design. In preparation (1991).

Diwekar U. M. and K. P. Madhavan, Multicomponent batch distillation column design. *Ind. Engng Chem. Res.* Accepted for publication (1991).

Diwekar U. M., R. K. Malik and K. P. Madhavan, *Computers chem. Engng* **11,** 629 (1987).

Diwekar U. M., K. P. Malik and R. E. Swaney, *Ind. Engng Chem. Res.* **29,** 1011 (1989).

Domenech S. and M. Enjalbert, *Chem. Engng Sci.* **29,** 1529 (1978).

Simulation Sciences Inc., *BASIS User Manual.* Fullerton, CA (1989).

Stewart R. E., E. Weisman, B. M. Goodwin and C. E. Speight, *Ind. Engng Chem. Process. Des. Dev.* **12,** 130 (1973).