An application of qualitative analysis of ordinary differential equations to azeotropic batch distillation

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Recently, a new approach to automate the qualitative analysis of dynamic systems has emerged in the AI literature. This approach has been successful in automatically constructing the phase portraits of explicitly specified second-order nonlinear dynamic systems, using the mathematics of nonlinear dynamics. In this paper, we extend the capability of the existing techniques to implicitly defined equations and apply it to the batch distillation of ternary azeotropic systems.

Rigorous models for the batch distillation of azeotropic systems are computationally complex, and the derivation of properties, such as feasible regions of operation does not seem possible. In this paper, we develop *abstract models (short-cut models)* for ternary azeotropic batch distillation based on simplifying assumptions to rigorous models. These abstract models are computationally simpler to analyze without compromising fidelity and would allow the derivation of a feasible region of operation. A knowledge of *distillation boundaries* and *azeotropic points* is essential for the proposed process of abstraction. The derivation of the distillation boundaries requires a qualitative analysis of ordinary differential equations describing the simple distillation operation.

Key words: qualitative analysis, nonlinear dynamic systems, phase portraits, automation, batch distillation, ternary azeotropes, residue-curve maps, short-cut models.

1 INTRODUCTION

Most previous work on qualitative reasoning literature in AI[1,2] has attempted to identify the qualitative properties of a dynamic system by performing a 'qualitative simulation'. Here, the term 'qualitative' is used to mean that the state variables (of a given set of differential equations) are represented by intervals such as $(+, 0, -)$ and the functional relations are also converted to monotonic relations ('confluences'). The dynamic system is simulated by letting the system evolve for a given set of interval initial values. Given the ambiguous nature of interval arithmetic, even for simple cases these simulations are plagued with multiple results, some of which are often physically infeasible. As a result, the use

of these methods for engineering analysis has been severely limited.

Recently, in a position paper, Sacks and Doyle[3] have outlined the shortcomings of the 'qualitative simulation' approach and have suggested the use of the mathematical theory of nonlinear dynamics to automate the qualitative analysis of dynamic systems. Some initial work along this direction has been reported in the literature,[4–6] which has demonstrated the ability to automate the qualitative analysis of second-order nonlinear autonomous differential equations. Although different programs differ in their ability to solve different classes of problems, they all nonetheless are able to construct automatically the phase portrait of highly nonlinear second-order systems. This direction of research provides the promise of useful applications of qualitative reasoning in engineering analysis and design. In this paper, we report the first such application where

the qualitative analysis of the simple distillation process for azeotropic systems is used to derive an abstract model which is computationally simpler to analyze.

Rigorous models for the batch distillation of *azeotropic* systems are computationally complex as they involve solving for a large number of stiff differential equations. Moreover, the derivation of a feasible region of operation using rigorous models does not seem possible. One approach for dealing with this computational complexity is to develop simplified models which are abstractions of rigorous models. The abstraction process is a trade-off between simplicity and fidelity. The usefulness of abstracted models depends on the ease with which they can be analyzed for global behavior, without comprising fidelity. It is precisely with these considerations that one of the authors of this paper has developed an abstract model for the analysis of binary azeotropic distillation columns. The abstract models † for *binary* azeotropic batch distillation can be analyzed about 200 to 300 times faster than rigorous models without sacrificing accuracy.[7] In this paper, we extend the process of abstraction to *ternary* azeotropic batch distillation. The *qualitative analysis of differential equations* is critical to this process of abstracting simple models from rigorous models of ternary azeotropic batch distillation and forms the primary focus of this paper.

In Section 2 we describe an AI based program, which automatically constructs the *residue curve maps* for ternary azeotropic systems. To illustrate this, we present the ethanol–water–cyclohexane ternary azeotropic system and its residue curve map derived by our program. Section 3 describes a process for abstracting simplified models for azeotropic batch distillation systems. This abstraction process is applied to the acetone–isopropanol–water to illustrate three points:

1. The need for constructing the *residue curve map* for simple distillation and its use in the abstraction process.
2. The high accuracy of the abstract model in comparison to rigorous models.
3. The substantial savings in the computational effort by using the abstract model.

Finally, in Section 4 we discuss the impact of this work for the preliminary analysis and optimization of ternary azeotropic batch distillation columns.

2 AUTOMATIC ANALYSIS OF ORDINARY DIFFERENTIAL EQUATIONS

Qualitative reasoning with dynamic systems involves drawing a phase portrait, that is, partitioning the phase

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†For reasons of consistency with the literature pertaining to this subject, we have used the terms *abstract models* and *shortcut methods* as synonyms in this paper.

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plane in which the behavior of the system is essentially similar. This requires identifying special solutions such as *equilibrium points, limit cycles* and *separatrices*. The qualitative theory of differential equations does not provide systematic methods to identify these solutions by purely analytic means. Symbolic reasoning must be supplemented with numeric simulation of behavior, with initial values judiciously chosen based on partial analysis. One of the authors of this paper has been involved in developing a program[6,8] which integrates the use of symbolic and numeric computational methods to construct *automatically* the phase portrait of a dynamic system. Symbolic methods are used to search for equilibrium points, separatrices and limit cycles, using heuristics based on the underlying *mathematical theory*. These results are then used to guide numerical simulation to identify the remaining features of the phase portrait.

2.1 Qualitative analysis of planar differential equations

In this subsection we provide a brief introduction to the qualitative analysis of differential equations. We restrict our discussion to planar systems described by

$$\frac{dx}{dt} = P(x, y), \quad \frac{dy}{dt} = Q(x, y) \qquad (1)$$

We assume that P and Q are nonlinear and satisfy conditions guaranteeing the existence and uniqueness of the solution for given initial values. Moreover, we assume that time does not appear explicitly in P and Q and hence the system is termed *autonomous*. The reader is referred to Coddington[9] for a detailed discussion of the theory of ordinary differential equations, and to Andronov *et al.*[10,11] for a detailed discussion of the qualitative theory of second order differential equations.

Any state (x, y) is represented by a point in the *phase plane*, which represents the set of all possible states of the system. The state variables x and y are functions of time $t : x = f(t)$, $y = g(t)$. As t varies, the state (x, y) moves along a *path*, which is also called a *trajectory*. A complete path represents the history of the system throughout all times. The totality of all paths represents all possible histories and it is called the *phase portrait*. One and only one path passes through each point in the phase plane for autonomous systems. So the precise knowledge of any single point on the path determines the entire path for the system.

Qualitative investigation entails the construction of a *phase portrait* which describes the partitioning of the phase plane into regions in which the behavior of the system is qualitatively similar. Three kinds of information are critical for the construction of the phase portrait. First, we need to identify the point trajectories or the *equilibrium points* of the system and the local behavior of the system around these points. The local behavior is derived by computing the eigenvalues and

eigenvectors of the Jacobian of the system around the equilibrium points. Second, we need to identify the existence or the nonexistence of closed paths called *limit cycles*, which are periodic solutions of the system. Lastly, we need to identify the global behavior of the trajectories that pass through equilibrium points. Such paths are called *separatrices*. For a more complete discussion, the reader is referred to a recent paper by Kalagnanam *et al.*[6]

2.2 Residue curve maps for azeotropic systems

Now we turn our attention to the thermodynamics of azeotropic distillation processes described by using differential equations. Doherty and coworkers[12-14] have shown the correspondence between the mathematical properties on the differential equations describing the simple distillation residue curve map and thermodynamic properties for azeotropic distillation.

A residue curve map for the simple distillation operation graphs the liquid composition paths which are solutions to the following set of ordinary differential equations:[12]

$$\frac{dx_i}{d\zeta} = x_i - y_i \quad i = 1, 2, \ldots, n-1 \quad (2)$$

where n is the number of components in the system (i.e. for a ternary system $n = 3$), the independent variable ζ is a monotonically increasing quantity related to real time, and

$$0 \le x_i \le 1, \quad 0 \le y_i \le 1$$

y_i, the vapor composition, is related to x_i, the liquid composition, by the following vapor–liquid equilibrium (VLE) relationship:

$$y_i = \frac{x_i \gamma_i p_i^s}{p} \quad i = 1, 2, \ldots, n$$

where the liquid nonideality in terms of the activity coefficients γ can be calculated using the Wilson equation given below:

$$\ln \gamma_i = -\ln \left(\sum_{j=1}^n x_j \Lambda_{ij} \right)$$
$$+ 1 - \sum_{k=1}^n \frac{x_k \Lambda_{ki}}{\sum_{j=1}^n x_j \Lambda_{kj}} \quad i = 1, 2, \ldots, n$$

and the Antoine vapor pressure equation:

$$\log \frac{p_i^s}{p} = A_i - \frac{B_i}{T + C_i} \quad i = 1, 2, \ldots, n$$

The temperature T (in degrees Kelvin) in the above equations is calculated using

$$\sum_{i=1}^n \frac{x_i \gamma_i p_i^s}{p} = 1$$

and A_i, B_i and C_i are constants associated with the ith component in the ternary system and Λ_{ij} is the interaction parameter between component i and component j given by

$$\Lambda_{ij} = \frac{V_j}{V_i} \exp \left(-\frac{(\lambda_{ij} - \lambda_{ii})}{RT} \right)$$

where V_i is the molar volume of pure liquid component i, and λ_{ij} is the interaction energy between component i and j; R is the gas constant. The vector coefficients $\vec{A}$, $\vec{B}$, $\vec{C}$, $\vec{V}$, $\vec{\lambda}$ depend on the specific system under consideration. The actual values of the coefficients for the acetone–isopropanol–water and the ethanol–water–cyclohexane system are provided in Tables 1 and 2. Notice that the relation between x_i and y_i is given by an implicit relation which involves temperature T. A residue curve map is a phase portrait of the system in the composition space. The azeotropes correspond to the equilibrium points of the system, and the separatrices along with the boundaries of the phase portrait form the distillation boundaries.

The topological structure of the residue map is severely constrained by the thermodynamics of azeotropic distillation. Since x_i is the liquid composition, $\Sigma_i x_i = 1$ and the residue curve map is defined on a simplex. The vertices correspond to pure component compositions, and the equilibrium points are binary and ternary azeotropes. For $n = 3$ the residue curve map is defined on a right-angled triangle. The temperature surface is a naturally occurring Lyapunov function for the above differential equations. The movement of the liquid composition x_i is always in a direction which makes the temperature increase. The temperature function can be used to show that the above differential equations do *not* possess limit cycles. This constraint is extremely useful in constructing the residue map since it eliminates the computationally intensive search for the existence or nonexistence of limit cycles. Moreover, it has also been shown that the equilibrium points of this system are isolated and are either *saddles or nodes*.[15] This information severely restricts the search for the global configuration of the separatrices.

In the following subsection, we extend our previous work[6] to generate residue curve maps automatically for ternary solutions with binary and ternary azeotropes. These methods incorporate the use of the thermodynamics and the mathematical theory of dynamic systems to derive the residue maps. We also illustrate these methods by deriving the residue curve map for the ethanol–water–cyclohexane system.

2.3 Design and implementation

The procedure for constructing the residue curve map and extracting regions of qualitatively similar behavior bounded by distillation curves has been implemented using *Mathematica*.[16] The flow chart for this procedure

Table 1. System parameters for acetone–isopropanol–water ternary azeotropic system and input parameters for the batch distillation columns (Figs 2 and 3)

	System parameters for acetone–isopropanol–water							
Component i	Antoine constants				Wilson constants			Rel. vol.
	A_i	B_i	C_i	V_i	λ_{i1}	λ_{i2}	λ_{i3}	model
Acetone	4·23633	1210·595	−43·336	74·05	1·0	−203·114	679·487	2·790
Isopropanol	5·99476	2010·330	−20·364	76·92	593·183	1·0	556·390	1·000
Water	5·19050	1730·630	−39.574	18·07	1251·917	1294·715	1·0	0·367

	Input parameters for the batch distillation columns (Fig. 6)	
Component i	Feed composition	
	Case (a)	Case (b)
Acetone	0·05	0·10
Isopropanol	0·40	0·40
Water	0·55	0·50
Number of plates	5	5
Molar vapor rate	5·0	5·0
Molar feed	100·0	100·0
Holdup (%)	6·0	0·6

Table 2. System parameters for ethanol–water–cyclohexane ternary azeotropic system

Component i	Antoine constants				Wilson constants		
	A_i	B_i	C_i	V_i	λ_{i1}	λ_{i2}	λ_{i3}
Ethanol	5·2314	1592·864	−46·816	56·68	1·0	288·9156	1894·2908
Water	5·1905	1730·630	−39·574	18·07	962·0073	1·0	18155·835
Cyclohexane	3·9706	1206·470	−49·864	108·75	399·2968	35623·307	1·0

is presented in Fig. 1. We have also indicated in the figure how the use of the thermodynamics allows us to bypass the search for limit cycles.

For a given system of differential equations we first identify the equilibrium points and the topological structure of the paths in the neighborhood of these points. The stability of these equilibrium points and their local behavior provides the first, although local, indication of where the system might settle in the long run. Sometimes the local behavior about the equilibrium points cannot be determined based on linear approximations. Such points are called *nonelementary* equili-
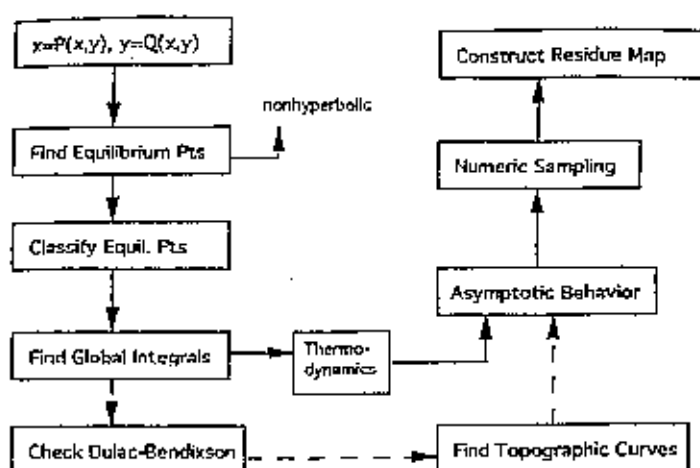

Fig. 1. Flow chart for residue curve map analysis.

brium points and we have not dealt with such points in this paper. Finally, the program examines the asymptotic behavior of the paths as $t \to \infty$. This is done by configuring the global behavior of the separatrices by using geometric constraints about adjacency.

2.3.1 Finding the equilibria

At equilibrium, $(dx/dt) = 0$, $(dy/dt) = 0$. The equations cannot be solved explicitly and hence the program has to use numerical methods to identify the equilibrium points. We have used *secant methods* to identify binary equilibrium points and *generalized secant methods* for ternary equilibrium points since the derivatives of the simple distillation equations are not easily characterized. The convergence of numerical methods depends critically on the initial values provided to the subroutines. For the distillation process, the region of search is severely constrained by the conditions $\Sigma_i x_i = 1$. We have found that by sampling the simplex uniformly we are able to identify all the azeotropes in all the examples we have examined. It appears that the secant methods provide robust methods for identifying the binary and ternary azeotropes.

For example consider the ethanol–water–cyclohexane system. The vector coefficients $\bar{A}$, $\bar{B}$, $\bar{C}$, $\bar{V}$, $\bar{\Lambda}$ for this system are provided in Tables 1 and 2. This system has *three* binary azeotropes $(0.457,0)$, $(0,0.299)$, $(0.89,0.11)$. Notice that the points $(0,0)$, $(0,1)$, $(1,0)$ correspond to pure compositions. The system has *one* ternary azeotrope $(0.316,0.15)$.

2.3.2 Classifying the equilibria

The classification of the equilibrium points is based on the local behaviour of the system about the equilibrium points. In order to classify the equilibrium points we linearize the equations about the equilibrium points and evaluate the eigenvalues and the eigenvectors of the linear system. For a ternary system this procedure is straightforward, and the partial derivatives are calculated using perturbation methods. However, for equilibrium points on the boundaries such as the binary azeotropes and the vertices we need to remember to evaluate the partial along directions from within the simplex and then use these partials to evaluate the eigenvalues and eigenvectors. We use simple rules regarding the appropriate directions for evaluating the partials for the vertices and binary azeotropes.

For the ethanol–water–cyclohexane system, all the binary azeotropes are *saddles* and all the vertices are *stable nodes*. The ternary azeotrope is an *unstable node*.

2.3.3 Configuration of the separatrices

Once we have all the equilibrium points of a given system we can list all the separatrices of the system, since we know that saddlepoints give rise to *one* stable and *one* unstable separatrix, and stable (unstable) nodes give rise *two* stable (unstable) separatrices. We also have
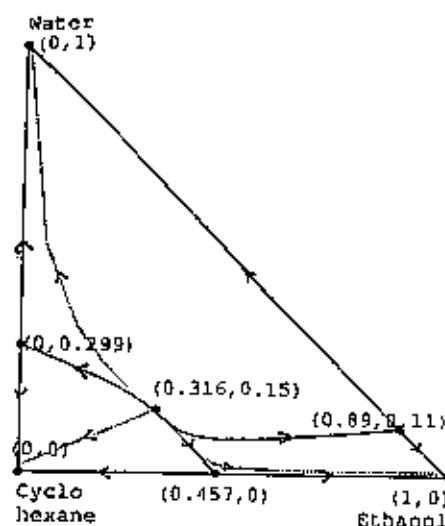

Water
(0,1)

(0,0.299)

(0.316,0.15)

(0.89,0.11)

(0,0)

Cyclo
hexane   (0.457,0)   (1,0)
Ethanol

Fig. 2. Residue curve map.

available to us the local behavior of these separatrices. The characterization of the global qualitative behavior of the separatrices is just the question of how to link up each separatrix beginning at one equilibrium point with its corresponding end at another (or the same) point. The search for the possible global configuration is constrained by rules derived from topological considerations. These rules are discussed in detail in Ref. 6. Here, we discuss how these rules constrain the separatrices for the ethanol-water-cyclohexane system.

Since all the binary azeotropes are saddlepoints and lie on the edges of the simplex, the edges are necessarily the separatrices of the binary azeotropes. Moreover, all the vertices are stable nodes, therefore the unstable separatrices emanating from each of the binary azeotropes terminate at the vertices moving along the edges (see Fig. 2). The unstable separatrices for each of the binary azeotropes emanate from the unstable ternary azeotrope and divide the residue curve map into *three* qualitative different regions. The unstable separatrices of the ternary azeotrope asymptotically evolve towards one of the vertices. The complete residue curve map for the ethanol-water-cyclohexane system is provided in Fig. 2.

2.4 Comparison with other work

In a recent paper, Foucher *et al.*[14] provide an automatic procedure for the determination of the structure of simple distillation residue curve maps for ternary mixtures. There are two main differences in the approach presented in this work. First, Foucher *et al.*[14] have assumed that the knowledge of the boiling temperatures and compositions of the azeotropes are known, whereas we use secant methods to determine the azeotropes. Second, Foucher *et al.*[14] use rules to classify the azeotropes as nodes or saddles, while we use

linearization along specific directions to classify the azeotropes as nodes or saddles. Although the procedure presented by Foucher *et al.*[14] is elegant for ternary systems, our approach is more general and can be easily extended to higher order azeotropes. In another recent paper, Bossen *et al.*[17] present the computational tools needed for the simulation, design and analysis of azeotropic distillation columns. However, they do not perform any qualitative analysis of the differential equations, in contrast they simulate the separatrices directly. In our approach, we first classify the azeotropes and determine their global configuration based on the nature of the azeotropes and then use this information to guide the numerical simulation of the separatrices. This approach provides a better handle for designing automatic procedures to determine the structure of simple distillation residue curve maps for ternary and higher order systems.

3 THE ABSTRACTION PROCESS

In Section 2 we described a program based on the qualitative analysis of different equations, which automatically constructs the residue curve maps for ternary azeotropic systems. In this section, we present the abstraction process used to derive simplified models of ternary azeotropic batch distillation. We describe the application of this abstraction process to the acetone–isopropanol—water system and use it to illustrate three points:

1. The need for constructing the *residue curve map* of the simple distillation process in the abstraction process.
2. The high accuracy of the abstract model in comparison to rigorous models.

3. The substantial savings in the computational effort by using the abstract model.

The process of abstraction for ternary azeotropic batch distillation columns is shown in Fig. 3. The qualitative analysis of the ordinary differential equations (described in Section 2.1) to construct the residue curve maps can provide an appropriate tool for generating the knowledge of azeotropic points and distillation boundaries. The mathematical theory of nonlinear dynamics and the underlying thermodynamics are used to extract automatically the azeotropic points and distillation boundaries of the simple distillation process. The knowledge of these boundaries is then used to derive simplified vapor–liquid equilibria (VLE) models for each of the regions in the composition space separated by the distillation boundaries. The abstract models are then constructed using these simplified VLE models.

3.1 The extended short-cut method

The short-cut method for batch distillation[18] is based on the assumption that the batch distillation column can be considered as a continuous distillation column with changing feed at any time instant. The short-cut method provides substantial savings in terms of the computational efforts, and their validity has been tested extensively for ideal as well as nonideal nonazeotropic systems, with and without holdup.[7,18] It has been found that the short-cut method can yield reasonably accurate results for nearly ideal systems and columns in which holdup effects are not severe. For columns with large holdup, a lumped dynamic element is introduced at the top of the column to account for the gradual variation of the product composition. The preliminary results of this modified short-cut method show that the inclusion
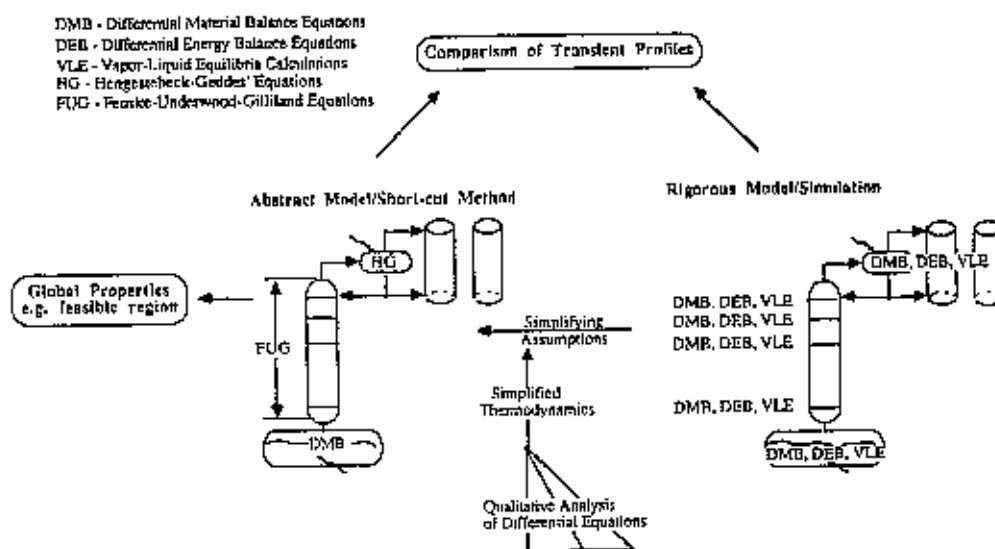

DMB - Differential Material Balance Equations
DEB - Differential Energy Balance Equations
VLE - Vapor-Liquid Equilibria Calculations
HG - Hengestebeck-Geddes' Equations
FUG - Fenske-Underwood-Gilliland Equations

Fig. 3. Schematic of the abstraction process.

of the dynamic effect in the short-cut method captures the holdup effect to a large extent.[19]

The short-cut methods are based on the assumption of constant relative volatility through the column, updated at each time instant, and use the following relationship for obtaining vapor–liquid equilibria:

$$y_i = \frac{\alpha_i x_i}{\sum\limits_{k=1}^{n} \alpha_k x_k}; \quad i = 1, 2, \ldots, n \quad (3)$$

where y_i is the vapor composition of the component i in equilibrium with the liquid composition x_i of the component i, and α_i is the relative volatility of the component i.

However, in the case of azeotropic systems this relation is no longer valid because of the azeotropic points (where the relative volatility becomes unity) and the distillation boundaries (which bounds the distillation paths). The azeotropic points and distillation boundaries offer impassable barrier/barriers. For binary azeotropic systems, Anderson and Doherty[20] transform the variables of binary VLE calculations by splitting the equilibrium curve into two regions. This approach is used for extending the short-cut method to binary azeotropic systems.[21] The bottom curve below the azeotropic composition of component 1 is represented by

$$x_1' = \frac{x_1}{x_1^{az}}; \quad x_2' = 1 - x_1'$$
$$y_1' = \frac{y_1}{y_1^{az}}; \quad y_2' = 1 - y_1' \quad (4)$$

and the top curve is given by

$$x_1' = \frac{x_1 - x_1^{az}}{1 - x_1^{az}}; \quad x_2' = 1 - x_1'$$
$$y_1' = \frac{y_1 - y_1^{az}}{1 - y_1^{az}}; \quad y_2' = 1 - y_2' \quad (5)$$

The equilibrium relationship for the binary system in terms of the transformed variables is represented by

$$y_1' = \frac{\alpha_1 x_1'}{1 + (\alpha_1 - 1)x_1'} \quad (6)$$

It has been found that the preliminary estimates of this extended short-cut method for ideal binary azeotropic systems compare very well with the rigorous models and it offers significant computational savings over the rigorous models (for some cases, the short-cut model was found to be 200 to 300 times faster than the rigorous models). For details of these preliminary studies please refer to the recent paper by Diwekar.[21]

For ternary systems, although the transformation of variables is key for extending the short-cut method, the impassable barriers are not represented by the azeotropic points as in the case of binary azeotropic batch
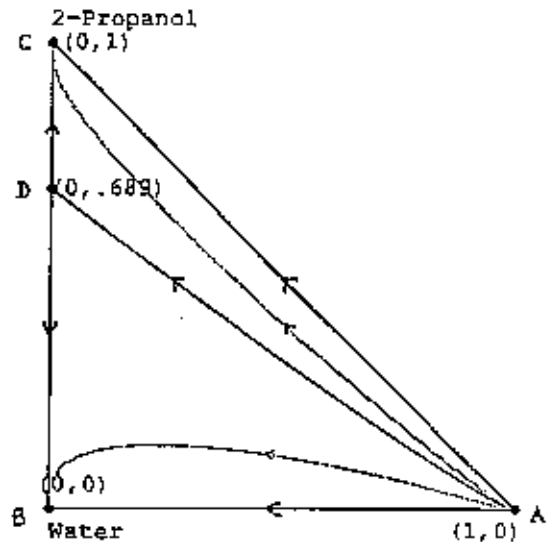

Fig. 4. Residue curve map for acetone–isopropanol–water.

distillation. Rather, the distillation boundaries play the important role of representing the impassable barriers. To identify the distillation boundaries, the construction of residue curve map is essential. These distillation boundaries can then be used to separate the distillation regions, and the triangular phase diagram can be divided accordingly. The variables are transformed in such a way that each region will form a separate triangular diagram. The thermodynamics of each region is represented by the constant relative volatility equations. The short-cut method and the modified short-cut method (for large holdup considerations) are then extended using these 'transformed variable' thermodynamic models.

3.2 Example of ternary azeotropic distillation

To illustrate the abstraction process and to demonstrate its advantages we present an example of a ternary system containing acetone–isopropanol–water. This system has one binary azeotrope and one separatrix† (see Fig. 4). As a first approximation this separatrix is approximated by a straight line. This results in two regions ABD and ADC. In Fig. 4, the triangle ABD is represented by the following transformed variables:

$$x_1' = x_1; \quad y_1' = y_1$$
$$x_2' = \frac{x_2}{x_2^{az}}; \quad y_2' = \frac{y_2}{y_2^{az}} \quad (7)$$
$$x_3' = 1 - x_1' - x_2'; \quad y_3' = 1 - y_1' - y_2'$$

The VLE data for the three components is generated by using the Wilson equation for liquid phase non-

†This residue curve map is generated using the automatic analysis of ordinary differential equations of the simple distillation process described in Section 2.
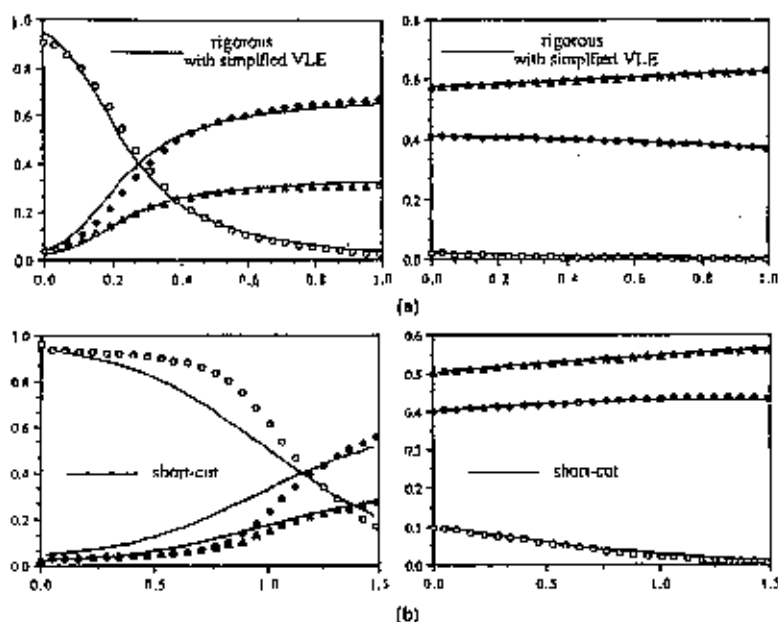
Fig. 5. Transient and still distillate composition profiles: (a) comparison of rigorous method with Wilson equation and rigorous method with simplified VLE equation: (b) Comparison of rigorous method with Wilson equation (with holdup effect) and short-cut method with simplified VLE equation. (○, Acetone; ●, isopropanol; ▲, water, x axes — composition: y axes — batch time (h).)

idealities. The vapor pressure equation constants and Wilson equation constants needed to correlate the vapor composition y_i to the liquid composition x_i are presented in **Tables 1** and **2** for this ternary system.† The constant relative volatility is obtained by averaging over the triangle ABD and using the transformed variables. In the tables, we have also provided the approximate equilibrium relationship in terms of the constant relative volatility model for the triangle ABD. The abstract model is computationally about 200 times faster to analyze. To check the thermodynamic approximation, the rigorous model for batch distillation is also extended to include the constant relative volatility transformed variable model. The results of both the extended short-cut method for the azeotropic system and the extended rigorous method (rigorous method with simplified VLE) are compared to the rigorous method with the real thermodynamic model. These comparisons are presented in Fig. 5. It can be seen that the agreement between the constant relative volatility transformed variable thermodynamic model and the actual Wilson equation model is very good (Fig. 5(a)). The extended short-cut method also compares very well with the rigorous model (Fig. 5(b)).

In short, this abstraction process involves:

- identification of distillation boundaries and azeotropic points;
- transforming the variables and generating simplified VLE model;

† In the Antoine equation the pressure is in atm and the temperature is in degrees Kelvin and the Wilson equation constants are given in cal/mol. Data obtained from Ref. 22.

- extending the short-cut methods using the transformed variables;
- validating the extended methods with rigorous models.

The encouraging preliminary results in the case of binary as well as ternary systems suggests that this approach will provide an efficient preliminary design tool.

4 CONCLUSIONS

This paper presents the first engineering application of a new approach to qualitative analysis of dynamic systems. This new approach in AI, which is based on the mathematical theory of nonlinear dynamics, represents a promising area for useful engineering applications. We have used this approach to analyze the thermodynamics underlying azeotropic batch distillation.

Residue curve maps for azeotropic distillation systems are automatically generated and used to derive computationally efficient and accurate models. These abstract models provide a powerful tool for preliminary analysis and optimization of ternary batch distillation.

Doherty and coworkers[12-15,20,23] have shown that a knowledge of residue curve maps provides insights into the problem of ternary azeotropic distillation. The automatic analysis framework presented in this paper will ease the process synthesis, design or optimization of ternary azeotropic continuous or batch distillation columns, as shown in the Fig. 6. This framework will
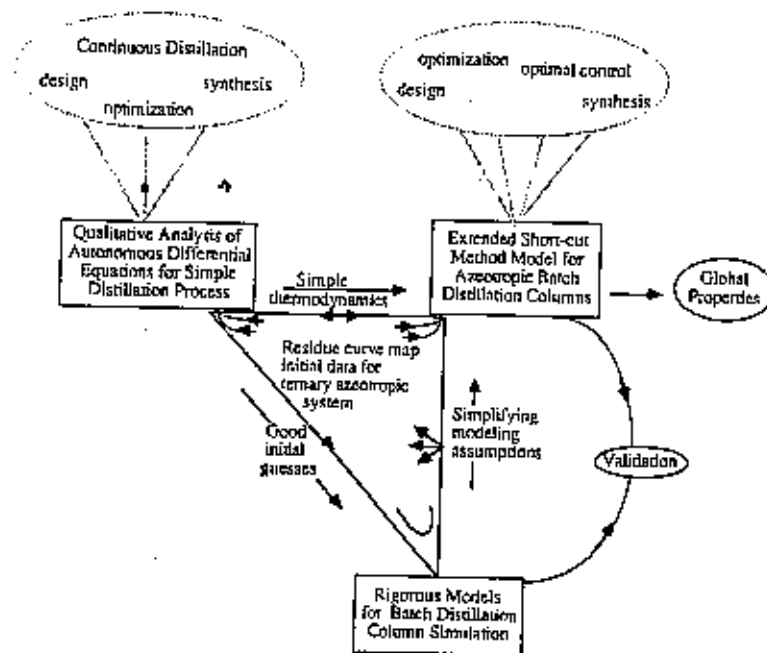
Fig. 6. Scope of the automatic analysis of residue curve map.

also allow one to explore the possible extension of this theory to azeotropic systems consisting of more than three components.

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