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IDENTIFYING MULTIPLE STEADY STATES
IN THE DESIGN OF
REACTIVE DISTILLATION PROCESSES

by

THOMAS KARL MILLS

A DISSERTATION

Presented to the Faculty of the Graduate School of the
MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

In Partial Fulfillment of the Requirements for the Degree

DOCTOR OF PHILOSOPHY

in

CHEMICAL ENGINEERING

2010

Approved by

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PUBLICATION DISSERTATION OPTION

This dissertation has been prepared in the style utilized by Computers and Chemical Engineering. Pages 18-32 and 33-47 will be submitted for publication in that journal. Appendices A, B, C, and D have been added for purposes normal to dissertation writing.

ABSTRACT

Global homotopy continuation is used to identify multiple steady states in ideal reactive flash and reactive distillation systems involving a reaction of the form $A+B \leftrightarrow C$ taking place in the liquid phase. The choice of specifications has an influence on the existence of multiple solutions for both the flash and the column. For the flash, specification of the heat input or withdrawal can give rise to multiplicities while specification of the split fraction does not. Specification of one internal energy balance variable and one external material balance variable does not produce multiplicities in the column; however, specification of two internal energy balance variables can produce multiplicities. This is seen to have implications for the selection of control variables for both the flash and the column.

The effects of the relative volatility between the light and heavy components, the forward rate constant, and the reaction equilibrium constant are studied. It is concluded that both the relative volatility spread and the equilibrium constant exhibit threshold values, below which only singular solutions are obtained. Above this threshold, multiplicities are to be found. The rate constant also affects the appearance of multiple solutions, but the multiplicities are found in regions bounded above and below by regions producing only singular solutions.

The cause of multiplicities in the idealized system studied is seen to be the interaction between consumption and creation of species by reaction and transfer of material between phases. The reaction rate appears to be the major contributor to this effect because it is able to reverse direction, assuming either positive or negative values.

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NOMENCLATURE

Symbol	Description
A_i, B_i	constants for component vapor pressure expression
D/F	vapor overhead to feed ratio
E_A	reaction activation energy, J/mol
F_j	molar bulk feed rate to stage j, mol/time
f_{ij}	component i feed rate to stage j, mol/time
h_j	liquid holdup on stage j, mol
H	stream enthalpy, J/mol
ΔH_r	heat of reaction, J/mol
ΔH_v	heat of vaporization, J/mol
K_{ij}	component i vapor-liquid distribution coefficient
$k_{f,0}$	reaction forward rate constant pre-exponential
k_f	reaction forward rate constant at temperature T
$K_{e,0}$	reaction equilibrium constant pre-exponential
K_e	reaction equilibrium constant at temperature T
L_j	molar liquid rate, mol/time
l_{ij}	component i liquid rate
p_i^*	component i vapor pressure, bar
P	pressure, bar
Q	heat added to the flash, J/time
R	gas constant
r_{ij}	component i production, moles per unit time
S_{lj}	liquid side-draw from stage j
S_{vj}	vapor side-draw from stage j
T_j	temperature, K
V_j	molar vapor rate, mol/time
v_{ij}	component i vapor rate, mol/time
x_{ij}	liquid mole fraction i
y_{ij}	component i vapor mole fraction

Greek letters

α_i	component i volatility relative to the heavy component
Φ	vapor-to-feed ratio
η_j	Murphree efficiency
λ_j	reaction extent, mol/time
ν_i	component i stoichiometric coefficient
Θ	unit of time

Subscripts

i	component index
j	stage index
l	liquid phase
v	vapor phase

1. INTRODUCTION

Most commercial chemical processes feature at least one chemical reaction, along with one or more separations, commonly distillation. Distillation has been an important part of chemical processing for a very long time; however, the rapid growth in computing capabilities in the last few decades has enabled a corresponding increase in the sophistication of design calculations. This in turn has allowed the use of more complex configurations to satisfy demands for increased performance and economy. In particular, reactive distillation, in which both chemical reaction and the separation of products from byproducts and residual reactants take place in the same equipment, has received increasing attention in recent years (Malone and Doherty 2000).

One of the issues needing to be addressed in reactive distillation is the potential existence of multiple steady states, which has been observed both in laboratory and plant practice as well as in design calculations (Mohl, Kienle, Gilles et al. 1999). Output multiplicities, in which a process may exhibit differing performance profiles for apparently identical operating parameters, are particularly troublesome from the standpoint of design and control. Standard design calculation techniques for such processes may converge to different solutions, depending on the starting estimates used for process variables, but are typically able to find only a single profile for any given set of inputs (Taylor and Krishna 2000). When constructed on the basis of these design methods, the reactive distillation unit may not exhibit the expected profile, depending on the initial conditions at startup or the states imposed by transients during the operation of the unit. Performance and/or safety issues can be the result.

1.1. CHEMICAL / THERMODYNAMIC MODEL

Of the many systems for which reactive distillation has been studied or commercialized, several involve reactions of the form $A+B\leftrightarrow C$ (Luyben and Yu 2008). A small sampling of these systems is presented in Table 1.1.

Table 1.1 - Some three-component reactive distillation systems

A	B	C
acetaldehyde	acetic anhydride	vinyl acetate
acetone	hydrogen	isopropanol
benzene	ethylene	ethylbenzene
isoamylene	water	tert-amyl alcohol
methanol	isobutene	methyl tert-butyl ether
methanol	isoamylene	tert-amyl methyl ether

For these systems, the mass-action rate law may be expressed as

$$r = k_{f,0} e^{(-E_A/RT)} (x_A x_B - x_C / K_{e,0} e^{(-\Delta H_r/RT)})$$

Systems with reactions of the form $2A \leftrightarrow C$ or $A \leftrightarrow B + C$ and with similarly structured rate laws have also been studied or commercialized.

For modeling the vapor-liquid equilibrium behavior of the system, it is desirable to represent the system with a minimal number of specified parameters. For this reason, it is convenient to assume that Raoult's law and the Clausius-Clapeyron equation are descriptive. From Raoult's law

$$y_i = x_i(p_i^*/P)$$

where y_i and x_i are the vapor and liquid mole fractions of component i , respectively, P is the total pressure, and p_i^* is the vapor pressure of component i . The Clausius-Clapeyron equation gives

$$\ln(p_i^*/p_i^{*0}) = (\Delta H_{Vi}/R)(1/T^0 - 1/T)$$

where ΔH_{Vi} is the component i heat of vaporization, R is the gas constant, p_i^{*0} is the component i vapor pressure at reference temperature T^0 , and T is the system temperature. This reduces to the more useful form

$$\ln p_i^* = [\ln p_i^{*0} + \Delta H_{Vi}/RT^0] - \Delta H_{Vi}/RT = A_i - B_i/T$$

where $A_i = \ln p_i^{*0} + \Delta H_{Vi}/RT^0$ and $B_i = \Delta H_{Vi}/R$. These values are easily determined by setting the reference temperature T^0 to the normal boiling point of the component.

Making the assumption that $\Delta H_{V1} = \Delta H_{V2} = \Delta H_{V3} = \dots = \Delta H_{Vn}$ gives

$$\ln \alpha_{ij} = \ln(p_i^*/p_j^*) = (\Delta H_V/R)(1/T_{bi} - 1/T_{bj})$$

which yields

$$T_{bj} = 1/[1/T_{bi} - R \ln \alpha_{ij} / \Delta H_V]$$

Assuming that both vapor and liquid heat capacities are negligible and that enthalpies are zero at the saturated liquid reference state further simplifies the computations.

1.2. COLUMN MODEL AND SOLUTION ALGORITHM

Perhaps the most straightforward approach to modeling distillation columns is the simultaneous correction scheme documented by Naphtali and Sandholm (1971), in which each stage is represented by a set of equations consisting of component material balances, stage energy balance, stream component summations, and component vapor-liquid distributions. For distillation with reactions occurring on the stages, Taylor and Krishna (2000) revised the equation set to incorporate the production or consumption of each component into the material balance functions:

$$\text{Material Balance: } (1+S_{l,j})/l_{i,j} + (1+S_{v,j})v_{i,j} - l_{i,j-1} - v_{i,j+1} - f_{i,j} - r_{i,j} = 0$$

$$\text{Equilibrium Functions: } (\eta_{i,j}K_{i,j})l_{i,j}/L_j - v_{i,j}/V_j + ((1-\eta_{i,j})v_{i,j+1})/V_{j+1} = 0$$

$$\text{Energy Balance: } (1+S_{l,j})H_{l,j} + (1+S_{v,j})H_{v,j} - H_{l,j-1} - H_{v,j+1} - H_{f,j} - Q_j = 0$$

Traditionally, the set of equations describing a column has been solved by a locally convergent approach such as Newton's method. One characteristic of these methods is that they are able to find only a single solution. Where the possibility of multiple solutions is an issue, a global solving algorithm is needed. Methods have been developed for finding multiple solutions to reactive distillation problems; however, these

methods have been predominantly graphical or algebraic (Bekiaris and Morari 1996; Bessling, Schembecker, and Simmrock 1997; Dalal and Malik 2003), and are thus limited in the precision they can offer and the number of species involved in the problems they can address. Homotopy continuation has been found useful because of its robustness and its ability to locate multiple solutions (Wayburn and Seader 1987; Kuno and Seader 1988; Lee and Dudukovic 1998; Sun and Seider 1995; Choi, Harney, and Book 1996). In the most common application of this approach, a vector of initial guesses x^0 is mapped to solution vectors x^* by a homotopy function $h(x,t) = tf(x) + (1-t)g(x^0)$ where $g(x^0)$ is a vector of “simple” functions, $f(x)$ is a vector of the functions to be solved, and t is the homotopy parameter. The solutions of $h(x,t) = 0$ form a homotopy path, which maps the solution of $g(x^0) = 0$ to a solution of $f(x^*) = 0$ as the value of t is varied from 0 to 1. Multiple solutions of $f(x)$ are found by global homotopy continuation, in which the homotopy path is exhaustively traced to locate solutions of $f(x) = 0$. Algorithms have been developed (Choi 1990; Choi, Harney, and Book 1996) to overcome the possibility of missing solutions by skipping from one segment of the homotopy path to another. However, Choi and Book (1991) demonstrated that all solutions may not be located on the single homotopy path emanating from the starting point. Therefore, these methods do not absolutely guarantee determination of all solutions.

Nonetheless, much of the published work in this area has dealt with specific systems of more-or-less nonideal components (Kovach III and Seider 1987; Singh et al. 2005). The problem of identifying parametric combinations or ranges of values for which multiplicities do or do not appear in generalized ideal systems has yet to receive adequate attention.

2. LITERATURE REVIEW

2.1. REACTIVE DISTILLATION APPLICATION

Harmsen (2007) discussed the increased application of reactive distillation, primarily in the last two decades. He cited more than 150 processes, in the range of 100-3000 ktonne/yr operating worldwide. He concluded that reactive distillation has become an established unit operation, and should be considered a front-runner in the field of process intensification.

Hoyme (2004) conducted parametric studies of several ideal reactive distillation systems. On the basis of these studies, he developed a set of heuristics for predicting the economic feasibility of a given reactive distillation process. He identified reaction equilibrium constant, volatility order, relative volatility, and reflux ratio as key parameters in economic feasibility estimation.

2.2. GRAPHICAL AND ALGEBRAIC MODELS

Barbosa and Doherty (1988a) presented a set of transformed composition variables to simplify design equations for single-feed reactive distillation columns. A method of calculating minimum reflux ratios for reactive columns was developed, based on these simplified equations.

Equations describing the distillation of homogeneous reactive mixtures were derived by Barbosa and Doherty (1988b), and were used to compute residue curve maps for ideal and non-ideal systems. It was shown that distillation boundaries could be either created or eliminated by allowing the mixture components to react.

Karimi and Inamdar (2002) noted that, although many systems are described by equations that cannot be reduced to a single equation, much of the work on bifurcation diagrams and identification of steady state multiplicities relies on either the assumption that such systems are reducible or some mathematical technique exists to reduce them. They presented a perturbation method for dealing with multiple equations without reduction, and used their method to study branching and stability of steady states near a singularity.

Monnigmann and Marquardt (2003) presented an approach to the optimization based design of processes in which uncertainty in some process parameters exists. Their approach operates by placing a lower bound on the distance of the nominal operating point from stability and feasibility boundaries in the space defined by the uncertain parameters. They discuss their method in the context of optimizing a process known to have a nontrivial stability boundary caused by steady state multiplicity and sustained oscillation.

Baur, Taylor, and Krishna (2003) compared the use of heterogeneous and pseudo-homogeneous reaction kinetic models in preparing a bifurcation analysis of a reactive distillation for the synthesis of t-amyl methyl ether. They concluded that the two models show similar performance, both indicating the possibility of multiple steady states. They attributed difference in performance to imprecision in the knowledge of liquid holdup and other hydrodynamic factors.

Barbosa and Doherty (1987a) derived expressions for the partial derivatives of intensive properties that characterize equilibrium states in two-phase systems with one chemical reaction. They found necessary and sufficient conditions for the occurrence of azeotropic transformation, and presented conditions under which reactive azeotropes are not equivalent to stationary points in the equilibrium surfaces.

Barbosa and Doherty (1987b) presented a transformed set of composition variables for representing phase diagrams where chemical reaction is present. They make the claim that this set of variables is superior to mole fractions in several respects, and give examples of phase diagrams to illustrate the claimed advantages.

Barbosa and Doherty (1988c) presented phase diagrams for simultaneous chemical reaction and phase equilibrium for both ideal and non-ideal systems. They showed that even for ideal mixtures, reactive azeotropes can occur. In addition, they concluded that for such reactive azeotropes to exist, volatilities of the reactants must be either all higher or all lower than the volatilities of the products.

Bekiaris et al. (1993) studied multiple steady states in homogeneous azeotropic distillation. Under the conditions of infinite reflux and an infinite number of trays (∞/∞ analysis), they constructed bifurcation diagrams with distillate flow as the

bifurcation parameter, and derived necessary conditions for the existence of multiple steady states.

Fien and Liu (1994) presented a review of published work on the use of ternary composition diagrams and residue curve maps for the analysis and design of azeotropic separation processes. Their analysis sought to clarify some contradictions in prior work, and highlighted the usefulness of this approach for preliminary system design.

Ung and Doherty (1995a) showed that the Gibbs free energy for reacting mixtures can be expressed as an unconstrained function of a set of transformed composition variables. From this, they developed a simplified representation of equilibrium and stability conditions in reactive systems that is similar to the non-reacting case.

Ung and Doherty (1995b) showed that in a transformed composition space, conditions for azeotropy in reactive mixtures take the same functional form as in non-reactive mixtures. However, reactive azeotropes generally do not correspond to points of equal mole (or mass) fraction in the coexisting phases.

Ung and Doherty (1995c) introduced a set of composition variables for evaluating phase equilibria in multicomponent, multireaction systems. They showed that their transformed variables simplified analysis by reducing the dimensionality of the problem. They found that reactive azeotropes occur at points of equal transformed composition in coexisting phases, but not at points of equal mole fraction.

Ung and Doherty (1995d) derived the differential equations describing simple distillation of mixtures with multiple chemical reactions. They found that the results are conveniently expressed in terms of composition coordinates transformed to reduce the dimensionality of the problem. From this, they prepared residue curve maps which provide visualization of the combined equilibria, and show the presence of reactive azeotropes as well as non-reactive azeotropes which survive the reactions.

Bekiaris, Meski, and Morari (1996) used the assumptions of infinite reflux ratio and infinite number of trays to construct bifurcation diagrams for ternary azeotropic systems. With distillate flow rate as the bifurcation parameter, they demonstrated that these diagrams could be used to predict the occurrence of multiple steady states. They also showed relevant implications for cases with finite reflux and a finite number of trays.

Bekiaris and Morari (1996) extended a previously presented method of analysis to quaternary mixtures, and elaborated on the implications for column design and simulation. They discussed the effect of thermodynamic phase equilibrium on the existence of multiplicities, and identified classes of mixtures for which multiplicities are inherent and robust. Finally, they discussed issues arising from their analysis that are relevant to the use of commercial simulators for computing the composition profiles of azeotropic distillation columns.

Bessling et al. (1997) studied the concept of residue curve maps based on transformed composition variables. From this study, they developed conditions under which a combination of reactive and non-reactive sections is needed within a given column.

Gehrke and Marquardt (1997) demonstrated the application of singularity theory to the analysis of a one-stage reactive distillation, in order to study the causes of multiple steady states. They identified causes which are common to non-reactive processes, as well as those that are connected to the interaction between chemical reaction and phase equilibrium.

Guttinger and Morari (1997) reviewed and demonstrated the ∞/∞ analysis of Bekiaris et al. (1993) for multicomponent azeotropic mixtures. They then extended the analysis by combining it with a singularity analysis to treat additional azeotropic systems, and by combining it with reactive residue curves to treat problems involving reaction. In addition, they related known multiplicities for the MTBE process to causative physical phenomena.

Karpilovskiy, Pisarenko, and Serafimov (1997) used distillation line diagrams and reaction stoichiometry to derive a criterion for predicting multiple steady states in a single-product reactive distillation. Their criterion successfully predicted multiplicity for butyl acetate synthesis, which prediction was confirmed by further analysis.

Song et al. (1998) studied the influence of heterogeneous catalysis on the kinetically controlled esterification of acetic acid with methanol in a reactive distillation system. They noted the role of pressure in regulating liquid boiling point and thus reaction temperature. They experimentally measured residue curves, and compared the results with predictions from a kinetic model.

Guttinger and Morari (1999a) present a method for predicting the existence of multiple steady states in columns consisting solely of reactive stages, for the limiting case of infinite column length and infinite internal flows. They applied geometric conditions to identify the region of feed compositions leading to multiplicities.

Guttinger and Morari (1999b) developed a graphical method for predicting multiple steady states in columns containing both reactive and nonreactive sections (“hybrid columns”). This extended their development of a method for analyzing columns having only reactive stages (“nonhybrid columns”). They showed their method to be capable of predicting the existence of, and feed regions giving rise to, multiple steady states.

Reder, Gehrke, and Marquardt (1999) applied the geometric ∞/∞ analysis to esterification reactions occurring in distillation columns, and transferred their findings to rigorous reactive column models, weakening the assumptions of infinite reflux and column length. They showed that where the ∞/∞ analysis can predict an infinite number of steady states, relaxation of the assumptions reduces the prediction to a finite number, and that at relatively small values of reaction rate, column length, or reflux rate, the multiplicities reduce to unique solutions.

Bekiaris et al. (2000) studied the observation of output multiplicities in numerical simulation of heterogeneous azeotropic distillation columns. They concluded that the accuracy of the thermodynamic description is a key factor in determining whether multiplicities can be observed. In addition, they studied reported multiplicities, and derived relationships to identify causative physical phenomena.

Jalali-Farahani and Seader (2000) investigated stability in nonideal chemical systems where reactions occur in more than one phase. They used a homotopy continuation method to identify solutions, and stability criteria were applied to determine the number of stable phases at equilibrium.

Melles et al. (2000) studied the effect of tray holdup in continuous kinetically controlled reactive distillation columns. They concluded that using tray holdup as a parameter aided the design and optimization of such columns.

Kenig et al. (2001) studied the synthesis of ethyl acetate by homogeneously catalyzed reactive distillation. They identified feasible configurations through the use of

residue curve map techniques, then used a rate-based simulator to predict concentrations and other relevant process variables. They found substantial agreement between experimental data and their predicted temperature and composition profiles.

Rodriguez, Zheng, and Malone (2001) studied the steady state behavior of an isobaric, adiabatic reactive flash for a two component system. They noted that vapor-liquid equilibrium can create or remove steady state multiplicities, relative to a single phase reactor. They related the presence of multiple steady states to a dimensionless parameter formed from the heats of reaction and vaporization along with the compositions in the system.

Rodriguez (2002) noted that, while combining a reaction step with a separation step can be economically efficient, it also reduces the degrees of freedom available for controlling the system. He applied bifurcation and singularity theory to derive algebraic expressions that describe the possibility of steady state multiplicities. His work considered both the reactive (multistage) column and the two-phase reactor (reactive flash).

Rodriguez, Zheng, and Malone (2002) studied steady state solutions for an isobaric, adiabatic, reactive flash, and showed that the existence of the second phase affects the presence or absence of steady state multiplicities. They related the existence of multiple steady states to a dimensionless quantity derived from the heats of reaction and vaporization along with the vapor-liquid equilibrium behavior.

Huss et al. (2003) illustrated an approach to the design of reactive distillation columns, using methyl acetate production as an example. They demonstrated that in the limit of both phase and reaction equilibrium, there are both minimum and maximum reflux limits, and that multiple steady states persist throughout the range of feasible reflux ratios. For finite reaction rates, they showed that desired compositions are achievable over a wide range of reaction rates, and that multiplicities occur at high reflux ratios beyond the range of normal operation.

Rodriguez, Zheng, and Malone (2004) noted that steady state multiplicity is caused by interaction between reaction and separation in systems with sufficiently large activation energy and boiling temperature versus composition gradient. They established necessary conditions for multiplicity in an isobaric flash with constant split fraction, and

determined that multiplicity is possible in endothermic systems as well as those with a small heat of reaction.

2.3. SIMULATIONS OTHER THAN WITH HOMOTOPY CONTINUATION

Naphtali and Sandholm (1971) presented an approach to separation calculations in which component material balances, enthalpy balances, and equilibrium relationships were arranged to be solved simultaneously. Their construct formed the basis which others subsequently extended to include the effect of chemical reaction.

Taylor and Krishna (2000) presented a comprehensive review of models for reactive distillation, noting that multiple steady states had been predicted by theoretical studies as early as the 1970's. They cited several models which had been used to make these predictions, primarily through altering the parameters of standard simulation models or use of singularity theory or bifurcation analysis. Their review covered only real-component systems, and noted several experimental studies verifying these predictions.

Seferlis and Grievink (2001) presented a method for screening control configurations to identify manipulated variables that perform poorly in the presence of multiple disturbances and parameter variations. In particular, they developed a comparison between reactive distillation configurations and conventional reactor-separator schemes.

Tang et al. (2005) studied the esterification of acetic acid using five different low molecular weight alcohols, and identified three different types of flowsheets. For each flowsheet type, they presented a design procedure and explored economic potential.

Grosser, Doherty, and Malone (1987) proposed a model for reactive distillation in a system where extreme purity is required in the overhead vapor. They concluded that economical operation of such systems is enhanced by the use of a reactive entrainer. They also presented guidelines for the use of reactive entrainers in the separation of closely boiling mixtures.

Hua, Brennecke, and Stadtherr (1996) demonstrated an initialization independent interval analysis technique for reliably solving phase stability problems. They concluded

that their technique, properly implemented, guarantees that all correct solutions have been found.

Reneaume, Meyer, Letourneau, and Joulia (1996) described an approach to phase equilibrium problems in which they found Gibbs energy minima by resolving a mixed integer nonlinear programming problem into nonlinear programming subproblems. Global optima for each subproblem were then found by homotopy continuation.

Sneesby, Tade, and Smith (1997, 1998) discussed three types of steady state multiplicity, and the implications of each for column control. They concluded that input multiplicity, or the existence of the same output for several different sets of inputs, placed restrictions on the selection of controlled variables. Output and pseudo-multiplicities were thought to have less significant impacts, but were seen to influence the choice of control structure and operating region.

Okasinski and Doherty (1998) presented a design methodology for kinetically controlled reactive distillation columns featuring a single liquid phase reaction and nonideal vapor-liquid equilibrium. They considered their method to be useful for developing a set of feasible designs over a range of design specifications, and provided several examples of its application, including one in which the use of reactive distillation removed a distillation boundary normally existing in the system being separated.

Mohl et al. (1999) studied the dynamic behavior of reactive distillation columns for the production of methyl t-butyl ether and t-amyl methyl ether, with an emphasis on steady state multiplicity as identified by bifurcation analysis of pilot plant columns. Sources and physical causes of multiple steady states were discussed, as were some of their implications.

Peng et al. (2002) compared equilibrium and rate-based models for packed reactive distillation columns to produce tert-amyl methyl ether and methyl acetate. Both models gave good agreement with experimental data, and predicted the existence of an optimum pressure and reflux ratio. The rate-based model was found to be much more complicated, and more difficult to converge, than the equilibrium model.

Dalal and Malik (2003) applied an optimization algorithm for systems of nonlinear equations to study methanol-propanol and ethanol-water-benzene columns.

They were able to find multiple solutions in both cases, but concluded that a more robust solver would represent an improvement.

Waschler, Pushpavanam, and Kienle (2003) analyzed the behavior of two-phase reactors under boiling conditions. Focusing on a simple reaction of the form $A \rightarrow B$, they identified three necessary conditions for the existence of steady state multiplicities: the reactant A must be the light component, the boiling point difference between A and B has to be sufficiently large, and the order of the reaction must be less than a measure of the self-inhibition of the reaction driven by phase equilibrium.

Yermakova and Anikeev (2005) constructed a model of a two-phase CSTR, or reactive flash, for the liquid phase hydrogenation of benzene, under the assumption of phase equilibrium. They demonstrated that under certain conditions, there exists the possibility of a multiplicity of solutions, which were attributed to nonlinearity of the kinetic reaction expressions and nonideality of the reacting mixture.

Yang et al. (2006) used the ASPEN PLUS simulation package to study reactive distillation processes for ethylene glycol and ethyl t-butyl ether, with liquid holdup volume and boilup ratio as parameters. Through the use of different initial guesses, they were able to demonstrate steady state multiplicities for both processes.

Qi and Sundmacher (2006) investigated reactive distillation for the production of high purity isobutene and diisobutene by dehydration of t-butyl alcohol. They noted that mild processing conditions, high per-pass conversion, and high selectivity were advantages offered by reactive distillation. Their analysis included examination of the influence of important process parameters.

Calvar, Gonzalez, and Dominguez (2007) studied the kinetics of the esterification of acetic acid with ethanol, using both heterogeneous and homogeneous catalyst systems. Their study was carried out using a packed bed reactive distillation column, and included an analysis of the effects of feed composition and reflux ratio.

Rovaglio and Doherty (1990) developed a dynamic model for heterogeneous azeotropic columns which was able to detect and account for multiple liquid phases on trays at each instant of time. They demonstrated the model by simulating the distillation of mixtures of ethanol, water, and benzene. They showed their results to be in substantial

agreement with prior work, and that the system under study can be expected to exhibit multiple steady states, complex dynamic behavior, and parametric sensitivity.

Jacobsen and Skogestad (1991) discussed two causes of multiple steady states in ideal two-product distillation. For systems specified in mass or volume units, they concluded that the transformation to molar units can become singular, resulting in multiple solutions. For units specified in molar units with an energy balance included in the model, their conclusion was that multiple solutions were caused by interaction between flows and compositions.

Jacobs and Krishna (1993) used a steady state equilibrium stage model to simulate a reactive distillation column for the production of methyl t-butyl ether. For identical configuration and feed specifications, they obtained two distinct results, corresponding to high and low conversion of isobutene. They showed that these two results were associated with residue curves having their starting points in distinctly different composition regions.

Baur et al. (2000) used two case studies to compare the equilibrium stage model with a nonequilibrium model which uses mass transfer rates across the vapor-liquid interface for modeling reactive distillation columns. It was shown that, while multiple steady states are exhibited in both approaches, the “window” for their occurrence is significantly smaller in the nonequilibrium case. It was also observed that some of the multiplicities found by the equilibrium approach could not be achieved in practice due to physical constraints.

Kumar et al. (2001) simulated a reactive distillation column for producing MTBE. They observed two steady states, one having high conversion at relatively low temperature and the other having lower conversion at relatively high temperature. They also studied the effects of methanol feed tray location, reflux ratio, catalyst loading, and other parameters on overall conversion and product purity.

Chen et al. (2002) developed a model for kinetic effects in reactive distillation, using a Damkohler number as the key parameter. For methyl t-butyl ether synthesis and t-amyl methyl ether synthesis, they traced solution branches as functions of the Damkohler number, reboil ratio, or reflux ratio, and found agreement with prior work at the reaction equilibrium limit. For the t-amyl methyl ether system, they found that multiplicities were

present in the kinetic regime, but disappeared above a critical value of the Damkohler number.

Lucia and Feng (2003) investigated a geometric terrain method for finding all solutions and singular points for chemical process simulation problems. They concluded that their method provided reliable and efficient performance, which was seen to be superior to differential arc homotopy continuation for some problems which exhibited parametric disconnectedness.

Svandova et al. (2009) compared the performance of equilibrium and non-equilibrium models for identifying hazardous situations or operability problems in reactive distillation columns. In particular, they studied the ability of the two models for predicting multiple steady states that can be the cause of operability issues. They observed that, while both models predict multiplicities, the non-equilibrium model is more realistic but requires more parameters as input and is thus more susceptible to errors in the input information.

2.4. HOMOTOPY METHOD DEVELOPMENT

Taylor et al. (2003) presented a comparison of rate-based and equilibrium models for nonreactive distillation. They concluded that, while much more complex than the equilibrium models, rate-based models become more feasible as available computing power increases, and that for definitive computations on existing columns, they should be used in preference to equilibrium models.

Kovach and Seider (1987) presented an algorithm for simulating three-phase azeotropic distillation towers and their associated phase separators. Their algorithm utilized a homotopy continuation method, with extensions to avoid limit points when multiple solutions were encountered or when two liquid phases exist on the trays. Extensions were also added to perform parametric studies by tracking solution paths. They demonstrated the ability of the algorithm to detect regions where multiple solutions exist, some of which had not been previously identified.

Vadapalli and Seader (2001) composed a method for incorporating an addition to standard process simulators which are normally only able to find single solutions, so that

these simulators are able to trace a solution path with respect to some input parameter, thus finding multiple solutions.

Wayburn and Seader (1987) applied homotopy continuation methods to the solution of difficult flowsheeting and design problems involving sets of simultaneous nonlinear equations. They described three circumstances under which homotopy continuation can fail, and discussed a potential remedy for two of the three failure modes.

Kuno and Seader (1988) investigated the application of global fixed-point homotopy continuation to the solution of systems of nonlinear equations. They concluded that the fixed-point approach offered the possibility of finding all real roots of a system, provided that the single starting point was selected according to a criterion that minimized the number of roots at an infinite value of the homotopy parameter. This characteristic would be advantageous for systems where it is not possible to pre-determine the number of real roots.

Choi and Book (1991) demonstrated that, for both the Newton and fixed-point global homotopies, there are problems that have solutions which are not reachable in either the real or complex domain from a single starting point. Therefore, these methods cannot offer an absolute guarantee that all roots of a problem will be located by starting from a single point.

Choi (1990) developed an algorithm designed to avoid jumping from one segment of a homotopy path to another by controlling the size of each computational step. This approach mitigated the tendency of earlier algorithms to miss solutions by failing to explore all parts of the path.

Sun and Seider (1995) presented an algorithm for the determination of phase equilibria at the global minimum of Gibbs energy. They used the Newton homotopy continuation method to locate multiple stationary points of a target-plane-distance function, and tested their method against several non-ideal mixtures. They concluded that, while slower than another comparable method, theirs provided similar reliability and enabled a simpler initialization strategy.

Choi, Harney, and Book (1996) proposed a path tracking algorithm designed to maintain tracking efficiency while improving the ability of homotopy continuation methods to avoid jumping from one path segment to another, thus enhancing detection of

all roots of a function. The distinguishing feature of the algorithm was the control of step size by restricting the amount of change in the determinant of the augmented Jacobian.

2.5. HOMOTOPY METHOD APPLICATION

Singh et al. (2005b) presented an approach for synthesizing control structures for reactive distillation columns, based on steady state analysis. Their idea was to identify pairings of input and output variables that are sensitive and avoid steady state multiplicities. They highlighted the impact of steady state multiplicities, and illustrated their approach with an example methyl t-butyl ether column.

Lin, Seader, and Wayburn (1987) demonstrated the use of a homotopy continuation method for finding multiple solutions to complex separation column configurations. They noted that for some approaches finding all solutions requires that the simulation be started from multiple initial points, and proposed an algorithm designed to overcome this difficulty.

Lee and Dudukovic (1998) presented a comparison between equilibrium and non-equilibrium models for ethyl acetate production by reactive distillation. They applied both Newton-Raphson and homotopy continuation methods to solution of the model equations, and concluded that homotopy continuation provided superior performance in terms of guaranteeing a solution.

PAPERS

I. MULTIPLE STEADY STATES IN THREE-COMPONENT REACTIVE DISTILLATION: EFFECT OF OPERATING PARAMETERS

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ABSTRACT

Global homotopy continuation is used to identify multiple steady states in reactive flash and reactive distillation systems involving a reaction of the form $A+B \leftrightarrow C$ taking place in the liquid phase. It is concluded that for both the flash and the column, the choice of specifications has an influence on the existence of multiple solutions. Multiple steady states have been identified when there are two energy constraints, but not otherwise. This has implications for the selection of control and operating strategies to avoid multiple steady states.

1. INTRODUCTION

Distillation has been an important part of chemical processing for a very long time; however, the rapid growth in computing capabilities in the last few decades has enabled a corresponding increase in the sophistication of design calculations. This in turn has allowed the use of more complex configurations to satisfy demands for increased performance and economy. In particular, reactive distillation, in which both chemical reaction and the separation of products from byproducts and residual reactants take place in the same equipment, has received increasing attention in recent years (Malone and Doherty 2000; Luyben and Yu 2008).

The existence of multiple steady states in distillation processes has been observed both in laboratory and plant practice, and in design calculations (Mohl et al. 1999).

Output multiplicities, in which a process may exhibit differing performance profiles for apparently identical operating parameters, are particularly troublesome from the standpoint of design and control, and have the potential for causing safety hazards. In operation, a column may approach different performance profiles, depending on the states imposed by process transients. Standard design calculation techniques for such processes may converge to different solutions, depending on the starting estimates used for process variables, but are typically able to find only a single profile for any given set of inputs (Taylor and Krishna 2000).

Methods have been developed for finding multiple solutions to reactive distillation problems. However, these methods have been predominantly graphical or algebraic, and are thus limited in the precision they can offer and the number of species involved in the problems they can address (Bekiaris and Morari 1996; Bessling, Schembecker, and Simmrock 1997; Dalal and Malik 2003). While global homotopy continuation has been found useful because of its robustness and its ability to locate multiple solutions, much of the published work in this area has dealt with specific systems of more-or-less nonideal components (Kovach III and Seider 1987; Singh et al. 2005). The problem of identifying parametric combinations or ranges of values for which multiplicities do or do not appear in generalized ideal systems has yet to receive adequate attention.

Of the many systems for which reactive distillation has been studied or commercialized, several involve reactions of the form $A+B \leftrightarrow C$ (Luyben and Yu 2008). A small sampling of these systems is presented in Table 1.

Table 1 – Commercial reactive distillation systems for $A+B \leftrightarrow C$

A	B	C
acetaldehyde	acetic anhydride	vinyl acetate
acetone	hydrogen	isopropanol
benzene	ethylene	ethylbenzene
isoamylene	water	tert-amyl alcohol
methanol	isobutene	methyl tert-butyl ether
methanol	isoamylene	tert-amyl methyl ether

For these systems, the mass-action rate law may be expressed as

$$r = k_{f,0} e^{(-E_A/RT)} (x_A x_B - x_C / K_{e,0} e^{(-\Delta H_r/RT)})$$

Systems with reactions of the form $2A \leftrightarrow C$ or $A \leftrightarrow B + C$, and having similarly structured rate laws, have also been commercialized.

2. THE REACTIVE FLASH

Figure 1 is a diagram of a reactive flash, two-phase CSTR, or single stage reactive distillation. F represents the molar flow rate of the saturated liquid feed, and is the sum of the component molar feed rates f_i . Additional energy entering the stage is represented by Q , while V is the vapor and L the liquid exiting the stage (the summations of the v_i and l_i , respectively). A single reaction of the form $A + B \leftrightarrow C$ takes place in the liquid phase.

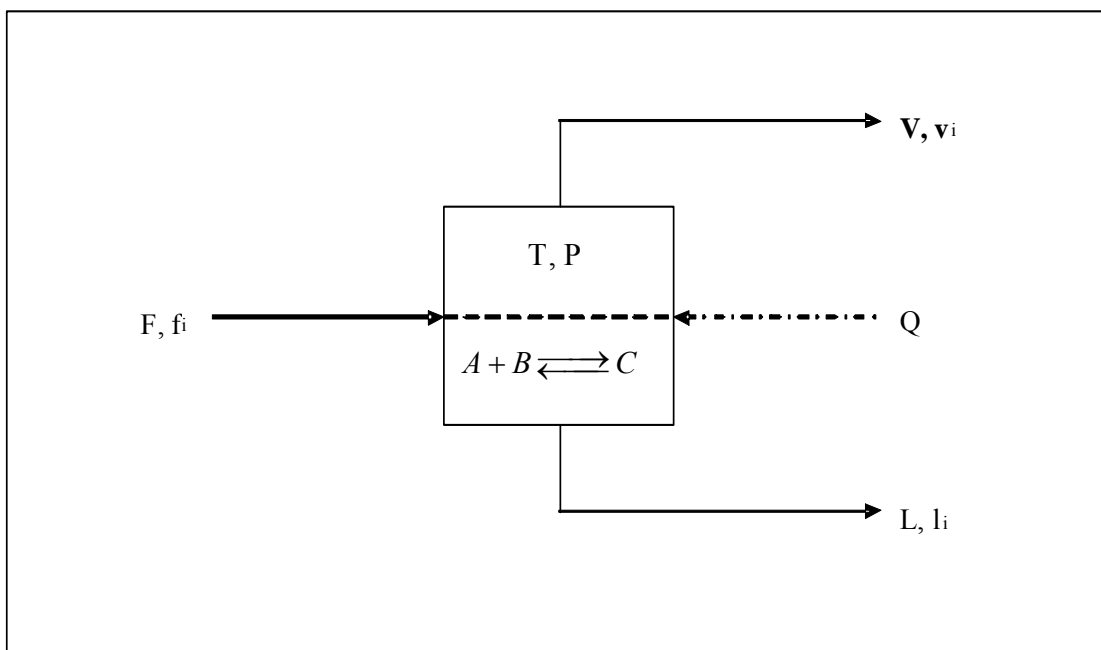


Figure 1 - Reactive flash

The stage operates at vapor-liquid equilibrium. It is assumed that Raoult's law applies for each species and that the Clausius-Clapeyron equation is valid for vapor pressures, so that $y_i = (p_i^*/P)x_i$ and $p_i^* = \exp(A_i - B_i/T)$, where $B_i = \Delta H_{v,i}/R$ for all i . It is

further assumed that all component heats of vaporization are equal and that sensible heat effects are negligible.

In order to model the performance of this system, it is necessary to obtain simultaneous solutions to the mass and energy balances and the equilibrium constraints (Taylor and Krishna 2000):

$$l_A + v_A - f_A - h\lambda v_A = 0$$

$$l_B + v_B - f_B - h\lambda v_B = 0$$

$$l_C + v_C - f_C - h\lambda v_C = 0$$

$$H_V + H_L - H_F - Q = 0$$

$$K_A l_A / L - v_A / V = 0$$

$$K_B l_B / L - v_B / V = 0$$

$$K_C l_C / L - v_C / V = 0$$

For finding multiple solutions, the reaction extent must be an element of the solution vector, rather than being fixed by other elements of the solution:

$$hk_f [(l'_A / L')(l'_B / L') - (1/K_e)(l'_C / L')] - \lambda = 0$$

where $l'_i = f_i - v_i$ and $L' = F - V$. Solutions are obtained using the Newton homotopy and a suitable path tracking algorithm to apply global homotopy continuation (Choi 1990; Choi, Harney, and Book 1996).

Parameters for the reactive flash base case are shown in Tables 2 and 3. The normal boiling points of the components are 294 K, 355 K, and 362 K for A, B, and C, respectively, and the heat of vaporization for all three components is 29,070 J/mol. Stream enthalpies are taken to be the composition weighted sum of component enthalpies. The reference state for the enthalpy is pure saturated liquid, and all sensible energy effects are neglected. The heat of reaction is -41,870 J/mol and the activation energy 125,600 J/mol. The reaction equilibrium constant is 20, and the forward rate

constant is 0.008 per unit of time, both at a reference temperature of 366 K. The feed is a bubble-point liquid consisting of 12.63 moles of A and 12.82 moles of B per unit time.

Figure 2 shows the fractional conversion of component A versus Damkohler number for a range of specified vapor-to-feed ratios. The Damkohler number is defined here as the product of holdup and the forward rate constant at the reference temperature, divided by the feed rate $Da = hk_{f,ref}/F$. It is seen that conversion increases with increasing Damkohler number (increasing holdup), but that the slope of the trace does not become negative, so multiplicities are not exhibited.

Table 2 - Operating parameters for base case flash

ΔH_v (J/mol)	29070 .	P (bar)	8
ΔH_r (J/mol)	-41870 .		
E_a (J/mol)	125600 .		
$K_{eq,ref}$	20 .		
$k_{f,ref}$ (Θ^{-1})	0.008		
T_{ref} (K)	366		

Table 3 - Material parameters for base flash case

Component	A	B (K)	T_{NBP} (K)	$T_{B,8bar}$ (K)	$\alpha_{i,C}$	Feed (mol/ Θ)
A	13.16	3862	294	348	12 .	12.63
B	10.90	3862	355	437	1.25	12.82
C	10.67	3862	362	450		

Figure 3 shows the fractional conversion of component A versus Damkohler number for a range of specified dimensionless heat inputs (Q'), defined here as the heat input divided by the feed flow times the heat of vaporization $Q' = Q/(F\Delta H_v)$. Vapor to feed ratios for the computations shown in this chart are in the range of 0.01 to 0.35, which are comparable to the range shown in Figure 2. The trace for each value of Q' exhibits an inflection around a region in which the conversion increases rapidly with Damkohler number. For dimensionless heat inputs between about -0.169 (heat withdrawal) and 0.068 (heat input), the flash exhibits multiple steady states. Dimensionless heat inputs greater than 0.068 resulted in singular solutions, and for

dimensionless heat withdrawals greater than 0.169 solutions were not found because the heat withdrawal exceeded the heat generated by the reaction, preventing the formation of a vapor phase. The apparent flatness in the upper part of the trace for $Q' = -0.169$ is caused by insufficient sampling frequency in that region.

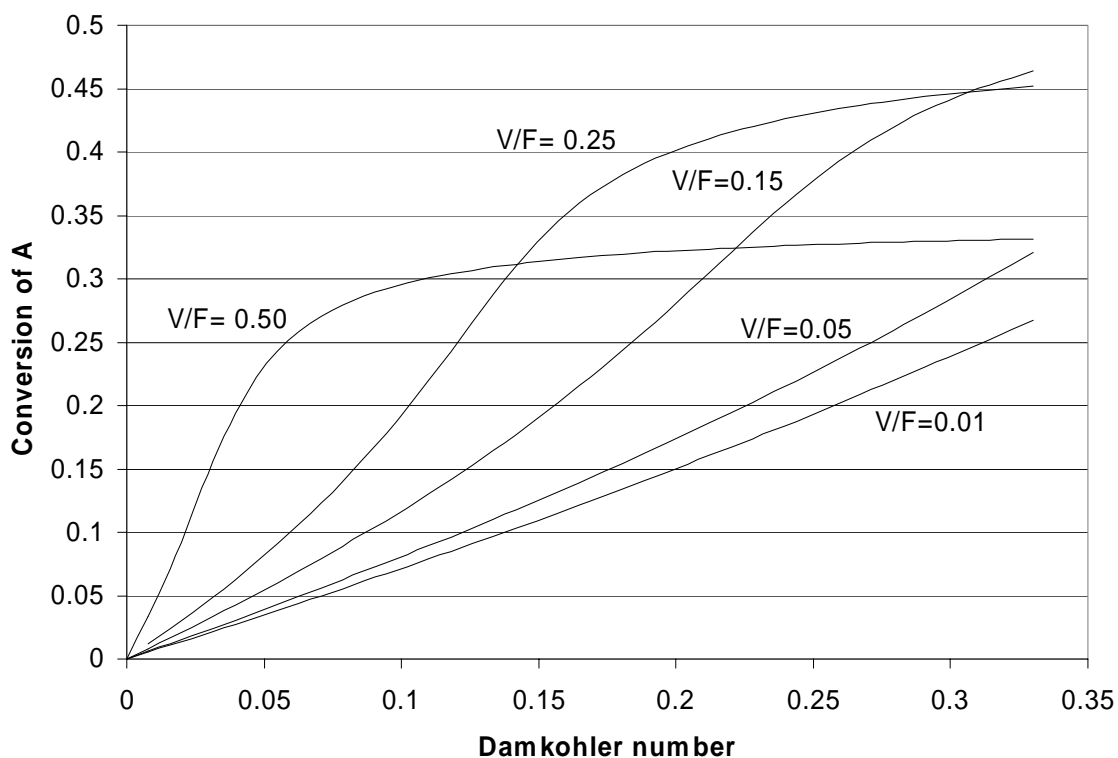


Figure 2 – Reactive flash with vapor-to-feed ratio specified

3. THE REACTIVE COLUMN

Figure 4 represents a multistage column in which a reaction $A+B \leftrightarrow C$ takes place in the liquid holdup on designated trays. Since the single product C is the heavy component and is ideally the only species leaving the column, non-reacting stages are placed at the column bottom to return components A and B to the reactive section at the top. In the model, nonreactive stages are modeled by specifying zero holdup for those stages. This is analogous to including stages without catalyst in heterogeneously catalyzed systems and would not be possible in homogeneously catalyzed systems. The heavier of the two reactants is fed at the top of the reactive section, while the lighter component is fed to the

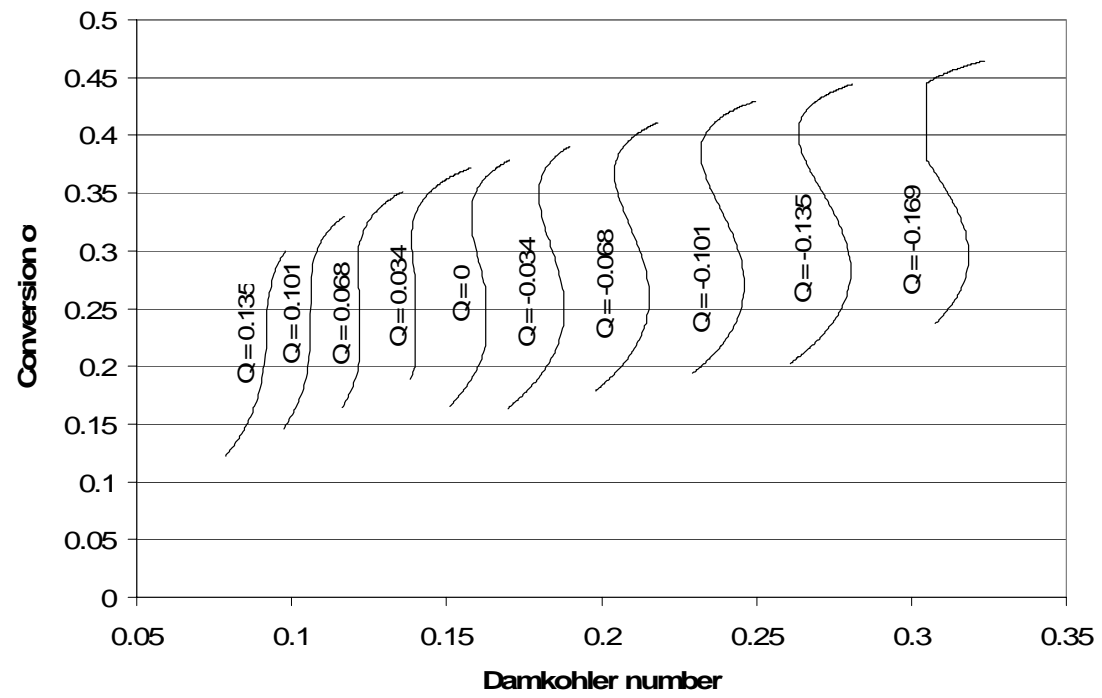


Figure 3 – Reactive flash with heat duty specified

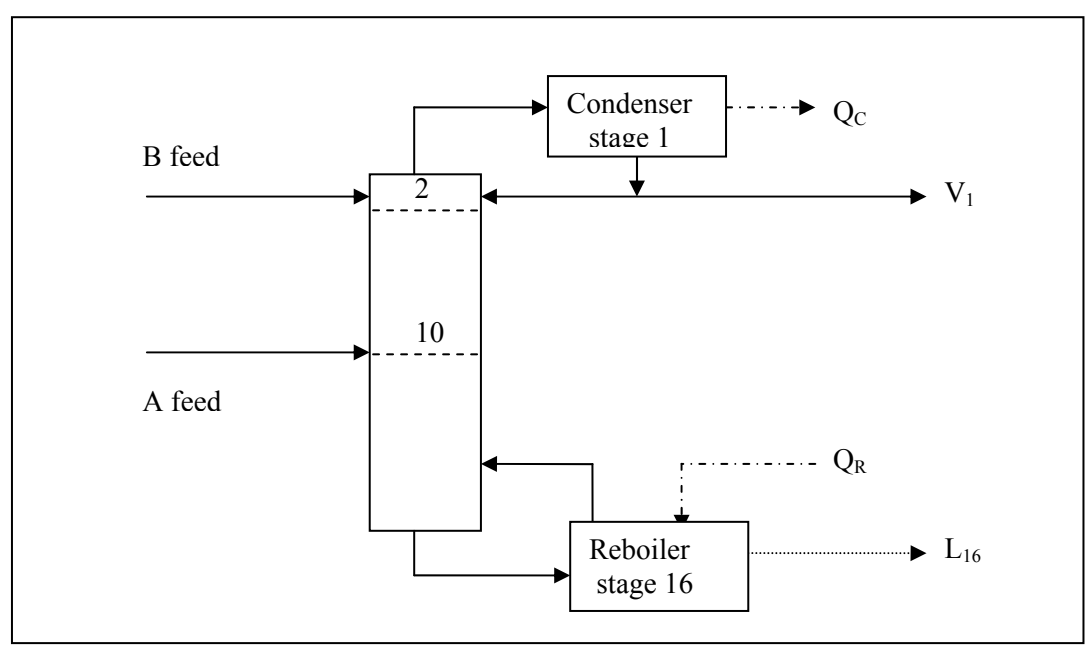


Figure 4 - Reactive column

lowest reactive stage. Modeling the column's performance is accomplished in the same way as for the flash, except that the equation set to be solved consists of the eight

material balance, energy balance, equilibrium, and reaction extent equations for each stage, for a total of $8n$ equations:

$$l_{A,j} + v_{A,j} - f_{A,j} - l_{A,j-1} - v_{A,j+1} - h\lambda_j v_A = 0$$

$$l_{B,j} + v_{B,j} - f_{B,j} - l_{B,j-1} - v_{B,j+1} - h\lambda_j v_B = 0$$

$$l_{C,j} + v_{C,j} - f_{C,j} - l_{C,j-1} - v_{C,j+1} - h\lambda_j v_C = 0$$

$$H_{V,j} + H_{L,j} - H_{F,j} - H_{L,j-1} - H_{V,j+1} - Q_j = 0$$

$$K_{A,j} l_{A,j} / L_j - v_{A,j} / V_j = 0$$

$$K_{B,j} l_{B,j} / L_j - v_{B,j} / V_j = 0$$

$$K_{C,j} l_{C,j} / L_j - v_{C,j} / V_j = 0$$

$$h_j k_f [(l'_{A,j} / L_j) (l'_{B,j} / L_j) - (1/K_e) (l'_{C,j} / L_j)] - \lambda_j = 0$$

Tables 4 and 5 contain the parameters for the column base case. The heat of reaction is $-41,870$ J/mol, activation energy $125,600$ J/mol, reaction equilibrium constant 20 , and forward rate constant 0.008 per unit of time at a reference temperature of 366 K. Component normal boiling points are 313 K, 338 K, and 353 K for A, B, and C respectively. This case corresponds to the ternary system without inerts presented by Luyben and Yu (2008). Column stages are taken to be adiabatic, with the exception of the reboiler and total condenser.

Figure 5 shows fractional conversion of A versus Damkohler number when the bottoms rate L_{16} (an external material balance variable) is specified in addition to boilup V_{16} (an internal energy balance variable). For this set of specifications, it is seen that conversion increases smoothly with Damkohler number, and no multiplicities are observed. These results compare well with the case as presented by Luyben and Yu, where the bottoms rate was specified at 12.86 mol per unit time and liquid holdup on the reactive trays was set at 1000 mol (the Damkohler number would then have been 0.1), and where no multiplicities were reported.

Table 4 - Operating parameters for base distillation case

ΔH_v (J/mol)	29070.	stages	16
ΔH_r (J/mol)	-41870.	react stages	2-10
E_a (J/mol)	125600.	B feed	stage 2
$K_{eq,ref}$	20.	A feed	stage 10
$k_{f,ref}$ (\ominus^{-1})	0.008	Condenser	Total
T_{ref} (K)	366.	P (bar)	8
		V_{16} (mol/ \ominus)	62.03

Table 5 - Component parameters for base distillation case

Component	A	B (K)	T_{NBP} (K)	$T_{B,8bar}$ (K)	$\alpha_{i,C}$	Feed (mol/ \ominus)
A	12.34	3862	313	376	4.	12.63
B	11.45	3862	338	412	1.6	12.82
C	10.96	3862	353	435		

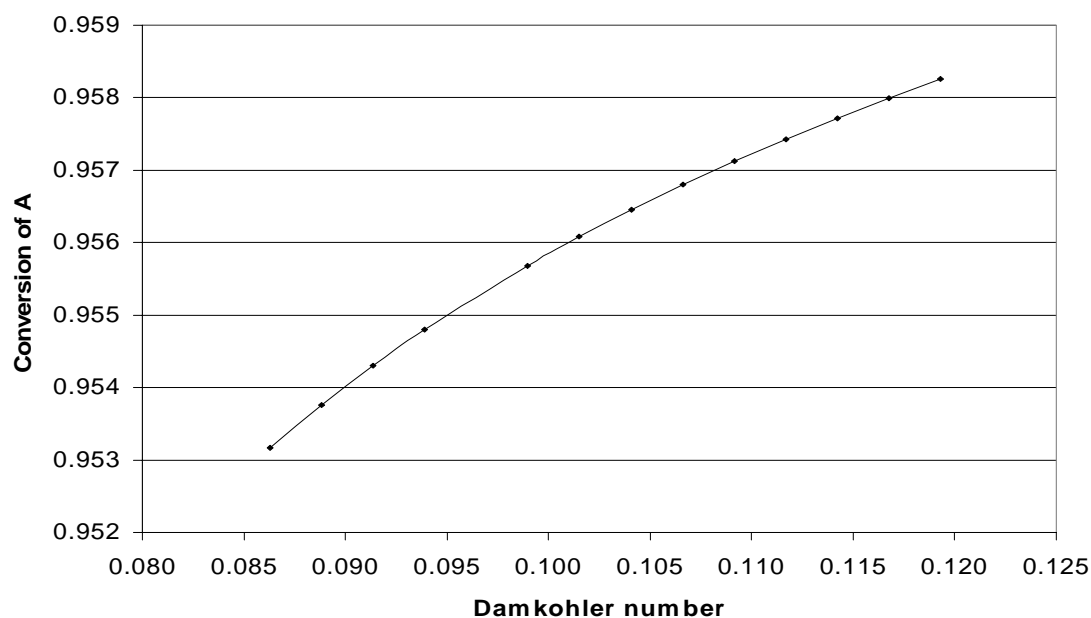
**Figure 5 – Reactive distillation with specified boilup and bottoms rates**

Figure 6 shows the temperature profiles obtained for the case where holdup on each reactive stage is 1000 mol (Damkohler number is 0.1) and the specifications were V_{16} (boilup, an internal energy balance variable) at 62.03 moles per unit time and L_1 (reflux, also an internal energy balance variable) at 78.5 moles per unit time. In this case three distinct solutions are obtained, with the profiles beginning to diverge at about the second reactive stage from the top of the column. Component A conversions for the three solutions are 94.6, 93.8, and 93.1 percent, respectively. While there is little difference in the temperatures at the bottom of the column, the divergence in the temperature profiles between stages 4 and 14 gives a clear indication of significant differences in the compositions at the bottom of the reactive section (stage 10). This difference in compositions at the bottom of the reactive section is shown in Figures 7, 8, and 9 which present the liquid composition profiles for components A, B, and C, respectively.

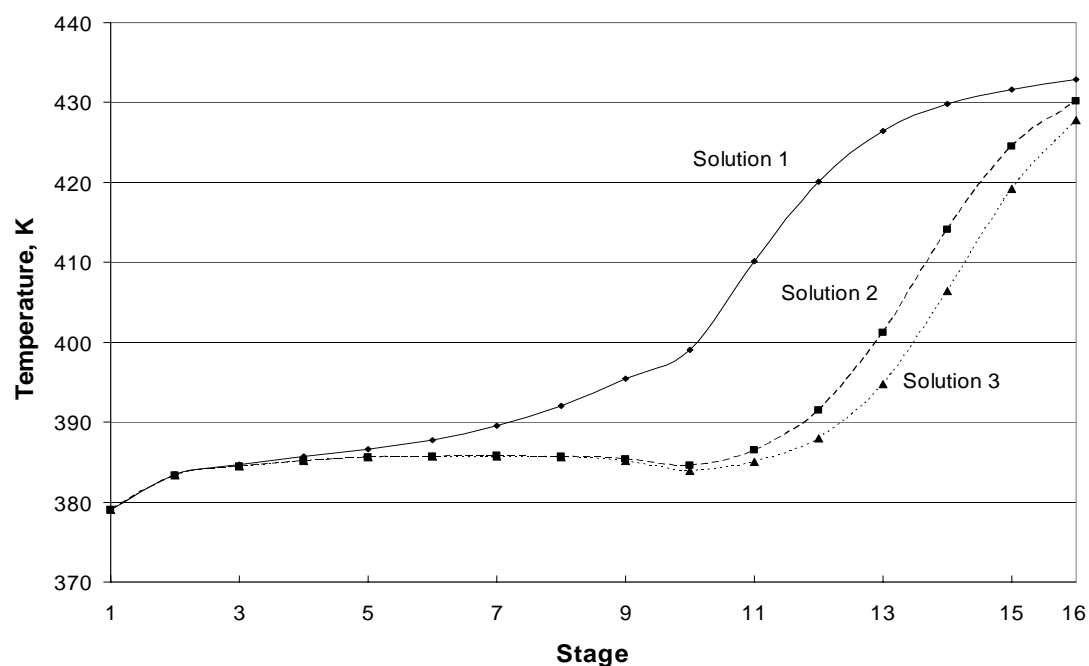


Figure 6 – Reactive distillation with boilup and reflux rate specified

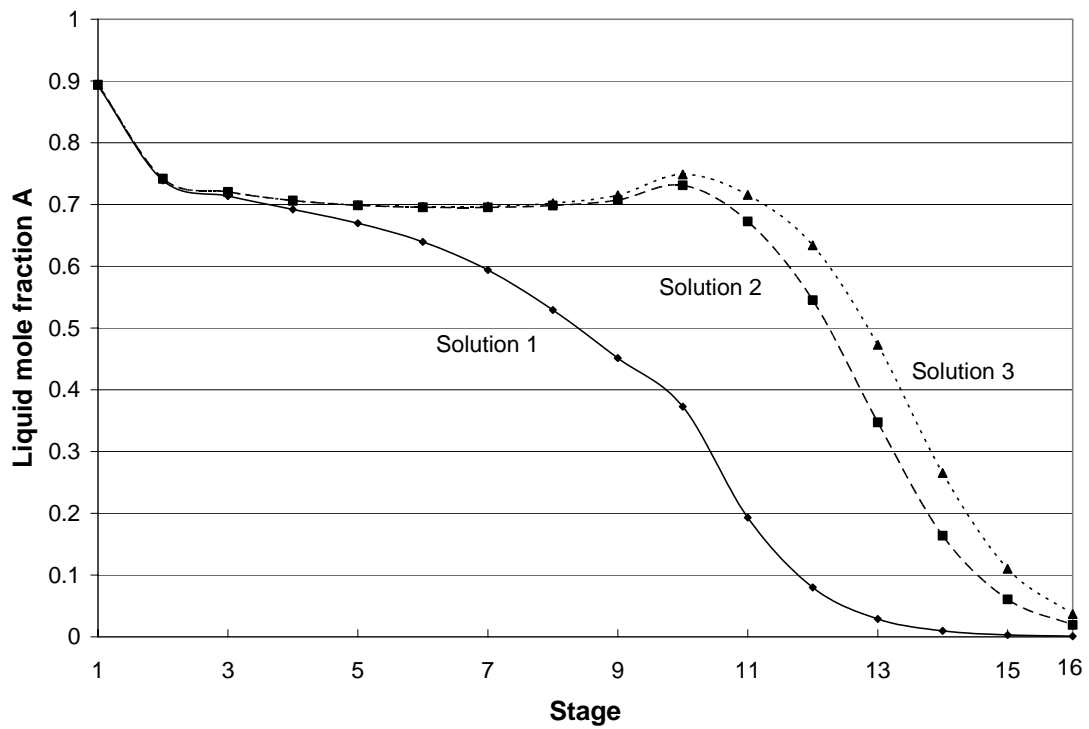


Figure 7 – Component A liquid compositions with boilup and reflux rate specified

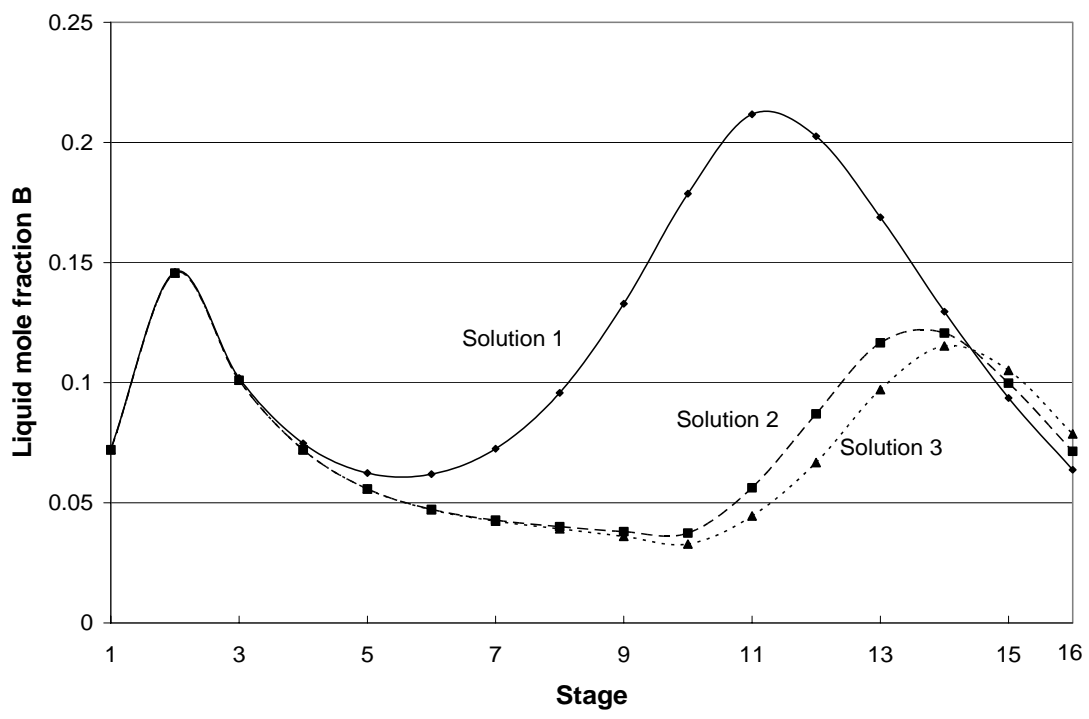


Figure 8 – Component B liquid compositions with boilup and reflux rate specified

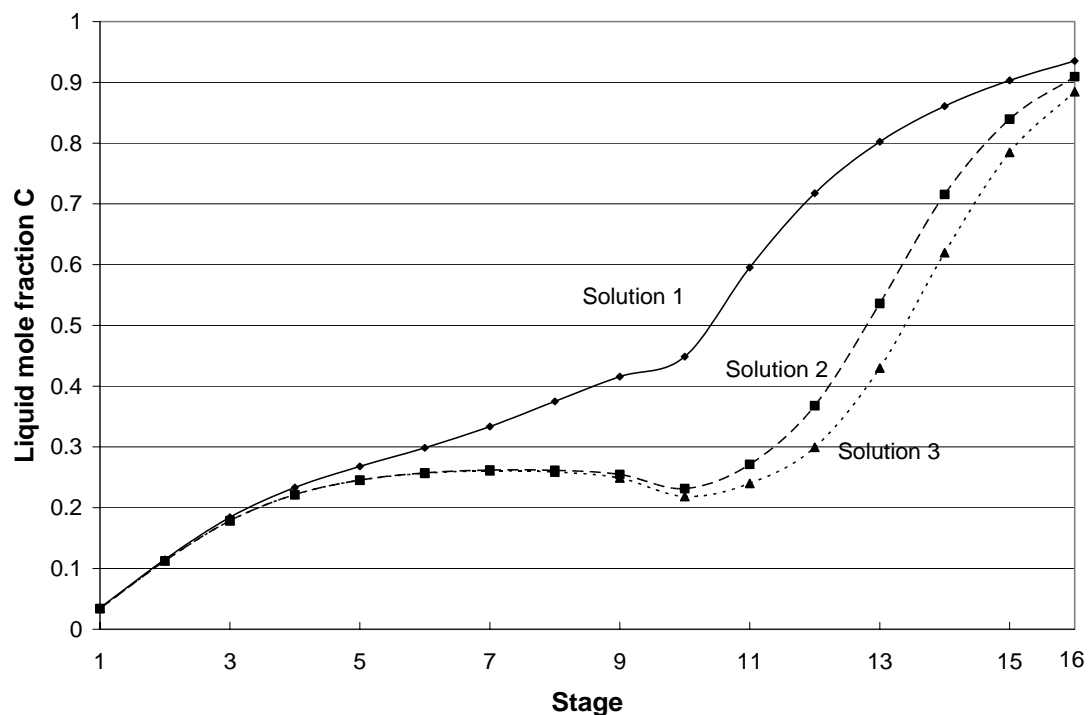


Figure 9 – Component C liquid compositions with boilup and reflux rate specified

4. CONCLUSIONS

Output multiplicities are found for both the reactive flash and the multistage reactive distillation, even for systems described by highly idealized models. For these ideal systems, the multiplicities appear to be caused by interaction between the components' relative rates of evaporation which do not change sign, and the rates of production or consumption which do change sign. Homotopy continuation is found to be a useful tool for identifying these multiplicities, and for locating them in parameter space.

The choice of specifications, or by analogy the choice of control variables in the physical operation, affects the occurrence of these multiplicities. In the reactive flash, specifying the heat input can give rise to multiplicities, while specifying the fraction of the feed vaporized does not. For the column, specifying the boilup and the bottoms rate - one being an internal energy balance variable, and the other an external material balance variable - fails to produce multiplicities. In contrast, specifying both the boilup and the reflux rate - both internal energy balance variables - can give rise to multiple solutions.

NOMENCLATURE

A_i, B_i constants for component vapor pressure expression

D/F vapor overhead to feed ratio

E_A reaction activation energy, J/mol

F_j molar bulk feed rate, mol/time

f_{ij} component i feed rate, mol/time

h_j liquid holdup on stage j , mol

ΔH_r heat of reaction, J/mol

ΔH_v heat of vaporization, J/mol

K_{ij} component i vapor-liquid distribution coefficient

$k_{f,0}$ reaction forward rate constant pre-exponential

k_f reaction forward rate constant at temperature T

$K_{e,0}$ reaction equilibrium constant

K_e reaction equilibrium constant at temperature T

L_j molar liquid rate, mol/time

l_{ij} component i liquid rate

P_i^* component i vapor pressure, bar

P pressure, bar

Q heat added to the flash, J/time

R gas constant

r_j rate of reaction, moles per unit time

T_j temperature, K

V_j molar vapor rate, mol/time

v_{ij} component i vapor rate, mol/time

x_{ij} liquid mole fraction i

y_{ij} component i vapor mole fraction

Greek letters

α_i component i relative volatility

Φ vapor-to-feed ratio

λ_j reaction extent, mol/time

ν_i component i stoichiometric coefficient

Θ unit of time

Subscripts

i component index

j stage index

l liquid phase

v vapor phase

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II. MULTIPLE STEADY STATES IN THREE-COMPONENT REACTION

SYSTEMS:

EFFECT OF COMPONENT PHYSICAL PROPERTIES

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ABSTRACT

The effects of relative volatility between the light and heavy components, forward rate constant, and reaction equilibrium constant are studied for a reaction of the form $A+B \leftrightarrow C$ taking place in the liquid phase of both a single stage flash (two phase reactor) and a multistage reactive distillation column. It is concluded that both the relative volatility spread and the equilibrium constant exhibit threshold values, below which singular solutions are obtained, and above which multiplicities are to be found. The rate constant also is seen to affect the appearance of multiple solutions, but the multiplicities are found in regions that are bounded above and below by regions where singular solutions are produced.

1. INTRODUCTION

Distillation has been an important part of chemical processing for at least several centuries; however, the rapid growth in computing capabilities in the last few decades has enabled a corresponding increase in the sophistication of design calculations. This in turn has allowed the use of more complex configurations to satisfy demands for increased performance and economy. In particular, reactive distillation, in which both chemical reaction and the separation of products from byproducts and residual reactants take place in the same equipment, has received increasing attention in recent years (Malone and Doherty 2000; Luyben and Yu 2008).

The existence of multiple steady states in distillation processes has been observed both in laboratory and plant practice, and in design calculations (Mohl et al. 1999). Output multiplicities, in which a process may exhibit differing performance profiles for

apparently identical operating parameters, are particularly troublesome from the standpoint of design, control, and safety. Standard design calculation techniques for such processes may converge to different solutions, depending on the starting estimates used for process variables, but are typically able to find only a single profile for any given set of inputs (Taylor and Krishna 2000). In operation, the column may approach different performance profiles, depending on startup conditions or the states imposed by process transients.

Methods have been developed for finding multiple solutions to reactive distillation problems. However, these methods have been predominantly graphical or algebraic, and are thus limited in the precision they can offer and the number of species involved in the problems they can address (Bekiaris and Morari 1996; Bessling, Schembecker, and Simmrock 1997; Dalal and Malik 2003). While homotopy continuation has been found useful because of its robustness and its ability to locate multiple solutions, much of the published work in this area has dealt with specific systems of more-or-less nonideal components (Kovach III and Seider 1987; Singh, Singh, Kumar et al. 2005). The problem of identifying parametric combinations or ranges of values for which multiplicities do or do not appear in generalized ideal systems has yet to receive adequate attention.

Of the many systems for which reactive distillation has been studied or commercialized, several involve reactions of the form $A+B \leftrightarrow C$ (Luyben and Yu 2008). A small sampling of these systems is presented in Table 1.

For these systems, the mass-action rate law may be expressed as

$$r = k_{f,0} e^{(-E_A/RT)} \left(x_A x_B - x_C / K_{e,0} e^{(-\Delta H_r/RT)} \right)$$

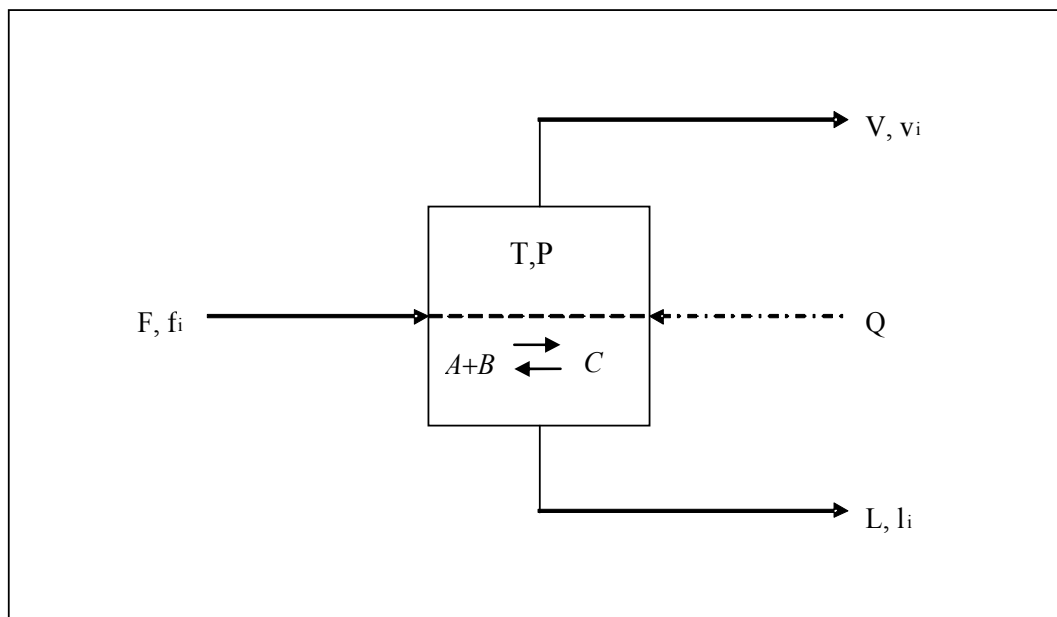
Systems with reactions of the form $2A \leftrightarrow C$ or $A \leftrightarrow B + C$, and having similarly structured rate laws have also been commercialized.

Table 1 - Some three-component reactive distillation systems

A	B	C
acetaldehyde	acetic anhydride	vinyl acetate
acetone	hydrogen	isopropanol
benzene	ethylene	ethylbenzene
isoamylene	water	tert-amyl alcohol
methanol	isobutene	methyl tert-butyl ether
methanol	isoamylene	tert-amyl methyl ether

2. THE REACTIVE FLASH

Figure 1 is a diagram of a reactive flash, two phase reactor or single stage, reactive distillation. F represents the feed, and is the sum of the component feeds f_i . Additional energy entering the stage is represented by Q , while V is the vapor and L the liquid exiting the stage (the summations of the v_i and l_i , respectively). A single reaction of the form $A+B \leftrightarrow C$ takes place in the liquid on the stage.

**Figure 1 – Reactive flash**

The stage operates at vapor-liquid equilibrium. It is assumed that Raoult's law applies for each species, and that the Clausius-Clapeyron equation is valid for vapor pressures, so that $y_i = (p_i^*/P)x_i$ and $p_i^* = \exp(A_i - B_i/T)$, where $B_i = \Delta H_{v,i}/R$ for all i . It is

further assumed that all component heats of vaporization are equal and that sensible heat effects are negligible.

In order to model the performance of this system, it is necessary to obtain simultaneous solutions to the mass and energy balances and the equilibrium constraints (Taylor and Krishna 2000):

$$l_A + v_A - f_A - h\lambda v_A = 0$$

$$l_B + v_B - f_B - h\lambda v_B = 0$$

$$l_C + v_C - f_C - h\lambda v_C = 0$$

$$H_V + H_L - H_F - Q = 0$$

$$K_A l_A / L - v_A / V = 0$$

$$K_B l_B / L - v_B / V = 0$$

$$K_C l_C / L - v_C / V = 0$$

For finding multiple solutions, the reaction extent must be an element of the solution vector, rather than being fixed by other elements of the solution:

$$hk_f [(l'_A / L')(l'_B / L') - (1/K_e)(l'_C / L')] - \lambda = 0$$

where $l'_i = f_i - v_i$ and $L' = F - V$. Solutions are obtained using the Newton homotopy and a suitable path tracking algorithm to apply global homotopy continuation (Choi 1990; Choi, Harney, and Book 1996).

Parameters for the reactive flash base case are shown in Tables 2 and 3. The normal boiling points of the components are 294 K, 355 K, and 362 K for A, B, and C, respectively, and all components have the same heat of vaporization, 29,070 J/mol. The heat of reaction is -41,870 J/mol, activation energy is 125,600 J/mol, reaction equilibrium constant is 20, and the forward rate constant is 0.008 per unit of time. The reference temperature for the equilibrium and rate constants is 366 K.

Table 2 - Operating parameters for base case flash

ΔH_v (J/mol)	29070.	P (bar)	8
ΔH_r (J/mol)	-41870.	Q (J/Θ)	0.
E_a (J/mol)	125600.		
$K_{eq,ref}$	20.		
$k_{f,ref}$ (Θ ⁻¹)	0.008		
T_{ref} (K)	366.		

Table 3 - Material parameters for base flash case

Component	A	B (K)	T_{NBP} (K)	$T_{B,8bar}$ (K)	$\alpha_{i,c}$	Feed (mol/Θ)
A	13.16	3862	294	348	12.	12.63
B	10.90	3862	355	437	1.25	12.82
C	10.67	3862	362	450		

The fractional conversion of component A versus Damkohler number (here taken to be the product of holdup and forward rate constant at the reference temperature, divided by the bulk feed rate, $Da = hk_{f,ref}/F$) is shown in Figure 2 for a range of values of the relative volatility of component A with respect to component C. Relative volatilities greater than 10 give rise to multiple solutions in the range of Damkohler numbers studied (holdups of 200 to 3600 mol). As the relative volatility increases above 10, the multiplicities appear at higher values, and across wider ranges of the Damkohler number. In this study, no upper limit to this effect was seen.

Figure 3 shows the fractional conversion of A versus Damkohler number for holdup values ranging from 480 to 542 mol at forward reaction rate constant values of 0.0070 (Damkohler numbers 0.132 to 0.151), 0.0080 (Damkohler numbers 0.151 to 0.179), and 0.0090 (Damkohler numbers 0.170 to 0.192). From the graph, it is observed that all results form a single curve, and that multiplicities are only observed for Damkohler numbers between 0.158 and 0.163. Outside this range, only singular solutions are found.

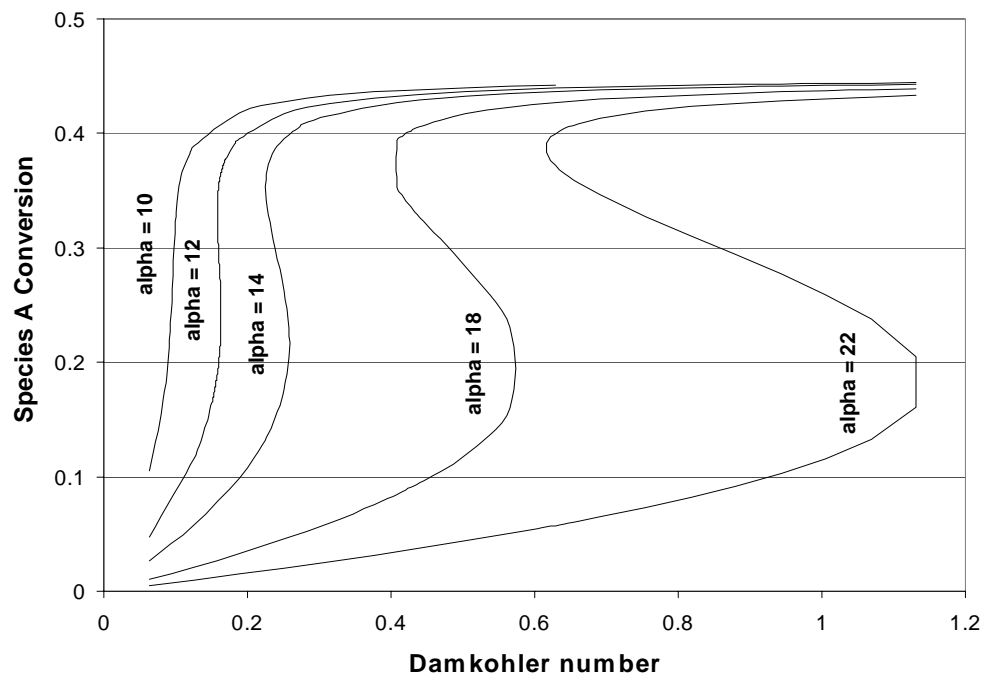


Figure 2 - Conversion versus Damkohler number for a range of species A relative volatilities

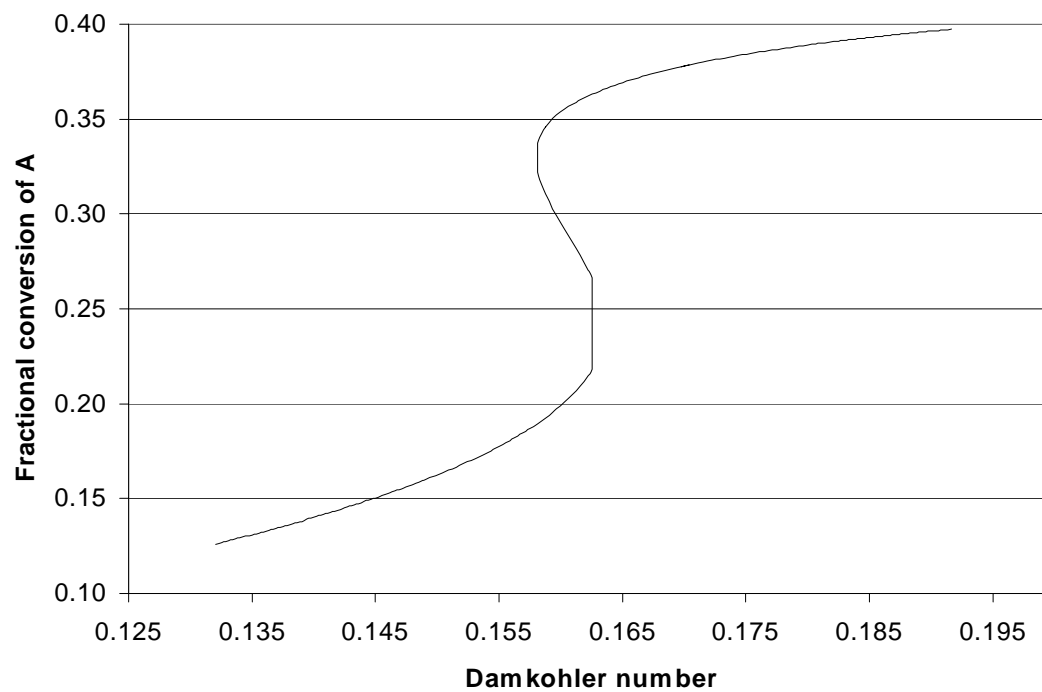


Figure 3 - Conversion versus Damkohler number for a range of rate constant values

Conversion versus Damkohler number for a range of reaction equilibrium constant values is shown in Figure 4. It can be seen that as the value of the chemical equilibrium constant increases, the range of Damkohler number for which multiplicities are observed grows wider and moves toward smaller values of the Damkohler number. For values of the equilibrium constant below about 15, singular solutions are obtained, and multiplicities are no longer found. For a reference temperature equilibrium constant of 18, multiplicities are found in a range of Damkohler numbers from about 0.162 to 0.165; when the equilibrium constant is 22, the range of Damkohler numbers is from about 0.154 to 0.162.

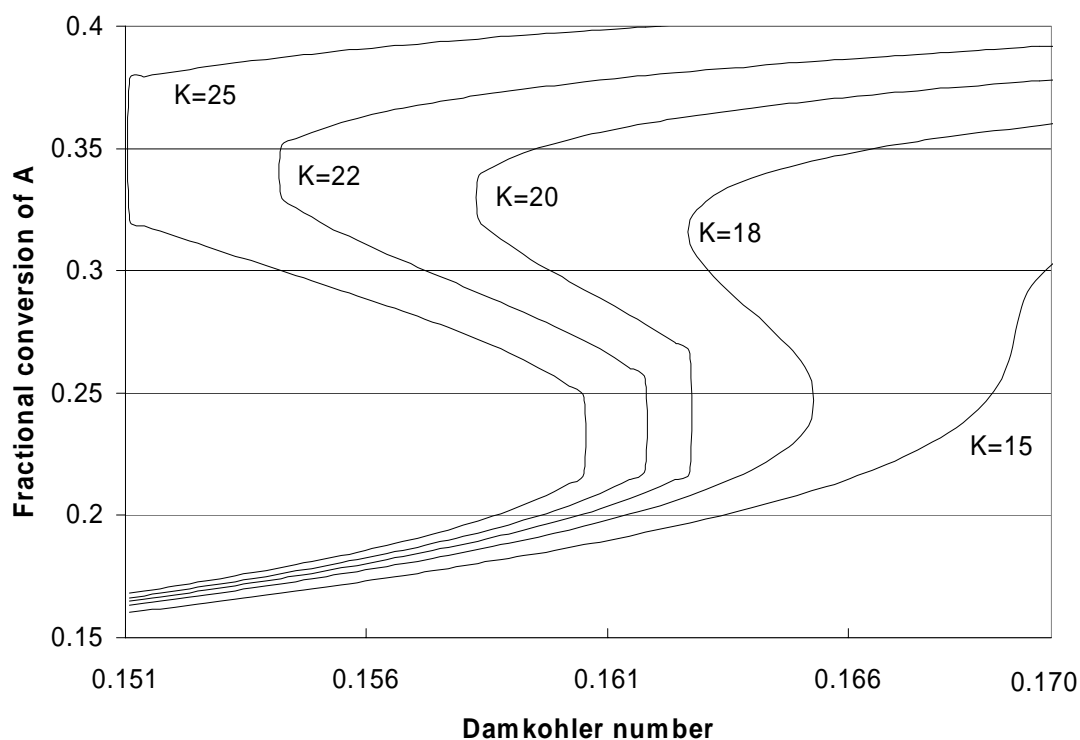


Figure 4 - Conversion versus Damkohler number for a range of equilibrium constant values

3. THE REACTIVE COLUMN

Figure 5 represents a multistage column in which a reaction $A+B \leftrightarrow C$ takes place in the liquid phase on designated trays. Nonreactive trays are specified by setting the holdup to zero for those stages. Since the single product C is the heavy component, and is ideally the only species leaving the column, non-reacting stages are placed at the column

bottom to return components A and B to the reactive section at the top. The heavier of the two reactants is fed at the top of the reactive section, while the lighter component is fed to the lowest reactive stage. Modeling the column's performance is accomplished in the same way as for the flash, except that the equation set to be solved consists of the eight material balance, energy balance, equilibrium, and reaction extent equations for each stage, or a total of $8n$ equations:

$$l_{A,j} + v_{A,j} - f_{A,j} - l_{A,j-1} - v_{A,j+1} - h\lambda_j v_A = 0$$

$$l_{B,j} + v_{B,j} - f_{B,j} - l_{B,j-1} - v_{B,j+1} - h\lambda_j v_B = 0$$

$$l_{C,j} + v_{C,j} - f_{C,j} - l_{C,j-1} - v_{C,j+1} - h\lambda_j v_C = 0$$

$$H_{Vj} + H_{Lj} - H_{Fj} - H_{Lj-1} - H_{Vj+1} - Q_j = 0$$

$$K_{A_j} l_{A_j} / L_j - v_{A_j} / V_j = 0$$

$$K_{B_j} l_{B_j} / L_j - v_{B_j} / V_j = 0$$

$$K_{C_j} l_{C_j} / L_j - v_{C_j} / V_j = 0$$

$$h_j k_j [(l'_{A_j} / L_j') (l'_{B_j} / L_j') - (1/K_e) (l'_{C_j} / L_j')] - \lambda_j = 0$$

Tables 4 and 5 contain the parameters for the column base case. The heat of reaction is $-41,870$ J/mol, activation energy $125,600$ J/mol, reaction equilibrium constant 20 , and forward rate constant 0.008 per unit of time at a reference temperature of 366 K. Component normal boiling points are 313 K, 338 K, and 353 K for A, B, and C respectively. These parameters are substantially the same as those describing the case presented by Luyben and Yu (2008), and except for the observation of solution multiplicities, comparable results were obtained.

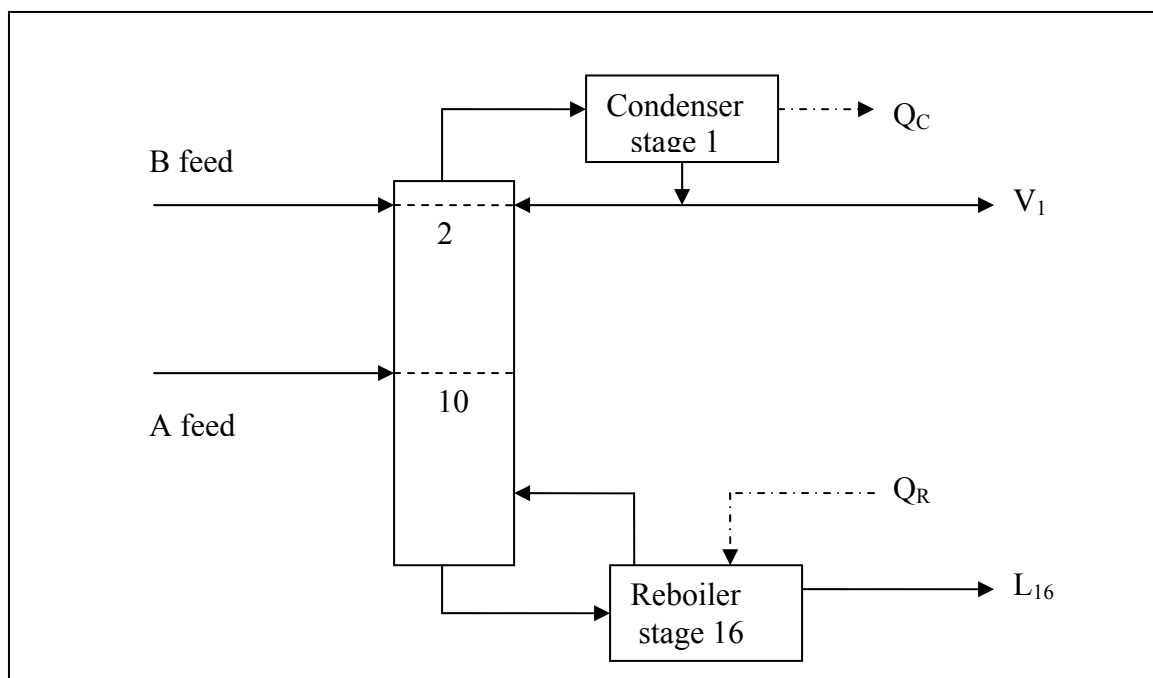


Figure 5 - Reactive column

Table 4 - Operating parameters for base distillation case

ΔH_v (J/mol)	29070.	stages	16
ΔH_r (J/mol)	-41870.	react stages	2-10
E_a (J/mol)	125600.	B feed	stage 2
$K_{eq,ref}$	20.	A feed	stage 10
$k_{f,ref}$ (Θ^{-1})	0.008	Condenser	Total
T_{ref} (K)	366.	P (bar)	8
		L_{16} (mol/ Θ)	12.85
		V_{16} (mol/ Θ)	62.03

Table 5 - Component parameters for base distillation case

Component	A	B (K)	T_{NBP} (K)	$T_{B,8bar}$ (K)	$\alpha_{i,c}$	Feed (mol/ Θ)
A	12.34	3862	313	376	4.	12.63
B	11.45	3862	338	412	1.6	12.82
C	10.96	3862	353	435		

Figure 6 shows the fractional conversion of A versus distillate-to-total-feed ratio (D/F) at various levels of the relative volatility spread between components A and C. For relative volatilities at or below 3.4, and in all cases for D/F less than about 0.016, singular solutions are obtained and multiplicities are not observed. For a relative volatility of 3.8, multiplicities are found for D/F in the range of about 0.019 to 0.022, and as the relative volatility increases, the range of D/F for which multiplicities are observed becomes wider and reaches higher D/F values. In the range of conditions studied, conversions as high as 97 percent were found where multiplicities existed. However, for a relative volatility spread of 3.4, singular solutions were found and maximum conversion was only 95.6 percent.

Figure 7 demonstrates the effect of varying the reference forward rate constant $k_{f,ref}$ on the relationship between conversion and D/F. As with the relative volatility spread, multiplicities are not observed for D/F less than about 0.014. In the range of values studied, smaller forward rate constants result in higher values and broader ranges of D/F for which multiple solutions are obtained.

The variation in conversion with D/F for several values of the reaction equilibrium constant K_e is shown in Figure 8. For values of K_e at or below 10, multiple solutions are not observed in the range of D/F studied. For values of K_e of 15 and above, increasing K_e leads to narrower ranges and lower values of D/F where multiple solutions are to be found.

4. CONCLUSIONS

The occurrence of steady-state multiplicities for both the single stage reactive flash and the multistage reactive column is influenced by both the vapor-liquid and reaction kinetic properties of the components involved. For the idealized ternary system studied, this has been examined in terms of the relative volatility between the lightest and heaviest components, and forward rate constant and equilibrium constant for the reaction. The occurrence of multiplicities appears to be caused by interaction between the relative rates of component evaporation which do not change sign, and the rates of production or consumption which can change sign.

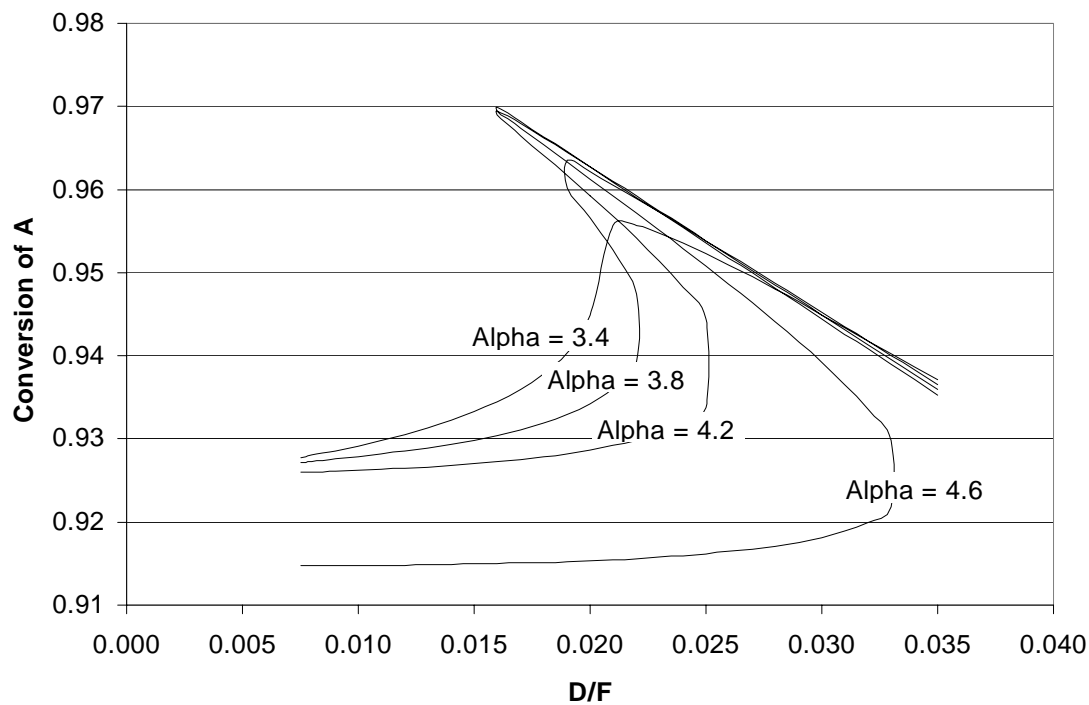


Figure 6 - Conversion versus distillate to feed ratio for a range of relative volatilities

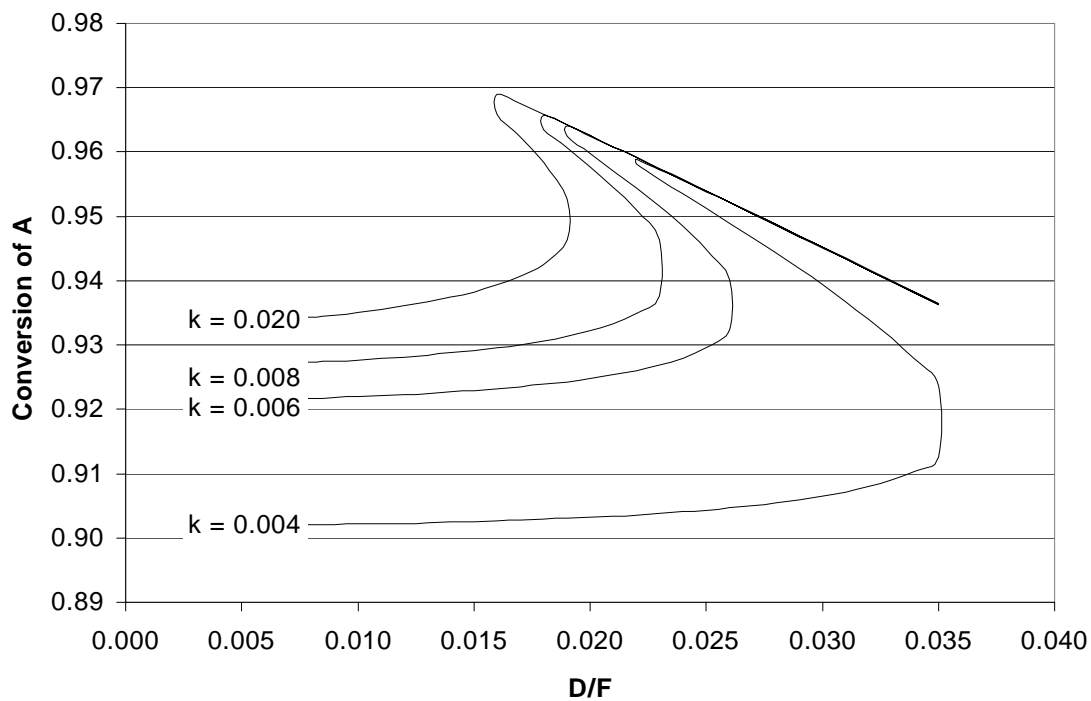


Figure 7 - Conversion versus distillate to feed ratio for a range of values of the forward rate constant

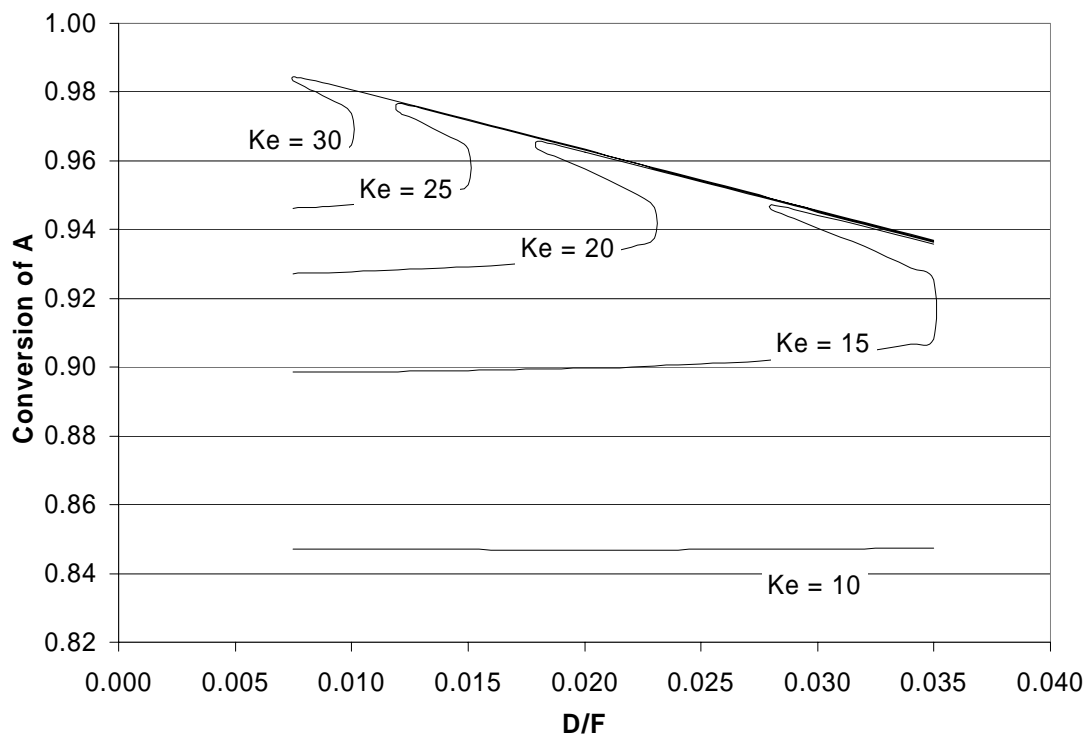


Figure 8 - Conversion versus distillate to feed ratio for a range of values of the reaction equilibrium constant

Multiplicities are observed only for values of the relative volatility spread above some minimum value, below which only singular solutions are found. As the relative volatility difference increases above the minimum, multiplicities are observed at increasing values of the Damkohler number in the case of the flash, and distillate to feed ratio in the case of the column. This could be accounted for by the greater tendency of the light reactant to leave the system rather than reacting as relative volatility increases.

In the flash, multiplicities appear to exist only for values of the Damkohler number between about 0.158 and 0.163, throughout the range of rate constant values studied. This can be attributed to the fact that higher rate constant and lower holdup have a tendency to offset each other in determining reaction extent. For the column, singular solutions are observed for distillate to feed ratio less than about 0.014. Above this threshold, increasing rate constant values correspond to the appearance of multiplicities at lower values and narrower ranges of distillate to feed ratio.

For the column, under the conditions studied, conversion was limited to 95.6 percent when the relative volatility was in a range where singular solutions were found.

Higher conversions were observed; however, they occurred in regions where solution multiplicities were encountered. For each of the three properties studied, the downward slope of the curves representing high conversion solutions indicates a limit imposed by removal of reactants in the overhead, rather than attainment of reaction equilibrium.

For both the flash and the column, there appears to be a threshold value of the equilibrium constant below which multiplicities are not exhibited. Above that threshold, multiplicities are found at lower values of the Damkohler number in the flash and distillate to feed ratio in the column, as the equilibrium constant increases.

NOMENCLATURE

A_i, B_i constants for component vapor pressure expression

D/F vapor overhead to feed ratio

E_A reaction activation energy, J/mol

F_j molar bulk feed rate, mol/time

f_{ij} component i feed rate, mol/time

h_j liquid holdup on stage j , mol

ΔH_r heat of reaction, J/mol

ΔH_v heat of vaporization, J/mol

K_{ij} component i vapor-liquid distribution coefficient

$k_{f,0}$ reaction forward rate constant pre-exponential

k_f reaction forward rate constant at temperature T

$K_{e,0}$ reaction equilibrium constant pre-exponential

K_e reaction equilibrium constant at temperature T

L_j molar liquid rate, mol/time

l_{ij} component i liquid rate

P_i^* component i vapor pressure, bar

P pressure, bar

Q heat added to the flash, J/time

R gas constant

r_j rate of reaction, moles per unit time

T_j temperature, K

V_j molar vapor rate, mol/time

v_{ij}	component i vapor rate, mol/time
x_{ij}	liquid mole fraction i
y_{ij}	component i vapor mole fraction
Greek letters	
α_i	component i relative volatility
Φ	vapor-to-feed ratio
λ_j	reaction extent, mol/time
ν_i	component i stoichiometric coefficient
Θ	unit of time
Subscripts	
i	component index
j	stage index
l	liquid phase
v	vapor phase

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SECTION

3. CONCLUSIONS

Output multiplicities are found for both the reactive flash and the multistage reactive distillation, even for systems described by highly idealized models. Multiplicities in these ideal systems are seen to be caused by interaction between components' relative rates of evaporation which cannot change sign, and rates of production or consumption which can change sign. Homotopy continuation is found to be a useful tool for identifying these multiplicities, and for locating regions in parameter space where they occur.

The occurrence of multiplicities for both the single stage reactive flash and the multistage reactive column is influenced by both the vapor-liquid and reaction kinetic properties of the components involved. For the idealized ternary system studied, this has been looked at in terms of the relative volatility between the lightest and heaviest components, and the reaction forward rate constant and equilibrium constant.

Multiplicities are observed only for values of the relative volatility spread above some minimum value; below this value, only singular solutions are found. As the relative volatility difference increases above the minimum, multiplicities are observed at increasing values of Damkohler number in the case of the flash, and distillate to feed ratio in the case of the column.

In the flash, multiplicities appear to exist only for values of Damkohler number between about 0.158 and 0.163, throughout the range of rate constant values studied. For the column, singular solutions are observed for distillate to feed ratio less than about 0.016. Above this threshold, increasing rate constant values correspond to the appearance of multiplicities at lower values and narrower ranges of distillate to feed ratio.

For both the flash and the column, there appears to be a threshold value of the equilibrium constant below which multiplicities are not exhibited. Above that threshold, multiplicities are found at lower values of Damkohler number in the flash and distillate to feed ratio in the column, as the equilibrium constant increases.

The choice of specifications, or by extension the choice of control variables in the physical operation, also affects the occurrence of these multiplicities. In the reactive flash, specifying the heat input can give rise to multiplicities, while specifying the fraction of the feed vaporized does not. For the column, specifying the boilup and the bottoms rate - one being an internal energy balance variable, and the other an external material balance variable - fails to produce multiplicities. In contrast, specifying both the boilup and the reflux rate - both internal energy balance variables - can give rise to multiple solutions. For both the flash and the column, when other specifications are favorable for the existence of multiplicities, they are exhibited for some ranges of Damkohler number values (as determined by holdup), but not for other values.

APPENDIX A.
COMPUTER PROGRAMS USED FOR THIS STUDY

The computer programs used in this study were coded in the FORTRAN 77 language, and compiled using the MINGW g77 compiler. The distillation program was prepared initially, and was then modified to create the flash program by removing the logic needed for unique handling of a condenser, reboiler, and multiple stages. Each program consists of routines for receiving problem specifications, constructing the vector of initial estimates, calling the solver routine, monitoring the state returned by the solver, and printing formatted results. The homotopy solver routine for both programs is as published by Choi (1990).

PROGRAM INPUT

Input to both the distillation and flash programs is through text files containing a series of “command” lines describing a case or series of cases to be run. For the distillation program, the input formats are presented in Table A.1. Table A.2 contains the input formats for the flash program, which differ from those for the distillation program only in that a single stage, rather than multiple stages, is specified for each case.

Table A.1

Distillation Program Input file "card" format and content

Case Identification string	(Required)
P1 <string>	
Case Description	
P2 <string>	
Case solution algorithm	(Default: Newton)
P3 <integer>	
1 => Newton solver (default)	
2 => Homotopy solver	
Thermodynamic model	(Ideal only for current thermodynamic subroutines)
P4 <integer>	
1=> Peng-Robinson EOS (default)	
2=> Soave-Redlich-Kwong EOS	
3=> Redlich-Kwong EOS	
4=> Van der Waals EOS	

Table A.1 (cont.)

Component specifications	(Required)
P5 <no. components> <"datafile name"> <"component name"> ... <"component name">	
Number of stages (incl. condenser and reboiler)	(Required)
P6 <integer>	
Condenser type	(Default: Total)
P7 <integer> 1 => Total (default) 2 => Partial	
Top specification	(Required)
P8 <spec type> <spec value> <component index> 1=> Qc (J) 2=> L/D 3=> D/F 4=> Di/Fi 5=> Tc (K) 11=> L1 (mol)	
Bottom specification	(Required)
P9 <spec type> <spec value> <component index> 6=> Tr (K) 7=> Bi/Fi 8=> B/F 9=> V/B 10=> Qr (J) 12=> Vn (mol)	
Condenser pressure and per-stage delta	(Required)
P10 <Pcond> <delta>	
Feed specifications	(Required)
P11 <no. feeds> <stage> <type> <pressure> <temperature> <feed 1> ... <feed nc> ... <stage> <type> <pressure> <temperature> 1=> Bubble point liquid (temperature is recalculated)	

Table A.1 (cont.)

	2=> Dew point vapor (temperature is recalculated)
	3=> Feed flashed at spec. temperature and stage pressure
Specified stage heat duties	(Default: 0.0 for all stages)
	P12 <Start stage> <End stage> <specified input(+) or withdrawal(-)>
Specified side-draws	(Default: 0.0 for all stages)
	P13 <no. specified>
	<stage> <type> <specified Sv/V or Sl/L>
	...
	<stage> <type> <specified Sv/V or Sl/L>
	1=> liquid
	2=> vapor
	note that both liquid and vapor side-draws can
	be specified for each stage
Specified Murphree (VLE) efficiencies	(Default: 1.0 for all stages)
	P14 <Start stage> <End stage> <specified efficiency>
Specified stoichiometric coefficients	(Default: 0.0 for all comps)
	P15 <c1> <c2> ... <cn>
	(+)=> reagent
	(-)=> product
	(0)=> inert
Specified stage reaction efficiencies	(Default: 0.0 for all stages)
	P16 <Start stage> <End stage> <specified efficiency>
Specified reaction equilibrium constant	(Default 0.0)
	P17 <spec. value>
	note that if the specified value is zero, program will use
	the value calculated from the thermodynamic model
Specified stage molar holdups	(Default: 0.0 for all stages)
	P18 <Start stage> <End stage> <specified holdup>
Specified homotopy solver parameters	
	P21 <param number> <value>
	1) dir tracking direction (default = 1 [positive t]; -1 for negative t)
	2) dso initial step size (default = 1.0d-01)
	3) dsmin minimum step size (default = 1.0d-20)

Table A.1 (cont.)

4)	dsmax	maximum step size	(default = 5.0d+04)
5)	xmax	continuation space boundary	(default = 1.0d+05)
6)	ecorc	continuation point tolerance	(default = 1.0d-04)
7)	ecorb	bisection point tolerance	(default = 1.0d-06)
8)	edet	max relative determinant change	(default = 5.0d-01)
9)	esol	solution point tolerance	(default = 1.0d-04)
10)	ebif	bifurcation point tolerance	(default = 1.0d-04)
11)	etur	turn point tolerance	(default = 1.0d-06)
12)	esta	start point tolerance	(default = 1.0d-04)
13)	easy	asymtotic behavior tolerance	(default = 1.0d-06)
14)	idom	compute in real or complex domain	(default = 0 [real domain])
15)	ihom	homotopy type	(default = 1 [newton]; 2 for fixed point)
16)	maxdet	maximum number of determinant evaluations	(default = 5)
17)	minasy	minimum steps to sense asymptote	(default = 5)
18)	maxasy	maximum steps to sense asymptote	(default = 20)

Parameters for simplified thermodynamic calculations

P31 <alpha> <tb1> <delhv> <delhr> <cpl> <cpv> <rxntref> <rxnk> <rxnkf> <rxefwd>

alpha	Component to component relative volatility
tb1	Boiling point of lightest component
delhv	Heat of vaporization (same for all components)
delhr	Heat of reaction
cpl	Liquid heat capacity (same for all components)
cpv	Vapor heat capacity (same for all components)
rxntref	Reference Temperature for reaction equilibrium and rate constants
rxnk	Reaction equilibrium constant at rxntref
rxkf	Reaction forward rate constant at rxntref
rxefwd	Activation energy (for forward rate constant)

Parameters for specified Antoine constants ($\ln P = A - B/T$)

P32 <Component index> <A>

Reaction coordinate for problem initialization

P33 <rx coord> (0 <= rxcoord <= 1)

0<=rxcoord<=1	initialization reaction coordinate
rxcoord>1 or <-1	initialization at full equilibrium
0>rxcoord>-1	initialize at fract approach to equilibrium

Table A.1 (cont.)

Component flow scaling for problem initialization	
P34 <scinit>	
Multiply component flows by scinit for starting vector	
End of current case	
XC	

Table A.2

Input file "card" format and content for flash program	
Case Identification string	(Required)
P1 <string>	
Case Description	
P2 <string>	
Case solution algorithm	(Default: Newton)
P3 <integer>	
1 => Newton solver (default)	
2 => Homotopy solver	
Thermodynamic model	(Ideal only for current thermodynamic subroutines)
P4 <integer>	
1=> Peng-Robinson EOS (default)	
2=> Soave-Redlich-Kwong EOS	
3=> Redlich-Kwong EOS	
4=> Van der Waals EOS	
Component specifications	(Required)
P5 <no. components> <"datafile name">	
<"component name">	
...	
<"component name">	
Number of stages (incl. condenser and reboiler)	(Required)
P6 <integer>	

Table A.2 (cont.)

Condenser type	(Default: Total)
P7 <integer>	
1 => Total (default)	
2 => Partial	
Top specification	(Required)
P8 <spec type> <spec value> <component index>	
1=> Spec V/F	
2=> Spec T	
3=> Spec Q	
Flash pressure and per-stage delta	(Required)
P10 <Pflash>	
Feed specifications	(Required)
P11 <no. feeds>	
<stage> <type> <pressure> <temperature> <feed 1> ... <feed nc>	
...	
<stage> <type> <pressure> <temperature>	
1=> Bubble point liquid (temperature is recalculated)	
2=> Dew point vapor (temperature is recalculated)	
3=> Feed flashed at spec. temperature and stage pressure	
Specified stoichiometric coefficients	(Default: 0.0 for all comps)
P15 <c1> <c2> ... <cn>	
(+)=> reagent	
(-)=> product	
(0)=> inert	
Specified stage reaction efficiencies	(Default: 0.0 for all stages)
P16 <specified efficiency>	
Specified stage molar holdups	(Default: 0.0 for all stages)
P18 <specified holdup>	
Specified homotopy solver parameters	
P21 <param number> <value>	
1) dir tracking direction (default = 1 [positive t]; -1 for negative t)	
2) dso initial step size (default = 1.0d-01)	
3) dsmin minimum step size (default = 1.0d-20)	
4) dsmax maximum step size (default = 5.0d+04)	
5) xmax continuation space boundary (default = 1.0d+05)	

Table A.2 (cont.)

6)	ecorc	continuation point tolerance	(default = 1.0d-04)
7)	ecorb	bisection point tolerance	(default = 1.0d-06)
8)	edet	max relative determinant change	(default = 5.0d-01)
9)	esol	solution point tolerance	(default = 1.0d-04)
10)	ebif	bifurcation point tolerance	(default = 1.0d-04)
11)	etur	turn point tolerance	(default = 1.0d-06)
12)	esta	start point tolerance	(default = 1.0d-04)
13)	easy	asymtotic behavior tolerance	(default = 1.0d-06)
14)	idom	compute in real or complex domain	(default = 0 [real domain])
15)	ihom	homotopy type	(default = 1 [newton homotopy])
16)	maxdet	maximum number of determinant evaluations	(default = 5)
17)	minasy	minimum steps to sense asymptote	(default = 5)
18)	maxasy	maximum steps to sense asymptote	(default = 20)

Parameters for simplified thermodynamic calculations

P31 <alpha> <tbl> <delhv> <delhr> <cpl> <cpv> <rxntref> <rxnk> <rxnkf> <rxefwd>

alpha	Component to component relative volatility
tbl	Boiling point of lightest component
delhv	Heat of vaporization (same for all components)
delhr	Heat of reaction
cpl	Liquid heat capacity (same for all components)
cpv	Vapor heat capacity (same for all components)
rxntref	Reference Temperature for reaction equilibrium and rate constants
rxnk	Reaction equilibrium constant at rxntref
rxkf	Reaction forward rate constant at rxntref
rxefwd	Activation energy (for forward rate constant)

Parameters for specified Antoine constants ($\ln P = A - B/T$)

P32 <Component index> <A>

Reaction coordinate for problem initialization

P33 <rx coord> (0 <= rxcoord <= 1)
 (rxcoord >1 or <=-1 full equil)
 (-1<rxcoord<0 partial equil)

Initialization scale factor

P34 <scinit>

End of current case

XC

PARAMETERS FOR THE HOMOTOPY SOLVER

Originally, Choi's path tracking algorithm was presented with a set of default parameters suitable for problems having two- or three-dimensional solution vectors. For the distillation problems involved in this study, solution vectors are commonly in excess of 100-dimensional. To obtain solutions to these larger problems in a reasonable number of steps, it was found necessary to increase the default initial step size, as shown in Table A.3. For some specific problems, it was also found useful to increase the minimum step size and to tighten the tolerance for identifying continuation points.

Table A.3

Parameter	Description	Choi value	Value used
dir	Tracking direction		1 (t incr.)
dso	Initial step size	1.0d-02	1.0d-01
dsmin	Minimum step size	1.0d-20	1.0d-20
dsmax	Maximum step size	5.0d+04	5.0d+04
xmax	Continuation space boundary	1.0d+05	1.0d+05
ecorc	Continuation point tolerance	1.0d-04	1.0d-04
ecorb	Bisection point tolerance	1.0d-06	1.0d-06
edet	Maximum relative determinant change	5.0d-01	5.0d-01
esol	Solution point tolerance	1.0d-04	1.0d-04
ebif	Bifurcation point tolerance	1.0d-04	1.0d-04
etur	Turn point tolerance	1.0d-06	1.0d-06
esta	Start point tolerance	1.0d-04	1.0d-04
easy	Asymptotic behavior tolerance	1.0d-06	1.0d-06
idom	Compute in real or complex domain		0 (real)
ihom	Homotopy type		1 (Newton)
maxdet	Maximum determinant evaluations	5	5
minasy	Minimum steps to sense asymptote	5	5
maxasy	Maximum steps to sense asymptote	20	20

PROGRAM USE AND VALIDATION

Table A.4 shows the program input for an example problem corresponding to the ternary case described by Luyben and Yu (2008). In this example, the light component, A, is fed to stage 10, and the intermediate boiling component, B, is fed to stage 2 of a column totaling 16 stages, including a total condenser. Reflux is specified at 78.5 moles per time unit, and boilup is 62.03 moles. Stages 11 through 16 and the condenser (stage 1) are specified to have no liquid holdup, and are thus nonreacting. On stages 2 through 10, holdup is specified at 1000 moles, and the reaction of A and B to form C proceeds.

Table A.4

```

P1  EX-001
P2  "Multiple Soln Example Case  h=1000"
P3  2
P5  3  "scomps.dat"
"A"
"B"
"C"
P6  16
P7  1
P8  11  78.50  0
P9  12  62.03  0
P10 8.000  0.
P11 2
      2  1  8.000  0.  0.  12.82  0.
      10 1  8.000  0.  12.63  0.  0.
P15 -1. -1. 1.
P18 1 16 0.0
P18 2 10 1000.
P21 1 1.
P21 3 1.d-06
P21 6 1.d-06
P21 10 0.
P21 13 1.d-04
P31 2.0 352 29070. -41870. 0. 0. 366. 20.0 0.008 125600.
P32 1 12.34 3862.
P32 2 11.45 3862.
P32 3 10.96 3862.
XC

```

The results of the example case are presented in Table A.5. As can be seen in that table, three unique solutions are found, with component A conversions of 94.6, 93.8, and 93.1 percent, respectively. From the table, it is seen that for each solution, and all stages below the condenser, the liquid bubble points and vapor dew points are equal, which indicates that vapor-liquid equilibrium on the stages is accurately determined. Table A.6 gives a summary of the material balances for the three solutions, and it is seen that the component material balance errors in each of the three cases is equal to or less than 0.0001 mole. Table A.7 presents a similar analysis of the energy balance for each solution, showing that for all solutions, the error is less than or equal to 0.01 kJ.

Table A.5

```

Feasible solution 1:
  Jacobian Determinant:  -6.4151569E-020

  Case ID:  EX-001
Multiple Soln Example Case  h=1000
Stages:  16   Components:   3   Condenser: Total
Component information:
      alpha      Hv      Hr      CpL      CpV      Krx
      2.00  29070.00 -41870.00   0.00   0.00  20.00
      nu      Tb      CpL      CpV      Hr
  A      -1.00   313.30   0.00   0.00   0.00
  B      -1.00   337.68   0.00   0.00   0.00
  C       1.00   352.80   0.00   0.00 -41870.00

Feeds:
Stg:   2   Temp(K):  412.1419  Press(bar):   8.0000  Enthalpy(J):   0.00
      Liquid      Vapor
  A           0.0000   0.0000
  B          12.8200   0.0000
  C           0.0000   0.0000
Stg:  10   Temp(K):  376.3928  Press(bar):   8.0000  Enthalpy(J):   0.00
      Liquid      Vapor
  A          12.6300   0.0000
  B           0.0000   0.0000
  C           0.0000   0.0000

Condenser duty(kJ):  -2303.66917
Reboiler duty(kJ):   1803.2121

```

Table A.5 (cont.)

Column profiles:

Stg	Q(kJ)	L s/d	V s/d	VLE eff	Rxn eff	Rx(mol)	Rx(kJ)
1	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
Stg	P(bar)	T(K)	L(mol)	V(mol)	H err	L(kJ)	V(kJ)
1	8.0000	379.0299	78.5000	0.7456	0.0000	-116.6714	-1.1081
						-1.4863	-1.4863
2	8.0000	383.4764	79.0314	79.2456	0.0000	-386.2836	2185.8897
						-4.8877	27.5837
3	8.0000	384.7029	71.2751	71.9926	0.0000	-556.6481	1916.2774
						-7.8099	26.6177
4	8.0000	385.6978	66.9209	67.4147	0.0000	-658.7248	1745.9129
						-9.8433	25.8981
5	8.0000	386.6226	64.5933	64.8448	0.0000	-727.9711	1643.8363
						-11.2701	25.3503
6	8.0000	387.7843	63.2327	63.4711	0.0000	-792.4642	1574.5899
						-12.5325	24.8080
7	8.0000	389.5321	62.1564	62.6680	0.0000	-869.2428	1510.0969
						-13.9848	24.0968
8	8.0000	392.1110	61.0314	62.0328	0.0000	-958.9623	1433.3183
						-15.7126	23.1058
9	8.0000	395.4112	60.1642	61.3687	0.0000	-1047.6754	1343.5988
						-17.4136	21.8939
10	8.0000	399.0068	74.7818	60.8569	0.0000	-1404.1432	1254.8856
						-18.7765	20.6203
11	8.0000	410.1494	74.7818	62.0300	0.0000	-1863.4536	898.4179
						-24.9186	14.4836

Table A.5 (cont.)

12	8.0000	420.1300	74.7818	62.0300	0.0000	-2246.3074	439.1075
						-30.0382	7.0790
13	8.0000	426.4226	74.7818	62.0300	0.0000	-2511.8416	56.2537
						-33.5890	0.9069
14	8.0000	429.7994	74.7818	62.0300	0.0000	-2694.8914	-209.2806
						-36.0367	-3.3739
15	8.0000	431.6652	74.7818	62.0300	0.0000	-2828.0138	-392.3303
						-37.8169	-6.3248
16	8.0000	432.8257	12.7518	62.0300	0.0000	-499.3489	-525.4528
						-39.1592	-8.4709

Vapor flows/compositions:

	A	B	C
1	0.6656	0.0536	0.0265
	0.892671	0.071832	0.035497
2	70.7403	5.6923	2.8130
	0.892671	0.071832	0.035497
3	64.0695	3.7065	4.2166
	0.889946	0.051485	0.058570
4	59.7006	2.6071	5.1071
	0.885571	0.038673	0.075756
5	56.9320	2.1521	5.7607
	0.877973	0.033188	0.088839
6	54.8454	2.1648	6.4608
	0.864101	0.034107	0.101791
7	52.5960	2.6284	7.4436
	0.839280	0.041942	0.118778
8	49.5212	3.6753	8.8363
	0.798307	0.059248	0.142445
9	45.3693	5.4814	10.5180
	0.739290	0.089319	0.171391
10	40.5861	7.9894	12.2815
	0.666910	0.131281	0.201809
11	27.8693	12.5511	21.6096
	0.449287	0.202339	0.348373
12	14.4282	15.0222	32.5795
	0.232601	0.242177	0.525222
13	5.9655	14.3411	41.7234
	0.096172	0.231196	0.672632
14	2.1461	11.8186	48.0653
	0.034598	0.190531	0.774871
15	0.7112	8.8817	52.4371

Table A.5 (cont.)

	0.011465	0.143184	0.845351
16	0.2187	6.1948	55.6165
	0.003525	0.099868	0.896607
Liquid flows/compositions:			
	A	B	C
1	70.0747	5.6388	2.7865
	0.892671	0.071832	0.035497
2	58.3683	11.4373	9.2258
	0.738546	0.144719	0.116736
3	50.8209	7.1595	13.2947
	0.713025	0.100448	0.186526
4	46.2681	4.9202	15.7326
	0.691385	0.073523	0.235093
5	43.2277	3.9791	17.3865
	0.669229	0.061603	0.269168
6	40.4208	3.8852	18.9268
	0.639238	0.061443	0.299319
7	36.9049	4.4910	20.7605
	0.593742	0.072254	0.334004
8	32.2920	5.8361	22.9033
	0.529105	0.095624	0.375271
9	27.1534	7.9887	25.0221
	0.451322	0.132781	0.415897
10	27.8811	13.3649	33.5358
	0.372833	0.178719	0.448449
11	14.4400	15.8360	44.5057
	0.193096	0.211763	0.595141
12	5.9773	15.1549	53.6496
	0.079930	0.202654	0.717415
13	2.1579	12.6324	59.9914
	0.028856	0.168924	0.802220
14	0.7230	9.6955	64.3633
	0.009668	0.129650	0.860682
15	0.2305	7.0086	67.5427
	0.003082	0.093721	0.903198
16	0.0118	0.8138	11.9262
	0.000925	0.063819	0.935256
Component creation & consumption:			
	A	B	C
1	0.0000	0.0000	0.0000
2	-5.0357	-5.0357	5.0357

Table A.5 (cont.)

3	-3.1784	-3.1784	3.1784
4	-1.7843	-1.7843	1.7843
5	-0.9538	-0.9538	0.9538
6	-0.5576	-0.5576	0.5576
7	-0.4410	-0.4410	0.4410
8	-0.4610	-0.4610	0.4610
9	-0.3554	-0.3554	0.3554
10	0.8145	0.8145	-0.8145
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000
Vapor/Liquid equilibrium ratios:			
	A	B	C
1	0.1074E+01	0.4410E+00	0.2702E+00
	0.1000E+01	0.1000E+01	0.1000E+01
2	0.1209E+01	0.4964E+00	0.3041E+00
	0.1209E+01	0.4964E+00	0.3041E+00
3	0.1248E+01	0.5126E+00	0.3140E+00
	0.1248E+01	0.5126E+00	0.3140E+00
4	0.1281E+01	0.5260E+00	0.3222E+00
	0.1281E+01	0.5260E+00	0.3222E+00
5	0.1312E+01	0.5387E+00	0.3301E+00
	0.1312E+01	0.5387E+00	0.3301E+00
6	0.1352E+01	0.5551E+00	0.3401E+00
	0.1352E+01	0.5551E+00	0.3401E+00
7	0.1414E+01	0.5805E+00	0.3556E+00
	0.1414E+01	0.5805E+00	0.3556E+00
8	0.1509E+01	0.6196E+00	0.3796E+00
	0.1509E+01	0.6196E+00	0.3796E+00
9	0.1638E+01	0.6727E+00	0.4121E+00
	0.1638E+01	0.6727E+00	0.4121E+00
10	0.1789E+01	0.7346E+00	0.4500E+00
	0.1789E+01	0.7346E+00	0.4500E+00
11	0.2327E+01	0.9555E+00	0.5854E+00
	0.2327E+01	0.9555E+00	0.5854E+00
12	0.2910E+01	0.1195E+01	0.7321E+00
	0.2910E+01	0.1195E+01	0.7321E+00
13	0.3333E+01	0.1369E+01	0.8385E+00

Table A.5 (cont.)

	0.3333E+01	0.1369E+01	0.8385E+00
14	0.3579E+01	0.1470E+01	0.9003E+00
	0.3579E+01	0.1470E+01	0.9003E+00
15	0.3720E+01	0.1528E+01	0.9360E+00
	0.3720E+01	0.1528E+01	0.9360E+00
16	0.3811E+01	0.1565E+01	0.9587E+00
	0.3811E+01	0.1565E+01	0.9587E+00
Reaction equilibrium ratios:			
	From thermo	From flows	
1	0.1246E+02	0.5536E+00	
2	0.1068E+02	0.1092E+01	
3	0.1025E+02	0.2604E+01	
4	0.9905E+01	0.4625E+01	
5	0.9601E+01	0.6529E+01	
6	0.9233E+01	0.7621E+01	
7	0.8711E+01	0.7786E+01	
8	0.8001E+01	0.7417E+01	
9	0.7187E+01	0.6940E+01	
10	0.6408E+01	0.6730E+01	
11	0.4548E+01	0.1455E+02	
12	0.3397E+01	0.4429E+02	
13	0.2847E+01	0.1646E+03	
14	0.2594E+01	0.6866E+03	
15	0.2466E+01	0.3127E+04	
16	0.2390E+01	0.1584E+05	
Stream bubble/dew points:			
Stg	L bubble	V dew	
1	379.0299	383.4764	
2	383.4764	383.4764	
3	384.7029	384.7029	
4	385.6978	385.6978	
5	386.6226	386.6226	
6	387.7843	387.7843	
7	389.5321	389.5321	
8	392.1110	392.1110	
9	395.4112	395.4112	
10	399.0068	399.0068	
11	410.1494	410.1494	
12	420.1300	420.1300	
13	426.4226	426.4226	
14	429.7994	429.7994	

Table A.5 (cont.)

15	431.6652	431.6652					
16	432.8257	432.8257					

Feasible solution 2:
 Jacobian Determinant: 1.28299782E-022

Case ID: EX-001
 Multiple Soln Example Case h=1000
 Stages: 16 Components: 3 Condenser: Total
 Component information:

	alpha	Hv	Hr	CpL	CpV	Krx
	2.00	29070.00	-41870.00	0.00	0.00	20.00
	nu	Tb	CpL	CpV	Hr	
A	-1.00	313.30	0.00	0.00	0.00	
B	-1.00	337.68	0.00	0.00	0.00	
C	1.00	352.80	0.00	0.00	-41870.00	

Feeds:

Stg:	2	Temp(K):	412.1419	Press(bar):	8.0000	Enthalpy(J):	0.00
		Liquid		Vapor			
A		0.0000		0.0000			
B		12.8200		0.0000			
C		0.0000		0.0000			

Stg:	10	Temp(K):	376.3928	Press(bar):	8.0000	Enthalpy(J):	0.00
		Liquid		Vapor			
A		12.6300		0.0000			
B		0.0000		0.0000			
C		0.0000		0.0000			

Condenser duty(kJ): -2299.00564
 Reboiler duty(kJ): 1803.2121

Column profiles:

Stg	Q(kJ)	L s/d	V s/d	VLE eff	Rxn eff	Rx(mol)	Rx(kJ)
1	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000

Table A.5 (cont.)

12	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
Stg	P(bar)	T(K)	L(mol)	V(mol)	H err	L(kJ)	V(kJ)
1	8.0000	378.9958	78.5000	0.5852	0.0000	-113.9276	-0.8492
						-1.4513	-1.4513
2	8.0000	383.3806	79.1048	79.0852	0.0000	-378.5018	2184.2288
						-4.7848	27.6187
3	8.0000	384.4695	71.4351	71.8755	0.0000	-540.6285	1919.6546
						-7.5681	26.7080
4	8.0000	385.1900	67.1896	67.3488	0.0000	-628.3629	1757.5279
						-9.3521	26.0959
5	8.0000	385.5858	65.0355	64.8430	0.0000	-671.7372	1669.7935
						-10.3288	25.7513
6	8.0000	385.7628	63.9989	63.5716	0.0000	-691.1663	1626.4192
						-10.7997	25.5841
7	8.0000	385.7940	63.5167	62.9598	0.0000	-697.1946	1606.9901
						-10.9765	25.5241
8	8.0000	385.6891	63.2872	62.6752	0.0000	-692.6990	1600.9618
						-10.9453	25.5438
9	8.0000	385.3603	63.0842	62.5397	0.0000	-671.2774	1605.4574
						-10.6410	25.6710
10	8.0000	384.4676	75.0536	62.4199	0.0000	-723.0612	1626.8790
						-9.6339	26.0635
11	8.0000	386.3712	75.0536	62.0300	0.0000	-841.7239	1575.0952
						-11.2150	25.3925
12	8.0000	391.0974	75.0536	62.0300	0.0000	-1133.9842	1456.4325
						-15.1090	23.4795
13	8.0000	400.5705	75.0536	62.0300	0.0000	-1654.4803	1164.1722
						-22.0440	18.7679
14	8.0000	413.4042	75.0536	62.0300	0.0000	-2225.5214	643.6761
						-29.6524	10.3769
15	8.0000	424.0695	75.0536	62.0300	0.0000	-2626.0451	72.6349
						-34.9889	1.1710
16	8.0000	429.9966	13.0236	62.0300	0.0000	-494.9443	-327.8887
						-38.0037	-5.2860
Vapor flows/compositions:							
	A	B	C				
1	0.5231	0.0418	0.0203				

Table A.5 (cont.)

	0.893894	0.071444	0.034662
2	70.6938	5.6501	2.7413
	0.893894	0.071444	0.034662
3	64.1787	3.6422	4.0546
	0.892915	0.050674	0.056412
4	60.0889	2.4760	4.7839
	0.892205	0.036763	0.071031
5	57.8350	1.8685	5.1395
	0.891923	0.028815	0.079261
6	56.7129	1.5659	5.2927
	0.892111	0.024632	0.083256
7	56.2182	1.4096	5.3320
	0.892923	0.022388	0.084689
8	56.0849	1.3119	5.2784
	0.894850	0.020931	0.084218
9	56.2346	1.2282	5.0770
	0.899182	0.019638	0.081180
10	56.7694	1.1684	4.4822
	0.909476	0.018718	0.071807
11	54.7610	1.8208	5.4482
	0.882814	0.029354	0.087832
12	50.5686	3.1791	8.2823
	0.815229	0.051251	0.133521
13	41.3358	5.4318	15.2625
	0.666384	0.087567	0.246050
14	26.6579	7.6783	27.6937
	0.429759	0.123784	0.446457
15	12.6064	8.0915	41.3322
	0.203230	0.130444	0.666325
16	4.5469	6.5851	50.8980
	0.073301	0.106160	0.820539
Liquid flows/compositions:			
	A	B	C
1	70.1707	5.6083	2.7210
	0.893894	0.071444	0.034662
2	58.6500	11.4148	9.0399
	0.741422	0.144300	0.114278
3	51.4174	7.1057	12.9121
	0.719777	0.099470	0.180752
4	47.4237	4.7584	15.0075
	0.705819	0.070821	0.223360

Table A.5 (cont.)

5	45.4189	3.5732	16.0434
	0.698371	0.054942	0.246687
6	44.4994	2.9920	16.5074
	0.695316	0.046751	0.257933
7	44.1686	2.6968	16.6514
	0.695385	0.042458	0.262158
8	44.2242	2.5190	16.5440
	0.698785	0.039803	0.261412
9	44.6758	2.3760	16.0324
	0.708193	0.037664	0.254143
10	55.0266	2.7578	17.2692
	0.733165	0.036744	0.230092
11	50.8343	4.1160	20.1033
	0.677307	0.054841	0.267852
12	41.6014	6.3687	27.0835
	0.554290	0.084855	0.360855
13	26.9236	8.6153	39.5147
	0.358725	0.114788	0.526486
14	12.8721	9.0284	53.1531
	0.171505	0.120293	0.708202
15	4.8126	7.5220	62.7190
	0.064122	0.100222	0.835657
16	0.2657	0.9369	11.8210
	0.020399	0.071941	0.907660
Component creation & consumption:			
	A	B	C
1	0.0000	0.0000	0.0000
2	-5.0056	-5.0056	5.0056
3	-3.1429	-3.1429	3.1429
4	-1.7397	-1.7397	1.7397
5	-0.8827	-0.8827	0.8827
6	-0.4248	-0.4248	0.4248
7	-0.1976	-0.1976	0.1976
8	-0.0941	-0.0941	0.0941
9	-0.0832	-0.0832	0.0832
10	-0.2707	-0.2707	0.2707
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000

Table A.5 (cont.)

16	0.0000	0.0000	0.0000
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Vapor/Liquid equilibrium ratios:

	A	B	C
1	0.1073E+01	0.4406E+00	0.2699E+00
	0.1000E+01	0.1000E+01	0.1000E+01
2	0.1206E+01	0.4951E+00	0.3033E+00
	0.1206E+01	0.4951E+00	0.3033E+00
3	0.1241E+01	0.5094E+00	0.3121E+00
	0.1241E+01	0.5094E+00	0.3121E+00
4	0.1264E+01	0.5191E+00	0.3180E+00
	0.1264E+01	0.5191E+00	0.3180E+00
5	0.1277E+01	0.5245E+00	0.3213E+00
	0.1277E+01	0.5245E+00	0.3213E+00
6	0.1283E+01	0.5269E+00	0.3228E+00
	0.1283E+01	0.5269E+00	0.3228E+00
7	0.1284E+01	0.5273E+00	0.3230E+00
	0.1284E+01	0.5273E+00	0.3230E+00
8	0.1281E+01	0.5259E+00	0.3222E+00
	0.1281E+01	0.5259E+00	0.3222E+00
9	0.1270E+01	0.5214E+00	0.3194E+00
	0.1270E+01	0.5214E+00	0.3194E+00
10	0.1240E+01	0.5094E+00	0.3121E+00
	0.1240E+01	0.5094E+00	0.3121E+00
11	0.1303E+01	0.5353E+00	0.3279E+00
	0.1303E+01	0.5353E+00	0.3279E+00
12	0.1471E+01	0.6040E+00	0.3700E+00
	0.1471E+01	0.6040E+00	0.3700E+00
13	0.1858E+01	0.7629E+00	0.4673E+00
	0.1858E+01	0.7629E+00	0.4673E+00
14	0.2506E+01	0.1029E+01	0.6304E+00
	0.2506E+01	0.1029E+01	0.6304E+00
15	0.3169E+01	0.1302E+01	0.7974E+00
	0.3169E+01	0.1302E+01	0.7974E+00
16	0.3593E+01	0.1476E+01	0.9040E+00
	0.3593E+01	0.1476E+01	0.9040E+00

Reaction equilibrium ratios:

	From thermo	From flows
1	0.1248E+02	0.5428E+00
2	0.1072E+02	0.1068E+01
3	0.1033E+02	0.2525E+01
4	0.1008E+02	0.4468E+01

Table A.5 (cont.)

5	0.9943E+01	0.6429E+01
6	0.9883E+01	0.7935E+01
7	0.9873E+01	0.8879E+01
8	0.9908E+01	0.9399E+01
9	0.1002E+02	0.9528E+01
10	0.1033E+02	0.8541E+01
11	0.9682E+01	0.7211E+01
12	0.8271E+01	0.7672E+01
13	0.6100E+01	0.1279E+02
14	0.4129E+01	0.3433E+02
15	0.3039E+01	0.1300E+03
16	0.2580E+01	0.6185E+03

Stream bubble/dew points:

Stg	L bubble	V dew
1	378.9958	383.3806
2	383.3806	383.3806
3	384.4695	384.4695
4	385.1900	385.1900
5	385.5858	385.5858
6	385.7628	385.7628
7	385.7940	385.7940
8	385.6891	385.6891
9	385.3603	385.3603
10	384.4676	384.4676
11	386.3712	386.3712
12	391.0974	391.0974
13	400.5705	400.5705
14	413.4042	413.4042
15	424.0695	424.0695
16	429.9966	429.9966

Feasible solution 3:

Jacobian Determinant: -1.39064598E-022

Case ID: EX-001

Multiple Soln Example Case h=1000

Stages: 16 Components: 3 Condenser: Total

Table A.5 (cont.)

Component information:

	alpha	Hv	Hr	CpL	CpV	Krx
	2.00	29070.00	-41870.00	0.00	0.00	20.00
	nu	Tb	CpL	CpV	Hr	
A	-1.00	313.30	0.00	0.00	0.00	
B	-1.00	337.68	0.00	0.00	0.00	
C	1.00	352.80	0.00	0.00	-41870.00	

Feeds:

Stg:	2	Temp(K):	412.1419	Press(bar):	8.0000	Enthalpy(J):	0.00
		Liquid		Vapor			
A		0.0000		0.0000			
B		12.8200		0.0000			
C		0.0000		0.0000			
Stg:	10	Temp(K):	376.3928	Press(bar):	8.0000	Enthalpy(J):	0.00
		Liquid		Vapor			
A		12.6300		0.0000			
B		0.0000		0.0000			
C		0.0000		0.0000			

Condenser duty(kJ): -2295.38839
Reboiler duty(kJ): 1803.2121

Column profiles:

Stg	Q(kJ)	L s/d	V s/d	VLE eff	Rxn eff	Rx(mol)	Rx(kJ)
1	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
Stg	P(bar)	T(K)	L(mol)	V(mol)	H err	L(kJ)	V(kJ)
1	8.0000	378.9960	78.5000	0.4607	0.0000	-113.8996	-0.6685
						-1.4510	-1.4510

Table A.5 (cont.)

2	8.0000	383.3805	79.1015	78.9607	0.0000	-378.3938	2180.8203
						-4.7836	27.6190
3	8.0000	384.4687	71.4286	71.7492	0.0000	-540.4423	1916.3261
						-7.5662	26.7087
4	8.0000	385.1868	67.1811	67.2205	0.0000	-628.0268	1754.2776
						-9.3483	26.0974
5	8.0000	385.5768	65.0271	64.7136	0.0000	-671.0799	1666.6931
						-10.3200	25.7549
6	8.0000	385.7411	63.9930	63.4422	0.0000	-689.8317	1623.6400
						-10.7798	25.5924
7	8.0000	385.7457	63.5177	62.8319	0.0000	-694.4386	1604.8882
						-10.9330	25.5426
8	8.0000	385.5849	63.3041	62.5513	0.0000	-686.9398	1600.2813
						-10.8514	25.5835
9	8.0000	385.1367	63.1441	62.4253	0.0000	-659.0812	1607.7801
						-10.4377	25.7553
10	8.0000	383.9810	75.2644	62.3308	0.0000	-690.9530	1635.6387
						-9.1803	26.2413
11	8.0000	385.1268	75.2644	62.0300	0.0000	-762.2207	1603.7669
						-10.1272	25.8547
12	8.0000	388.1564	75.2644	62.0300	0.0000	-956.6980	1532.4992
						-12.7112	24.7058
13	8.0000	395.1443	75.2644	62.0300	0.0000	-1378.7362	1338.0219
						-18.3186	21.5706
14	8.0000	407.0119	75.2644	62.0300	0.0000	-1977.5218	915.9837
						-26.2743	14.7668
15	8.0000	419.6529	75.2644	62.0300	0.0000	-2488.7269	317.1981
						-33.0665	5.1136
16	8.0000	428.0019	13.2344	62.0300	0.0000	-491.5078	-194.0070
						-37.1386	-3.1276
Vapor flows/compositions:							
	A	B	C				
1	0.4118	0.0329	0.0160				
	0.893886	0.071460	0.034654				
2	70.5819	5.6425	2.7363				
	0.893886	0.071460	0.034654				
3	64.0660	3.6368	4.0464				
	0.892916	0.050688	0.056396				
4	59.9768	2.4712	4.7724				
	0.892241	0.036763	0.070997				

Table A.5 (cont.)

5	57.7270	1.8628	5.1237
	0.892039	0.028786	0.079175
6	56.6158	1.5572	5.2693
	0.892399	0.024545	0.083057
7	56.1447	1.3938	5.2934
	0.893570	0.022183	0.084247
8	56.0614	1.2813	5.2086
	0.896246	0.020484	0.083270
9	56.3174	1.1658	4.9420
	0.902157	0.018676	0.079167
10	57.0859	1.0339	4.2111
	0.915853	0.016587	0.067560
11	55.8167	1.4498	4.7634
	0.899835	0.023373	0.076793
12	53.2022	2.3622	6.4656
	0.857685	0.038082	0.104233
13	46.8376	4.0821	11.1103
	0.755080	0.065808	0.179112
14	34.4603	6.3796	21.1901
	0.555542	0.102848	0.341610
15	18.8599	7.6790	35.4911
	0.304044	0.123795	0.572161
16	7.4830	6.8465	47.7005
	0.120636	0.110374	0.768991
Liquid flows/compositions:			
	A	B	C
1	70.1701	5.6096	2.7203
	0.893886	0.071460	0.034654
2	58.6472	11.4170	9.0373
	0.741417	0.144333	0.114250
3	51.4138	7.1071	12.9076
	0.719793	0.099500	0.180707
4	47.4235	4.7582	14.9994
	0.705905	0.070827	0.223269
5	45.4295	3.5699	16.0277
	0.698625	0.054898	0.246477
6	44.5347	2.9828	16.4756
	0.695931	0.046611	0.257459
7	44.2566	2.6755	16.5856
	0.696761	0.042121	0.261118

Table A.5 (cont.)

8	44.4252	2.4725	16.4065
	0.701773	0.039057	0.259169
9	45.1280	2.2749	15.7411
	0.714683	0.036027	0.249289
10	56.2800	2.4820	16.5023
	0.747764	0.032978	0.219258
11	53.6655	3.3944	18.2045
	0.713026	0.045100	0.241873
12	47.3009	5.1143	22.8492
	0.628463	0.067951	0.303586
13	34.9236	7.4118	32.9290
	0.464012	0.098477	0.437511
14	19.3232	8.7112	47.2300
	0.256737	0.115741	0.627522
15	7.9463	7.8787	59.4394
	0.105579	0.104680	0.789741
16	0.4633	1.0322	11.7389
	0.035007	0.077994	0.886999
Component creation & consumption:			
	A	B	C
1	0.0000	0.0000	0.0000
2	-5.0069	-5.0069	5.0069
3	-3.1442	-3.1442	3.1442
4	-1.7405	-1.7405	1.7405
5	-0.8827	-0.8827	0.8827
6	-0.4238	-0.4238	0.4238
7	-0.1948	-0.1948	0.1948
8	-0.0875	-0.0875	0.0875
9	-0.0656	-0.0656	0.0656
10	-0.2088	-0.2088	0.2088
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000
Vapor/Liquid equilibrium ratios:			
	A	B	C
1	0.1073E+01	0.4406E+00	0.2699E+00
	0.1000E+01	0.1000E+01	0.1000E+01

Table A.5 (cont.)

2	0.1206E+01	0.4951E+00	0.3033E+00
	0.1206E+01	0.4951E+00	0.3033E+00
3	0.1241E+01	0.5094E+00	0.3121E+00
	0.1241E+01	0.5094E+00	0.3121E+00
4	0.1264E+01	0.5191E+00	0.3180E+00
	0.1264E+01	0.5191E+00	0.3180E+00
5	0.1277E+01	0.5243E+00	0.3212E+00
	0.1277E+01	0.5243E+00	0.3212E+00
6	0.1282E+01	0.5266E+00	0.3226E+00
	0.1282E+01	0.5266E+00	0.3226E+00
7	0.1282E+01	0.5267E+00	0.3226E+00
	0.1282E+01	0.5267E+00	0.3226E+00
8	0.1277E+01	0.5245E+00	0.3213E+00
	0.1277E+01	0.5245E+00	0.3213E+00
9	0.1262E+01	0.5184E+00	0.3176E+00
	0.1262E+01	0.5184E+00	0.3176E+00
10	0.1225E+01	0.5030E+00	0.3081E+00
	0.1225E+01	0.5030E+00	0.3081E+00
11	0.1262E+01	0.5182E+00	0.3175E+00
	0.1262E+01	0.5182E+00	0.3175E+00
12	0.1365E+01	0.5604E+00	0.3433E+00
	0.1365E+01	0.5604E+00	0.3433E+00
13	0.1627E+01	0.6683E+00	0.4094E+00
	0.1627E+01	0.6683E+00	0.4094E+00
14	0.2164E+01	0.8886E+00	0.5444E+00
	0.2164E+01	0.8886E+00	0.5444E+00
15	0.2880E+01	0.1183E+01	0.7245E+00
	0.2880E+01	0.1183E+01	0.7245E+00
16	0.3446E+01	0.1415E+01	0.8670E+00
	0.3446E+01	0.1415E+01	0.8670E+00
Reaction equilibrium ratios:			
	From thermo	From flows	
1	0.1248E+02	0.5425E+00	
2	0.1072E+02	0.1068E+01	
3	0.1033E+02	0.2523E+01	
4	0.1008E+02	0.4466E+01	
5	0.9946E+01	0.6427E+01	
6	0.9891E+01	0.7937E+01	
7	0.9889E+01	0.8897E+01	
8	0.9943E+01	0.9455E+01	
9	0.1010E+02	0.9682E+01	

Table A.5 (cont.)

10	0.1050E+02	0.8891E+01
11	0.1010E+02	0.7521E+01
12	0.9119E+01	0.7109E+01
13	0.7249E+01	0.9575E+01
14	0.4999E+01	0.2112E+02
15	0.3444E+01	0.7146E+02
16	0.2725E+01	0.3249E+03
Stream bubble/dew points:		
Stg	L bubble	V dew
1	378.9960	383.3805
2	383.3805	383.3805
3	384.4687	384.4687
4	385.1868	385.1868
5	385.5768	385.5768
6	385.7411	385.7411
7	385.7457	385.7457
8	385.5849	385.5849
9	385.1367	385.1367
10	383.9810	383.9810
11	385.1268	385.1268
12	388.1564	388.1564
13	395.1443	395.1443
14	407.0119	407.0119
15	419.6529	419.6529
16	428.0019	428.0019

Table A.6

	Feed	Converted	Overhead	Bottoms	Error
Solution 1					
A	12.63	-11.9527	0.6656	0.118	0.0001
B	12.82	-11.9527	0.0536	0.8138	0.0001
C		11.9527	0.0265	11.9262	<0.0001
Solution 2					
A	12.63	-11.8413	0.5231	0.2657	0.0001
B	12.82	-11.8412	0.0418	0.9369	<0.0001
C		11.8413	0.0203	11.8210	<0.0001
Solution 3					
A	12.63	-11.7548	0.4118	0.4633	0.0001
B	12.82	-11.7548	0.0329	1.0322	0.0001
C		11.7548	0.0160	11.7389	0.0001

Table A.7

	Reaction	Reboiler Duty	Condenser Duty	Error
Solution1	500.46	1803.21	2303.67	<0.01
Solution 2	495.80	1803.21	2299.01	<0.01
Solution 3	492.17	1803.21	2295.39	0.01

APPENDIX B.
REACTIVE DISTILLATION PROGRAM SOURCE CODE

MAIN PROGRAM

```

program scdist
!   Distillation computation by simultaneous correction method.
!   Revised main program
!   Written by: T. Mills
!   Date:   Feb 22, 2007   Revised 04/04/09
!
!
!   Specification statements:
implicit real*8 (a-h,o-z)
logical c_in, f_in, dflag, quit, first, feasible, rstart
integer ioflag, kthermo, nargs, nc, ns, method
!
!   Set parameter values
include "pgm_params.f"
parameter (dflag = .false.)
!
!   Define local storage areas
integer nnull, nnullv(nvmax)
real*8 tmpdfx(nvmax,nvmax), tmpfx(nvmax), tmpwrk(nvmax), solndet
!
!   Define common storage areas
include "cmn_params.f"
include "cmn_spec.f"
include "cmn_thermo.f"
!
!   Define i/o channels
data in_spc,out_spc,out_log,out_sol,in_cdata/ 10,11,12,13,14/
data out_pth/ 15/
!
!-----
!   Executable statements begin here
!
!   Check to see if input file specified on the command line, then
!   determine whether Problem spec. from file or console
nargs=iargc()
if (iargc() .ge. 1) then
  call getarg(1,psname_in)
else
  write (*,'(a$)') " Problem Specification file: "
  read (*,*) psname_in
  if ( psname_in .eq. ' ') stop
end if
inquire(file= psname_in, exist= f_in)
if (f_in) then
  open (in_spc, file = psname_in, status = "old" )
  rewind in_spc
else
  open (out_spc, file = psname_in )
  in_spc = 5
end if
!
first = .true.
do
  ! while ( .not. quit)
!-----

```

```

!   Get problem specification
call probspec(f_in,method,first,quit)
!   Exit if no new case to solve
if (quit) then
  write (*,*) "Termination signal given"
  stop
end if
!   Open files for log and problem solutions
open (out_log, file = pdname_out(1:LnBlnk(pdname_out))//'.log' )
open (out_sol, file = pdname_out(1:LnBlnk(pdname_out))//'.sol' )
if (method .eq. 2) open (out_pth, file =
&      pdname_out(1:LnBlnk(pdname_out))//'.pth' )
!
!-----
!   Set up initial profile guesses
call initprob
!
!-----
!   Initial profiles are set, now time to solve the problem.
write (*,*)
write (*,*)"Case: ",pdname_out
write (*,*)c_desc
write (*,*)
if (method .eq. 2) then !use homotopy continuation
  write(out_log,*)"Initial estimates..."
  call display(out_log)
  do j=1,ns*(2*nc+2) !Save initial starting point
    vars0(j) = vars(j)
  end do
  kstatus = 0
  maxits = 5000
  nsoln = 0; nturn = 0; nstart = 1; nfeas = 0; nstalls = 3
  do while (.true.)
    call solver(vars,ns*(2*nc+2),1.d-6,1.d-06,100,
&      kstatus,nits,error,out_log,out_pth)
    write (*,*)"Homotopy parm ",error," after ",nits," steps."
    write (out_log,*)"Homotopy parm ",error," after ",nits,
&      " steps."
    if (kstatus .lt. 100) nstalls = 3
    if (kstatus .eq. 1) then !Solution point found
      feasible = .true.
      do j=1,ns*(2*nc+2)
        if (mod(j,(2*nc+2)) .ne. (nc+2) .and. vars(j) .lt.
&          -1.d-20) feasible = .false.
      end do
      call funcv(vars(1),tmpfx,ns*(2*nc+2),nnull)
      call fdjac(vars(1),tmpfx,tmpdfx,ns*(2*nc+2),nvmax)
      call ludcmp(tmpdfx,ns*(2*nc+2),nvmax,nnullv,tmpwrk,
&      solndet,nnull)
      nsoln = nsoln + 1
      if (feasible) then
        nfeas = nfeas + 1
        write (*,*) "Feasible solution ",nfeas,":"
        write (out_sol,*) "Feasible solution ",nfeas,":"
        write (out_log,*) "Feasible solution ",nfeas,":"
        write (*,*) "Jacobian Determinant: ",solndet

```

```

write (out_sol,*) "Jacobian Determinant: ",solndet
write (out_log,*) "Jacobian Determinant: ",solndet
! write column profiles to console for excel
call display2
else
write (*,*) "Infeasible solution"
write (out_sol,*) "Infeasible solution:"
write (out_log,*) "Infeasible solution:"
write (*,*) "Jacobian Determinant: ",solndet
write (out_sol,*) "Jacobian Determinant: ",solndet
write (out_log,*) "Jacobian Determinant: ",solndet
end if
call display(out_sol)
call display(out_log)
kstatus = 1
else if (kstatus .eq. 2) then !Bifurcation found
write (*,*) "Bifurcation found..."
kstatus = 1
else if (kstatus .eq. 3) then !Trifurcation found
write (*,*) "Trifurcation found..."
kstatus = 1
else if (kstatus .eq. 4) then !Turning point found
nturn = nturn + 1
write (*,*) "Turning point ",nturn,":"
kstatus = 1
else if (kstatus .eq. 5) then !Starting point found
nstart = nstart + 1
write (*,*) "Starting point ",nstart,":"
rstart = .true. !test for repeated start point
do j=1,ns*(2*nc+2)
if (abs(vars0(j)-vars(j))/abs(vars0(j)) .ge. 1.d-6)
& rstart = .false.
end do
if (rstart) then
nstart = nstart - 1
write (*,*) "Path returns to original start point..."
write (out_log,*) "returns to original start point..."
exit
end if
kstatus = 1
else if (kstatus .eq. 10) then !Step count exceeded
kstatus = -1
else if (kstatus .eq. 20 .or. kstatus .eq. 21) then
! Path goes to infinity
write (*,*) "Path goes to infinity..."
write (out_log,*) "Path goes to infinity..."
exit
else if (kstatus .eq. 101) then !Step size too small
write (*,*) "Stopped due to small step size..."
write (out_log,*) "Stopped due to small step size..."
nstalls = nstalls - 1
if (nstalls .eq. 0) exit
kstatus = 1
else if (kstatus .eq. 102) then !Process is stagnant
write (*,*) "Stopped due to stagnation..."
write (out_log,*) "Stopped due to stagnation..."

```

```

    nstalls = nstalls - 1
    if (nstalls .eq. 0) exit
    kstatus = 1
  else if (kstatus .eq. 105) then  !Singular homotopy matrix
    write (*,*) "Homotopy matrix is singular..."
    write (out_log,*) "Homotopy matrix is singular..."
    exit
  else if (kstatus .eq. 106) then  !No tangent vector
    write (*,*) "Tangent vector not obtained..."
    write (out_log,*) "Tangent vector not obtained..."
    exit
  else if (kstatus .eq. 201) then  !Start point out of bounds
    write (*,*) "Start point out of domain..."
    write (out_log,*) "Start point out of domain..."
    exit
  else if (kstatus .eq. 202) then  !Base point out of bounds
    write (*,*) "Base point out of domain..."
    write (out_log,*) "Base point out of domain..."
    exit
  end if
  if (nits .ge. maxits) then
    write (*,*) "Maximum steps exceeded..."
    exit
  end if
end do
write (*,*)
write (*,*)"Solutions: ",nsoln," Feasible: ",nfeas
write (*,*)"Start points: ",nstart," Turn points: ",nturn
write (*,*)
write (*,*)
else
  write(out_log,*)"Initial estimates..."
  call display(out_log)
  call nsolver(vars(1),ns*(2*nc+2),1.d-6,1.d-06,100,
&      kstatus,nits,error,out_log,out_sol)
  if (kstatus .lt. 0) then
    write(*,*)"Failed to converge..."
  else
    write(*,*)"Solution found..."
  end if
  write (*,*)"Error was ",error," after ",nits," iterations."
  write (out_log,*)"Error was ",
&      error," after ",nits," iterations."
  call display(out_sol)
  write(out_log,*)"Iterated results..."
  call display(out_log)
!
end if
!
close (out_log)
close (out_sol)
if (method .eq. 2) close (out_pth)
!
end do
stop
end

```


!

```

=====
      subroutine probspec(f_in,method,first,quit)
!      Subroutine to get problem specification from console or file
!      Parameters:
!          f_in      logical, TRUE if input to be from file
!          in_spc    integer, channel # for input
!          out_spc   integer, channel # for saving problem spec
!          in_cdata  integer, channel # for component props file
!          kstatus   integer, ?
!
!      Specification statements:
implicit real*8 (a-h,o-z)
logical f_in, c_in, dflag, quit, first, cdflag
integer ioflag, kthermo, nargs, nc, ns, method
character*80 ans
character*24 cname_in, formula, casno, cdfile
character*6 command
logical P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,P11,P12,P13,P14,P15,P16,
& P17,P18,P21,P31
save P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,P11,P12,P13,P14,P15,P16,
& P17,P18,P21,P31
!
!      Set parameter values
include "pgm_params.f"
!
!      Define common storage areas
include "cmn_params.f"
include "cmn_cspec.f"
include "cmn_thermo.f"
include "cmn_hsparms.f"
!
common /rxn/ sprxk
save /hsparms/
!
quit = .true.
rgas=8.314510d0                !Energy units are joules
!-----
!      Set default values if first call
if (first) then
  P1=.false.;P2=.false.;P3=.false.;P4=.false.;P5=.false.
  P6=.false.;P7=.false.;P8=.false.;P9=.false.;P10=.false.
  P11=.false.;P12=.false.;P13=.false.;P14=.false.;P15=.false.
  P16=.false.;P17=.false.;P18=.false.;P21=.false.;P31=.false.
  ns=0; nc=0; kcond=1; method=1; kthermo=1
  kspec(1)=0;kspec(2)=0;xspec(1)=0.d0;xspec(2)=0.d0
  pdname_out=' '; c_desc=' '
  do i=1,ncmax
    cname(i)=' ';rxsto(i)=0.d0
  end do

```

```

do j=1,nsmax
  p(j)=0.d0;fd_pres(j)=0.d0;fd_temp(j)=0.d0
  q(j)=0.d0;sd_v(j)=0.d0;sd_l(j)=0.d0;stg_mv(j)=1.d0
  rxeff(j)=0.d0;holdupl(j)=0.d0
  do i=1,ncmax
    fd_ctot(i,j)=0.d0
  end do
end do
rxcoord = 0.d0
scinit = 1.d0
sprxk = 0.d0
idom = 0; ihom = 1; dir = 1.d0; dso = 1.d-01
dsmin = 1.d-20; dsmax = 5.d04; xmax = 1.d05
ecorc = 1.d-04; ecorb = 1.d-06; edet = 5.d-01
esol = 1.d-04; ebif = 1.d-04; etur = 1.d-06
esta = 1.d-04; easy = 1.d-06; maxdet = 5
minasy = 5; maxasy = 20
first = .false.
end if
!-----
!   Branch on whether input from file (f_in = .true.) or console
!   if (.not. f_in) then
!
!-----
!   Get Case Identification string
!   write (*,(/a$)) "Case ID String: "
!   read (in_spc,(a)) pdname_out
!   if (pdname_out .eq. ' ') return
!   write (out_spc,*) "P1  "//pdname_out !write to pspec file
!   P1=.true.
!
!-----
!   Get Case Description String
!   write (*,(a$)) "Case Description: "
!   read (in_spc,(a)) c_desc
!   if (c_desc .eq. ' ') return
!   write (out_spc,(4a)) " P2  ",c_desc(1:len_trim(c_desc)),
&
!                               !write to pspec file
!   P2=.true.
!
!-----
!   Get Solution Algorithm   (default = Newton)
!   write (*,(a$)) "Solution Algorithm (1 = Newton; "//
&   "2 = Homotopy): "
!   read (in_spc,*) method
!   if ( method .lt. 1 .or. method .gt. 2) method = 1
!   write (out_spc,*) "P3  ",method !write to probspec file
!   P3=.true.
!
!-----
!   Get Thermodynamic model to use: (default = Peng-Robinson)
!
!   write (*,(a$)) "Thermo model (1: Peng-Robinson, "//
&   "2: SRK, 3: RK, 4: VdW): "
!   read (in_spc,*) kthermo

```

```

if (kthermo .lt. 1 .or. kthermo .gt. 4) kthermo = 1 !PR default
write (out_spc,*) "P4  ",kthermo !write to probspec file
P4=.true.
!
!-----
! Get component list / component properties
!
write (*,(a$)) "Component data file: "
read (in_spc,*) cdfile
inquire (file=cdfile, exist= cdflag)
if (.not. cdflag) return
open (in_cdata, file = cdfile )
nc=0
write (*,(a))
do i=1,ncmax
write (*,(a$)) "Component name: "
read (in_spc,(a)) cname_in
if ( LnBlnk(cname_in) .eq. 0) exit
nc=nc+1
rewind in_cdata
! Find component in the database
do
read (in_cdata,*,IOSTAT=ioflag)icomp, cname(nc), formula,
& casno, cmolwt(nc), tmelt(nc), tboil(nc), tcrit(nc),
& pcrit(nc), vcrit(nc), zcrit(nc), acfac(nc), delhf(nc),
& delgf(nc), tcpmin(nc), tcpmax(nc), cpa0(nc), cpa1(nc),
& cpa2(nc), cpa3(nc), cpa4(nc), ieq, vpa(nc), vpb(nc),
& vpc(nc), pvpmin(nc), pvpmax(nc), tvpmin(nc),
& tvpmax(nc)
if (cname(nc) .eq. cname_in ) exit
if (ioflag .ne. 0) then
write (*, '(2a)') "Component not found: ", cname_in
nc=nc-1
exit
end if
end do
end do
close (in_cdata)
if (nc .eq. 0) return ! Stop if no components specified
! Write component data file name, nc, and component ID's to file
write (out_spc,*) "P5  ",nc,
& ' '//cdfile(1:Len_Trim(cdfile))//""
do i=1,nc
write (out_spc,*)""//cname(i)(1:Len_Trim(cname(i))//""
end do
P5=.true.
!
!-----
! Get no. stages - stop if blank or out of range
!
write (*,(/a$)) "No. stages (Including "//
& "condenser and reboiler): "
read (in_spc,*) ns
if (ns .le. 0 .or. ns .gt. nsmax) return
write (out_spc,*) "P6  ",ns !write to probspec file
P6=.true.

```

```

!
!-----
!   Get Condenser type: Total or partial - default to total
!
!   write (*,(a$)) "Condenser type (1: total, "//
&       "2: partial): "
!   read (in_spc,*) kcond
!   if (kcond .ne. 2) kcond = 1
!   write (out_spc,*) "P7  ",kcond !write to probspec file
!   P7=.true.
!
!-----
!   Get top specification
!   write (*,(a$)) "Top specification"//
&       "(1:Qc, 2:L/D, 3:D/F, 4:Di/Fi, 5:Tc): "
!   read (in_spc,*) kspec(1)
!   write (*,(a$)) "Value, (i): "
!   if (kspec(1) .eq. 4) then
!       read (in_spc,*) xspec(1),ispec(1)
!   else
!       read (in_spc,*) xspec(1)
!       ispec(1) = 0
!   end if
!
!                               !write to probspec file
!   write (out_spc,*) "P8  ",kspec(1),xspec(1),ispec(1)
!   P8=.true.
!   Set condenser duty if specified
!   if (kspec(1) .eq. 1) q(1) = xspec(1)
!
!-----
!   Get bottom specification
!   write (*,(a$)) "Bottom specification"//
&       "(6:Tr, 7:Bi/Fi, 8:B/F, 9:V/B, 10:Qr): "
!   read (in_spc,*) kspec(2)
!   write (*,(a$)) "Value, (i): "
!   if (kspec(2) .eq. 7) then
!       read (in_spc,*) xspec(2),ispec(2)
!   else
!       read (in_spc,*) xspec(2)
!       ispec(2) = 0
!   end if
!
!                               !write to probspec file
!   write (out_spc,*) "P9  ",kspec(2),xspec(2),ispec(2)
!   P9=.true.
!   Set reboiler duty if specified
!   if (kspec(2) .eq. 10) q(ns) = xspec(2)
!
!-----
!   Get condenser pressure and stage delta
!
!   write (*,(a$)) "Condenser pressure, "//
&       "and per-stage delta P: "
!   read (in_spc,*) p(1), xtemp
!   write (out_spc,*) "P10  ",p(1), xtemp
!   P10=.true.
!

```

```

! Set stage pressures
  do j=2,ns
    p(j) = p(j-1) + xtemp
  end do
!
!-----
! Get column feed specs
!
  do j=1,ns
    ! Initialize feed storage areas
    fd_temp(j)=0.d0; fd_pres(j)=0.d0; fd_enth(j)=0.d0
    fd_totl(j)=0.d0; fd_psi(j)=0.d0; kfeed(j)=0
    do i=1,nc
      fd_liq(i,j)=0.d0; fd_vap(i,j)=0.d0; fd_ctot(i,j)=0.d0
    end do
  end do
  nf = 0
  !Count number of feeds
!
  write (*,'(a)') "Feed Types ==> "//
&      "(1: BP liquid, 2: DP vapor, 3: Flash at spec. T"
  do
    write (*,'(a$)') "Stage, type, P, (T): "
    read (in_spc,'(a80)') ans
    if ( ans .eq. ' ') exit
    read (ans,*) j
    if (j .lt. 1 .or. j .gt. ns ) exit
    if (kfeed(j) .ne. 0) then
      write(*,*)"Feed at stage ",j," already specified."
      cycle
    end if
    read (ans,*) j, kfeed(j)
    if (kfeed(j) .eq. 3) then
      read (ans,*) j, kfeed(j), fd_pres(j), fd_temp(j)
    else
      read (ans,*) j, kfeed(j), fd_pres(j) ; fd_temp(j) = 0.d0
    end if
    write (*,'(a)') "Feed molar flows: "
    do i=1,nc,5
      ic = nc; if (ic .gt. i+4) ic = i+4
      write (*,'(5a16)') (cname(ii),ii=i,ic)
      read (in_spc,*) (fd_ctot(ii,j),ii=i,ic)
    end do
    nf = nf+1
  end do
!
! Write feed info to case data file
  write (out_spc,*) "P11 ",nf
  do j=1,ns
    if (kfeed(j) .ne. 0) write (out_spc,*) j,kfeed(j),
&      fd_pres(j),fd_temp(j), (fd_ctot(i,j),i=1,nc)
  end do
  P11=.true.
!
!-----
! Get stage heat duties (default = 0)
!
  do j=1,ns

```

```

    q(j)=0.d0
end do
nq = 0          !count heat duty stages
do
  write (*,'(a$)') "Heat duty stage, value: "
  read (in_spc,'(a80)') ans
  if ( ans .eq. ' ') exit
  read (ans,*) j
  if (j .lt. 1 .or. j .gt. ns ) exit
  if (q(j) .ne. 0.d0) then
    write (*,*)"Stage ",j," duty already specified..."
    cycle
  end if
  read (ans,*) j, q(j)
  nq = nq+1
end do
! write heat duty stage info to case data file
if (nq .ne. 0) then
  write (out_spc,*) "P12 ",nq
  do j=1,ns
    if (q(j) .ne. 0.d0) write (out_spc,*),q(j)
  end do
end if
P12=.true.
!
!-----
! Get sidedraw values (liquid or vapor)
!
  do j=1,ns
    sd_l(j)=0.d0; sd_v(j)=0.d0
  end do
  nq = 0          !Count sidedraw stages
  do
    write (*,'(a$)') "Sidedraw stage, "//
    & "type(1: liquid, 2: vapor), value: "
    read (in_spc,'(a80)') ans
    if ( ans .eq. ' ') exit
    read (ans,*) j
    if (j .lt. 1 .or. j .gt. ns ) exit
    read (ans,*) j, ktemp, xtemp
    if (ktemp .eq. 2) then
      sd_v(j) = xtemp
    else
      sd_l(j) = xtemp
    end if
    nq = nq+1
  end do
! Write sidedraw info to case data file
if (nq .ne. 0) then
  write (out_spc,*) "P13 ",nq
  do j=1,ns
    if (sd_l(j) .ne. 0.d0) write (out_spc,*),j," 1",sd_l(j)
    if (sd_v(j) .ne. 0.d0) write (out_spc,*),j," 2",sd_v(j)
  end do
end if
P13=.true.

```

```

!
!-----
! Get stage murphree efficiencies (default = 1.)
!
  do j=1,ns
    stg_mve(j)=1.d0
  end do
  nq = 0          !count stages with MVE spec
  do
    write (*,'(a$)') "Murphree efficiency stage1, "//
& "stage2, value: "
    read (in_spc,'(a80)') ans
    if ( ans .eq. ' ') exit
    read (ans,*) j1, j2, xtemp
    if (j1 .gt. j2) then
      ktemp=j1; j1=j2; j2=ktemp
    end if
    if (j1 .lt. 1 .or. j2 .gt. ns ) exit
    do j=j1,j2
      stg_mve(j)=xtemp
    end do
    nq = nq+j2-j1+1
  end do
! Write MVE info to case data file
  if (nq .ne. 0) then
    write (out_spc,*) "P14 ",nq
    do j=1,ns
      if (stg_mve(j) .ne. 1.d0) write (out_spc,*)j,stg_mve(j)
    end do
  end if
  P14=.true.
!
!-----
! Get Stoichiometric coefficients for reaction
! reactants (neg); products (pos); inerts (zero); default = 0
!
  do i=1,nc
    rxsto(i) = 0
  end do
  write (*,'(a)') "Reaction stoichiometric coeffs: "
  do i=1,nc,5
    ic = nc; if (ic .gt. i+4) ic = i+4
    write (*,'(5a16)') (cname(ii),ii=i,ic)
    read (in_spc,*) (rxsto(ii),ii=i,ic)
  end do
  write (out_spc,*) "P15 ",(rxsto(i),i=1,nc)
  P15=.true.
!
!-----
! Get per-stage fractional approach to reaction equilibrium
! default = 0.
!
  do j=1,ns
    rxeff(j)=0.d0
  end do
  nq = 0          !Count rxn efficiency stages

```

```

do
  write (*,'(a$)') "Reaction efficiency stage1, "//
&   "stage2, value: "
  read (in_spc,'(a80)') ans
  if ( ans .eq. ' ') exit
  read (ans,*) j1, j2, xtemp
  if (j1 .gt. j2) then
    ktemp=j1; j1=j2; j2=ktemp
  end if
  if (j1 .lt. 1 .or. j2 .gt. ns ) exit
  do j=j1,j2
    rxeff(j)=xtemp
  end do
  nq = nq+j2-j1+1
end do
! Write Reaction efficiency info to case data file
if (nq .ne. 0) then
  write (out_spc,*) "P16 ",nq
  do j=1,ns
    if (rxeff(j) .ne. 0.d0) write (out_spc,*)j,rxeff(j)
  end do
end if
P16=.true.
!
! Write case termination signal
write (out_spc,*) "XC"
!-----
! Branch to here if input from file
else
  pdname_out = ' '; c_desc = ' ' !Clear filename & description
  P1 = .false.
  do
    read (in_spc,'(a80)',IOSTAT=ioflag) ans
    if (ioflag .ne. 0) exit
    read (ans,*) command
    if (command .eq. "XC") exit
    if (command .eq. "P1") then !Case ID string
      read (ans,*) command, pdname_out
      if (pdname_out(1:1) .eq. "")
&       pdname_out=pdname_out(2:len_trim(pdname_out))
      P1 = .true.
    else if (command .eq. "P2") then !Case Description
      read (ans,*) command, c_desc
      if (c_desc(1:1) .eq. "")
&       c_desc=c_desc(2:len_trim(c_desc))
      P2 = .true.
    else if (command .eq. "P3") then !Case Soln algorithm
      read (ans,*) command, method
      P3 = .true.
    else if (command .eq. "P4") then !Case Thermo model
      read (ans,*) command, kthermo
      P4 = .true.
    else if (command .eq. "P5") then !Case Components
      read (ans,*) command, nc, cdfile
      if (cdfile(1:1) .eq. "")
&       cdfile=cdfile(2:len_trim(cdfile))

```



```

inquire (file=cdf, exist=cdf)
if (.not. cdf) then
  quit=.true.; return
end if
open (in_cdata, file=cdf)
do i=1,nc
  read (in_spc,*) cname_in
  rewind in_cdata !find component in database
  do
    read (in_cdata,*,IOSTAT=iostat)comp, cname(i),
&    formula, casno, cmolwt(i), tmelt(i), tboil(i),
&    tcrit(i), pcrit(i), vcrit(i), zcrit(i),
&    acfac(i), delhf(i), delgf(i), tcpmin(i),
&    tcpmax(i), cpa0(i), cpa1(i), cpa2(i), cpa3(i),
&    cpa4(i), ieq, vpa(i), vpb(i), vpc(i),
&    pvpmin(i), pvpmax(i), tvpmin(i), tvpmax(i)
    if (iostat .ne. 0) then
      quit=.true.; return
    end if
    if (cname(i) .eq. cname_in) exit
  end do
end do
P5 = .true.
else if (command .eq. "P6") then !Case no. stages
  read (ans,*) command, ns
  P6 = .true.
else if (command .eq. "P7") then !Case Condenser type
  read (ans,*) command, kcond
  P7 = .true.
else if (command .eq. "P8") then !Case Top spec
  read (ans,*) command, kspec(1),xspec(1),ispec(1)
  if (kspec(1) .eq. 1) q(1)=xspec(1)
  P8 = .true.
else if (command .eq. "P9") then !Case Bottom spec
  read (ans,*) command, kspec(2),xspec(2),ispec(2)
  if (kspec(2) .eq. 10) q(ns)=xspec(2)
  P9 = .true.
else if (command .eq. "P10") then !Case Cond P & stg delta
  read (ans,*) command, p(1),xtemp
  do j=2,ns
    p(j)=p(j-1)+xtemp
  end do
  P10 = .true.
else if (command .eq. "P11") then !Case Feed spec
  do j=1,ns !Clear old spec
    kfeed(j)=0;fd_pres(j)=0.d0;fd_temp(j)=0.d0
  end do
  do i=1,nc
    fd_tot(i,j)=0.d0
  end do
  read (ans,*) command, nf
  do k=1,nf
    read (in_spc,*)j,kfeed(j),fd_pres(j),fd_temp(j),
&    (fd_tot(i,j),i=1,nc)
  end do
  P11 = .true.

```

```

else if (command .eq. "P12") then !Case Heat duties
  read (ans,*) command, j1, j2, xtemp
  if (j1 .gt. j2) then
    jtemp = j1; j1 = j2; j2 = jtemp
  end if
  jtemp = 1; if (kspec(1) .eq. 1) jtemp = 2
  if (j1 .lt. jtemp) j1 = jtemp
  jtemp = ns; if (kspec(2) .eq. 10) jtemp = ns-1
  if (j2 .gt. jtemp) j2 = jtemp
  do j=j1,j2
    q(j) = xtemp
  end do
  P12 = .true.
else if (command .eq. "P13") then !Case Sidedraws
  do j=1,ns !Clear old spec
    sd_v(j)=0.d0; sd_l(j)=0.d0
  end do
  read (ans,*) command, nq
  do k=1,nq
    read (in_spc,*)j,ktemp,xtemp
    if (ktemp .eq. 2) then
      sd_v(j) = xtemp
    else
      sd_l(j) = xtemp
    end if
  end do
  P13 = .true.
else if (command .eq. "P14") then !Case Murphree effs
  read (ans,*) command, j1, j2, xtemp
  if (j1 .gt. j2) then
    jtemp = j1; j1 = j2; j2 = jtemp
  end if
  if (j1 .lt. 1) j1 = 1
  if (j2 .gt. ns) j2 = ns
  do j=j1,j2
    stg_mve(j) = xtemp
  end do
  P14 = .true.
else if (command .eq. "P15") then !Case Stoich coeffs
  read (ans,*) command, (rxsto(i),i=1,nc)
  P15 = .true.
else if (command .eq. "P16") then !Case Rxn effs
  read (ans,*) command, j1, j2, xtemp
  if (j1 .gt. j2) then
    jtemp = j1; j1 = j2; j2 = jtemp
  end if
  if (j1 .lt. 1) j1 = 1
  if (j2 .gt. ns) j2 = ns
  do j=j1,j2
    rxeff(j) = xtemp
  end do
  P16 = .true.
else if (command .eq. "P17") then !Spec Reaction K
  read (ans,*) command, sprxk
  P17 = .true.
else if (command .eq. "P18") then !Stage molar holdups

```

```

read (ans,*) command, j1, j2, xtemp
if (j1 .gt. j2) then
  jtemp = j1; j1 = j2; j2 = jtemp
end if
if (j1 .lt. 1) j1 = 1
if (j2 .gt. ns) j2 = ns
do j=j1,j2
  holdupl(j) = xtemp
end do
P16 = .true.
else if (command .eq. "P21") then !Spec homo solver parms
  read (ans,*) command, nq
  P18 = .true.
  if (nq .eq. 1) read (ans,*) command, nq, dir
  if (nq .eq. 2) read (ans,*) command, nq, dso
  if (nq .eq. 3) read (ans,*) command, nq, dsmin
  if (nq .eq. 4) read (ans,*) command, nq, dsmax
  if (nq .eq. 5) read (ans,*) command, nq, xmax
  if (nq .eq. 6) read (ans,*) command, nq, ecorc
  if (nq .eq. 7) read (ans,*) command, nq, ecorb
  if (nq .eq. 8) read (ans,*) command, nq, edet
  if (nq .eq. 9) read (ans,*) command, nq, esol
  if (nq .eq. 10) read (ans,*) command, nq, ebif
  if (nq .eq. 11) read (ans,*) command, nq, etur
  if (nq .eq. 12) read (ans,*) command, nq, esta
  if (nq .eq. 13) read (ans,*) command, nq, easy
  if (nq .eq. 14) read (ans,*) command, nq, idom
  if (nq .eq. 15) read (ans,*) command, nq, ihom
  if (nq .eq. 16) read (ans,*) command, nq, maxdet
  if (nq .eq. 17) read (ans,*) command, nq, minasy
  if (nq .eq. 18) read (ans,*) command, nq, maxasy
else if (command .eq. "P31") then !input for simple thermo
  read (ans,*)command,alpha,tb1,delhv,delhr,cpl,cpv,
&      rxntref, rxnke0,rxkf0,rxefwd
  kinetic = .true. !default to kinetic reaction model
  xtemp=0.d0 !set up to allocate delhr
  do i=1,nc
    if (rxsto(i) .gt. 0.d0) xtemp=xtemp+rxsto(i)
  end do
  do i=1,nc
    cpa0(i)=cpl; cpa1(i)=cpv; delhf(i)=0.d0
    if (i .eq. 1) then !set component boiling points
      tboil(i)=tb1
    else
      tboil(i)=delhv/(delhv/tboil(i-1) - rgas*log(alpha))
    end if
    vpb(i) = delhv / rgas
    vpa(i) = 1.3163d-02 + vpb(i) / tboil(i)
    if (rxsto(i) .gt. 0.d0) delhf(i)=delhr*rxsto(i)/xtemp
  end do
  rxeeql = delhr !set constants for rxn equilibrium K
  if (rxkf0 .eq. 0.d0) kinetic = .false.
else if (command .eq. "P32") then !input for Antoine eq
  read (ans,*)command,i,vpa(i),vpb(i)
  tboil(i) = vpb(i) / ( vpa(i) - 1.3163d-02)
else if (command .eq. "P33") then !rx coord for init

```

```

        read (ans,*)command,rxcoord
    else if (command .eq. "P34") then !scale factor for init
        read (ans,*)command,scinit
    end if
end do
end if
!
! Determine whether or not to run a case
quit = .not. (P1 .and. P5 .and. P6 .and. P8 .and. P9 .and. P10
& .and. P11)
!
return
end
! End of problem specification input
!-----

```

```

=====
subroutine initprob
! Subroutine to set up initial solution estimates
!
!
! Specification statements:
implicit real*8 (a-h,o-z)
logical c_in, dflag, quit, trefset
integer ioflag, kthermo, nargs, nc, ns
character*80 ans
character*24 cname_in, formula, casno
!
! Set parameter values
include "pgm_params.f"
parameter (dflag = .false.)
!
! Define local storage areas
real*8 xnull, fvnull(ncmax),flnull(ncmax)
real*8 zfeed(ncmax), xfeed(ncmax), yfeed(ncmax),fctotal(ncmax),
& rxlim(ncmax),bulk_l(nsmax),bulk_v(nsmax),
& f(nsmax),g(ncmax,nsmax),vlek(ncmax,nsmax),
& fvalues(0:nvmax),fftf,ffvf
!
! Define common storage areas
include "cmn_params.f"
include "cmn_cspec.f"
include "cmn_thermo.f"
!
common /rxn/ sprxk
!-----
! Clear the feed variables
ffvf=0.d0; fftf=0.d0
tref=tboil(1)
do j=1,ns

```

```

    fd_enth(j)=0.d0; fd_totl(j)=0.d0; fd_psi(j)=0.d0
    do i=1,nc
        fd_liq(i,j)=0.d0; fd_vap(i,j)=0.d0
        fctotal(i) = 0.d0
    end do
end do
jfeed = 0; jfeedwt = 0
!
! Flash the feeds, or compute their temperatures
do j=1,ns
    if (kfeed(j) .ne. 0) then
        do i=1,nc
            zfeed(i) = fd_ctot(i,j)
        end do
        call flash(kfeed(j),zfeed,fd_temp(j),fd_pres(j),p(j),
&             xfeed,yfeed,fd_enth(j),fd_totl(j),fd_psi(j))
        do i=1,nc
            fd_liq(i,j) = xfeed(i)
            fd_vap(i,j) = yfeed(i)
            ffvf = ffvf + yfeed(i)
            fctotal(i) = fctotal(i) + zfeed(i)
            ffff = ffff + zfeed(i)
        end do
        jfeed = jfeed + int(fd_totl(j))
        jfeedwt = jfeedwt + j*int(fd_totl(j))
    end if
end do
ffvf = ffvf / ffff      !Fraction of total feed as vapor
jfeed = jfeedwt / jfeed  !"Average" feed stage
!
! React composite feed to start
if (rxcoord .ge. 0.d0 .and. rxcoord .le. 1.d0) then
    !Reaction coordinate is specified
    do i=1,nc      !Compute feed over stoich coeff for all cpds
        rxlim(i) = 0.d0
        if(rxsto(i) .ne. 0.d0) rxlim(i) = -fctotal(i)/rxsto(i)
    end do
    rxflim = 0.d0; rxblim = 0.d0
    do i=1,nc      !find limiting extents
        rxblim = min(rxblim,rxlim(i))
        rxflim = max(rxflim,rxlim(i))
    end do
    do i=1,nc
        if (rxsto(i) .gt. 0) rxblim = max(rxblim,rxlim(i))
        if (rxsto(i) .lt. 0) rxflim = min(rxflim,rxlim(i))
    end do
    rxext = rxcoord*(rxflim - rxblim) + rxblim !Reaction extent
else
    !Approach to equilibrium is specified
    if (rxcoord .ge. 1.d0 .or. rxcoord .le. -1.d0) rxcoord = -1.d0
        !limit values to 0>x>=-1
    avpres = (p(1) + p(ns))/2.d0      !Est avg P
    call flash(4,fctotal,avtemp,avpres,avpres,
&             flnull,fvnull,xnull,xnull,ffvf) !Est avg T
    rxext = rxex(fctotal,avtemp,avpres,nc,0,0) !Reaction extent
    rxext = -rxcoord * rxext

```

```

end if
fctsum = 0.d0
do i=1,nc
  fcttotal(i) = fcttotal(i) + rxsto(i)*rxext
  fctsum = fctsum + fcttotal(i)      !sum of reacted feed
end do
do i=1,nc
  fcttotal(i) = fcttotal(i)/fctsum  !convert to mol fractions
end do
!
! Set initial reaction extent estimates
do j=1,ns
  vars((j-1)*(2*nc+2)+nc+2) = 0.d0
!  vars((j-1)*(2*nc+2)+nc+2) = rxext
end do
!
! Set up initial profile guesses
!
! Approximate D/F and L1/D
do j=1,2                                !D/F
  if (kspec(j) .eq. 3 .or. kspec(j) .eq. 4) then
    fdf = xspec(j)
    exit
  else if (kspec(j) .eq. 7 .or. kspec(j) .eq. 8) then
    fdf = 1.d0 - xspec(j)
    exit
  else
    fdf = 0.5d0
  end if
end do
do j=1,2                                !L/D
  if (kspec(j) .eq. 2) then
    flv = xspec(j)
    exit
  else if (kspec(j) .eq. 9) then
    flv = xspec(j) + ffvf - fdf
    exit
  else if (kspec(j) .eq. 11) then
    flv = xspec(j) / (fftf*fdf)
    exit
  else if (kspec(j) .eq. 12) then
    flv = (xspec(j)/fftf + ffvf - fdf) / fdf
    exit
  else
    flv = 2.0d0
  end if
end do
!
! Get average column pressure
avpres = (p(1) + p(ns))/2.d0          !Avg pressure
!
! Estimate temperature profile
!
vars(nc+1)=bubpt(fcttotal,p(1)) !Condenser temp = BP of total feed
vars((ns-1)*(nc*2+2)+nc+1)=dewpt(fcttotal,p(ns))!Reboiler temp
!                                     Linear profile

```

```

xtemp = (vars((ns-1)*(nc*2+2)+nc+1) - vars(nc+1))/(ns - 1)
do j=2,ns
  jt = (j-1)*(2*nc+2)+nc+1
  vars(jt) = vars(jt-(2*nc+2)) + xtemp
end do
!
!   Tref = avg temperature
tref = (vars(nc+1) + vars((ns-1)*(nc*2+2)+nc+1))/2.d0
!
!   Set bulk flow profiles, assuming constant overflow
totv(1) = fdf * fctsum      !D
totl(1) = flv * totv(1)
do j=2,ns
  totv(j) = totv(j-1)
  if (j .eq. 2) totv(j) = totv(j-1) + totl(j-1)
  if (kfeed(j-1) .ne. 0) totv(j)=
&      totv(j-1)-fd_totl(j-1)*fd_psi(j-1)
  totl(j) = totl(j-1)
  if (kfeed(j) .ne. 0) totl(j)=
&      totl(j-1)+fd_totl(j)*(1.d0-fd_psi(j))
end do
totl(ns) = fctsum - totv(1)
!
!   Set component flow profiles
do j=1,ns
  jv=(j-1)*(2*nc+2); jl=jv+nc+2
  do i=1,nc
    vars(jv+i) = totv(j) * fcttotal(i) * scinit
    vars(jl+i) = totl(j) * fcttotal(i) * scinit
  end do
end do
!
  return
end
!-----
!   End of problem initialization
!=====
subroutine display(kchnl)
!   Write distillation problem/solution description to console or
!   log file.
!
!   INPUTS:
!     kchnl:  i/o channel to use for output
!
implicit real*8 (a-h,o-z)
include "pgm_params.f" !Program parameters
include "cmn_params.f" !No. stages and No. components
include "cmn_cspec.f" !Column specifications
include "cmn_thermo.f" !Thermodynamic data
!
common /rxn/ sprxk
real*8 xtemp(ncmax,nsmax)
!-----
!   Show case ID and Description
write (kchnl,*)

```

```

write (kchnl,*)"Case ID: ", pdname_out
write (kchnl,'(a)')c_desc
!
!-----
! Show thermodynamic model used
! write (kchnl,'(a$)')"Thermodynamic model: "
! if (kthermo .eq. 4) then
!   write (kchnl,'(a)')"Van der Waals"
! else if (kthermo .eq. 3) then
!   write (kchnl,'(a)')"Redlich-Kwong"
! else if (kthermo .eq. 2) then
!   write (kchnl,'(a)')"Soave-Redlich-Kwong"
! else
!   write (kchnl,'(a)')"Peng-Robinson"
! end if
!
!-----
! Show no. stages, no. components, and condenser type
write (kchnl,'(2(a,i3),a$)')"Stages: ",ns," Components: ",nc,
& " Condenser: "
if (kcond .eq. 2) then
  write (kchnl,'(a)')"Partial"
else
  write (kchnl,'(a)')"Total"
end if
!
!-----
! Show component data (simplified system)
write(kchnl,'(a)')"Component information:"
write(kchnl,'(a)')"      alpha   Hv   Hr"//
&"   CpL   CpV   Krx"
write(kchnl,'(8x,6f10.2)')alpha,delhv,delhr,cpl,cpv,rxnke0
write(kchnl,'(a)')"      nu   Tb   CpL"//
&"   CpV   Hr"
do i=1,nc
  write(kchnl,'(2x,a6,5f10.2)')cname(i),rxsto(i),tboil(i),cpa0(i),
&   cpa1(i),delhf(i)
end do
!
!-----
! Show material balance and energy balance specifications
do i=1,2
  if (kspec(i) .eq. 3) then
    write(kchnl,*)"Overhead recovery (D/D+B): ",xspec(i)
  else if (kspec(i) .eq. 8) then
    write(kchnl,*)"Bottoms recovery (B/D+B): ",xspec(i)
  else if (kspec(i) .eq. 4) then
    write(kchnl,*)"Overhead recovery (di/di+bi): ",xspec(i),
& " for ",cname(ispec(i))
  else if (kspec(i) .eq. 7) then
    write(kchnl,*)"Bottoms recovery (b1/di+bi): ",xspec(i),
& " for ",cname(ispec(i))
  else if (kspec(i) .eq. 2) then
    write(kchnl,*)"Reflux ratio (L/D): ",xspec(i)
  else if (kspec(i) .eq. 5) then
    write(kchnl,*)"Condenser temperature: ",xspec(i)

```



```

else if (kspec(i) .eq. 1) then
  write(kchnl,*)"Condenser heat duty: ",xspec(i)
else if (kspec(i) .eq. 9) then
  write(kchnl,*)"Boilup ratio (V/B): ",xspec(i)
else if (kspec(i) .eq. 6) then
  write(kchnl,*)"Reboiler temperature: ",xspec(i)
else if (kspec(i) .eq. 10) then
  write(kchnl,*)"Reboiler heat duty: ",xspec(i)
end if
end do
!
!-----
! Show reaction equilibrium constant if specified
if (sprxk .ne. 0.d0) write(kchnl,*)"Specified Reaction K: ",sprxk
!
!-----
! Show column feeds
write(kchnl,*)"Feeds:"
do j=1,ns
  if (fd_temp(j) .ne. 0) then
    write(kchnl,1010)"Stg: ",j," Temp(K): ",fd_temp(j),
    & " Press(bar): ",fd_pres(j),
    & " Enthalpy(J): ",fd_enth(j)
1010 format(a,i3,a,f9.4,a,f9.4,a,f9.2)
    write(kchnl,*)" " " Liquid Vapor"
    do i=1,nc
      write(kchnl,'(a12,2f10.4)')cname(i),fd_liq(i,j),
      & fd_vap(i,j)
    end do
  end if
end do
!
!-----
! Show Condenser and Reboiler duties.
qc = (- fd_enth(1) - hstream(vars(2*nc+3),vars(3*nc+3),p(2),nc,1)
& + (1.d0+sd_v(1))*hstream(vars(1),vars(nc+1),p(1),nc,kcond-1)
& + (1.d0+sd_l(1))*hstream(vars(nc+3),vars(nc+1),p(1),nc,0))
& /1.d3
write(kchnl,*)"Condenser duty(kJ): ",qc
jxr=(ns-1)*(2*nc+2); jxrm1=jxr-(2*nc+2)
qr = (- fd_enth(ns)
& - hstream(vars(jxrm1+nc+3),vars(jxrm1+nc+1),p(ns-1),nc,0)
& + (1.d0+sd_v(1))*hstream(vars(jxr+1),vars(jxr+nc+1),p(ns),nc,1)
& + (1.d0+sd_l(1))
& *hstream(vars(jxr+nc+3),vars(jxr+nc+1),p(ns),nc,0))
& /1.d3
write(kchnl,*)"Reboiler duty(kJ): ",qr
!
!-----
! Show pressure, temperature, heat duty, side draw, and
! efficiency profiles
write(kchnl,*)"Column profiles:"
write(kchnl,'(a)') "Stg Q(kJ) L s/d V s/d//"
& " VLE eff Rxn eff Rx(mol) Rx(kJ)"
do j=1,ns
  do i=1,nc

```

```

        xtemp(i,j)=-vars((j-1)*(2*nc+2)+i)+fd_liq(i,j)+fd_vap(i,j)
        if (j .ne. 1)xtemp(i,j)=xtemp(i,j)+
&           vars((j-2)*(2*nc+2)+nc+2+i)
        if (j .ne. ns)xtemp(i,j)=xtemp(i,j)+
&           vars(j*(2*nc+2)+i)
        end do
    end do
    do j=1,ns
        rxx = rxex(xtemp(1,j),vars((j-1)*(2*nc+2)+nc+1),p(j),nc,0,0)*
&           rxeff(j)
        write (kchnl,1000)j,q(j),sd_l(j),sd_v(j),stg_mve(j),rxeff(j),
&           rxx,rxx*delhr/1.d3
    end do
1000 format(i3,2x,7f11.4)
!
!-----
! Show Pressure, Temperature, Heat duty, and Bulk flow profiles.
write(kchnl,'(a)') "Stg  P(bar)  T(K)//
& "  L(mol)  V(mol)  H err  L(kJ)  V(kJ)"
do j=1,ns
    jstg = (j-1)*(2*nc+2)
    totv(j) = 0.d0
    totl(j) = 0.d0
    do i=1,nc
        totv(j) = totv(j) + vars(jstg+i)
        totl(j) = totl(j) + vars(jstg+nc+2+i)
        vlk(i,j) = vler(vars(jstg+nc+3),vars(jstg+1),
&           vars(jstg+nc+1),p(j),nc,i)
    end do
    hvap(j) = hstream(vars(jstg+1),vars(jstg+nc+1),p(j),nc,1)/
&           1000.d0
    if (j .eq. 1 .and. kcond .eq. 1)hvap(j) = hstream(vars(jstg+1),
&           vars(jstg+nc+1),p(j),nc,0)/1000.d0
    hliq(j) = hstream(vars(jstg+nc+2+1),vars(jstg+nc+1),p(j),nc,0)/
&           1000.d0
    rxk(j) = rxer(vars(jstg+nc+3),vars(jstg+nc+1),p(j),nc,0,0)
end do
do j=1,ns
    jstg = (j-1)*(2*nc+2)
    herr = fd_enth(j)+q(j)-hliq(j)-hvap(j)
    if (j .eq. 1 .and. q(j) .eq. 0.d0) herr = herr + qc
    if (j .eq. ns .and. q(j) .eq. 0.d0) herr = herr + qr
    if (j .ne. 1) herr = herr + hliq(j-1)
    if (j .ne. ns) herr = herr + hvap(j+1)
    write (kchnl,1000)j,p(j),vars(jstg+nc+1),totl(j),totv(j),
&           herr,hliq(j),hvap(j)
    write (kchnl,'(60x,2f11.4)')hliq(j)/totl(j),hvap(j)/totv(j)
end do
!-----
! Show Vapor flow profiles
write(kchnl,*)"Vapor flows/compositions:"
do ii=1,nc,5
    ij=ii+4
    if (ij .ge. nc) ij=nc
    write(kchnl,'(9x,5a12)')(cname(i),i=ii,ij)
do j=1,ns

```

```

        jj=(j-1)*(2*nc+2)
        write(kchnl,'(i3,2x,5f12.4)')j,(vars(jj+i),i=ii,ij)
        write(kchnl,'(5x,5f12.6)')(vars(jj+i)/totv(j),i=ii,ij)
    end do
end do
!
!-----
! Show Liquid flow profiles
write(kchnl,*)"Liquid flows/compositions:"
do ii=1,nc,5
    ij=ii+4
    if (ij .ge. nc) ij=nc
    write(kchnl,'(9x,5a12)')(cname(i),i=ii,ij)
    do j=1,ns
        jj=(j-1)*(2*nc+2)+nc+2
        write(kchnl,'(i3,2x,5f12.4)')j,(vars(jj+i),i=ii,ij)
        write(kchnl,'(5x,5f12.6)')(vars(jj+i)/totl(j),i=ii,ij)
    end do
end do
!
!-----
! Show component creation/consumption
write(kchnl,*)"Component creation & consumption:"
do j=1,ns
    do i=1,nc
        xtemp(i,j)=vars((j-1)*(2*nc+2)+i)+vars((j-1)*(2*nc+2)+nc+2+i)
        xtemp(i,j)=xtemp(i,j)-fd_liq(i,j)-fd_vap(i,j)
        if (j .ne. 1)xtemp(i,j)=xtemp(i,j)-
&          vars((j-2)*(2*nc+2)+nc+2+i)
        if (j .ne. ns)xtemp(i,j)=xtemp(i,j)-
&          vars(j*(2*nc+2)+i)
    end do
end do
do ii=1,nc,5
    ij=ii+4
    if (ij .ge. nc) ij=nc
    write(kchnl,'(9x,5a12)')(cname(i),i=ii,ij)
    do j=1,ns
        write(kchnl,'(i3,2x,5f12.4)')j,(xtemp(i,j),i=ii,ij)
    end do
end do
!
!-----
! Show VLE equilibrium ratios
write(kchnl,*)"Vapor/Liquid equilibrium ratios:"
do ii=1,nc,5
    ij=ii+4
    if (ij .ge. nc) ij=nc
    write(kchnl,'(9x,5a12)')(cname(i),i=ii,ij)
    do j=1,ns
        jv=(j-1)*(2*nc+2)
        jl=jv+nc+2
        write(kchnl,'(i3,2x,5e12.4)')j,(vlk(i,j),i=ii,ij)
        write(kchnl,'(5x,5e12.4)')(((vars(jv+i)*totl(j))/
&          (vars(jl+i)*totv(j))),i=ii,ij)
    end do
end do

```

```

    end do
!
!-----
! Show Reaction equilibrium ratios
write(kchnl,*)"Reaction equilibrium ratios:"
write(kchnl,'(6x,a,2x,a)')"From thermo", "From flows"
do j=1,ns
  rktemp = 1.d0
  do i=1,nc
    if (rxsto(i) .ne. 0.d0) rktemp=rktemp*
&      ((vars((j-1)*(2*nc+2)+nc+2+i)/totl(j))**rxsto(i))
  end do
  write(kchnl,'(i3,2x,2e12.4)')j,rxk(j),rktemp
end do
!
!-----
! Show Stream bubble and dew points
write (kchnl,*)"Stream bubble/dew points:"
write (kchnl,*)"Stg  L bubble  V dew"
do j=1,ns
  jstg=(j-1)*(2*nc+2)
  dbub=bubpt(vars(jstg+nc+3),p(j))
  ddew=dewpt(vars(jstg+1),p(j))
  write(kchnl,'(i3,2x,2f10.4)')j,dbub,ddew
end do

  return
end
!
=====
  subroutine display2
! Write solution description to console for excel
!
  implicit real*8 (a-h,o-z)
  include "pgm_params.f" !Program parameters
  include "cmn_params.f" !No. stages and No. components
  include "cmn_cspec.f" !Column specifications
  include "cmn_thermo.f" !Thermodynamic data
!
  real*8 xtemp(ncmax,nsmax)
!
!-----
! Show case ID
write (*,*)
write (*,*)"Case ID,", pdname_out
!
!-----
! Show Temperature and Bulk flow profiles.
write(*,*)"j,T,L,V,L/V"
do j=1,ns
  jstg = (j-1)*(2*nc+2)
  totv(j) = 0.d0
  totl(j) = 0.d0
  do i=1,nc
    totv(j) = totv(j) + vars(jstg+i)
    totl(j) = totl(j) + vars(jstg+nc+2+i)
  end do
end do

```

```

        end do
    end do
    do j=1,ns
        jstg = (j-1)*(2*nc+2)
        write (*,'(i3,4(" ",f12.6))')j,vars(jstg+nc+1),totl(j),
    &          totv(j),totl(j)/totv(j)
    end do
!-----
!   Show Vapor composition profiles
    write(*,*)"y's"
    do j=1,ns
        jstg = (j-1)*(2*nc+2)
        write(*,'(i3,10(" ",f12.6))')j,(vars(jstg+i)/totv(j),i=1,nc)
    end do
!
!-----
!   Show Liquid composition profiles
    write(*,*)"x's"
    do j=1,ns
        jstg = (j-1)*(2*nc+2)+nc+2
        write(*,'(i3,10(" ",f12.6))')j,(vars(jstg+i)/totl(j),i=1,nc)
    end do
!
!-----
!   Show component per stage conversion
    write(*,*)"Per stage conversion"
    do j=1,ns
        jstg = (j-1)*(2*nc+2)
        jm1 = jstg - (2*nc+2)+nc+2
        jp1 = jstg + (2*nc+2)
        do i=1,nc
            xtemp(i,j)=fd_ctot(i,j)
            if (j .ne. 1)xtemp(i,j) =xtemp(i,j)+vars(jm1+i)
            if (j .ne. ns)xtemp(i,j)=xtemp(i,j)+vars(jp1+i)
            xtemp(i,j)=1.d0-(vars(jstg+i)+vars(jstg+nc+2+i))/xtemp(i,j)
        end do
        write(*,'(i3,10(" ",f12.6))')j,(xtemp(i,j),i=1,nc)
    end do
    jm1 = 0
    jp1 = (ns-1)*(2*nc+2)
!   Show component overall conversion
    write(*,*)"Overall conversion"
    do i=1,nc
        xtemp(i,1)=0.d0
    end do
    do j=1,ns
        do i=1,nc
            xtemp(i,1)=xtemp(i,1)+fd_ctot(i,j)
        end do
    end do
    do i=1,nc
        xtemp(i,2)=0.d0
        if (xtemp(i,1) .ne. 0.d0) xtemp(i,2)=1.d0-
    &          (vars(jm1+i)+vars(jp1+nc+2+i))/xtemp(i,1)
    end do
    write(*,'(i3,10(" ",f12.6))')j,(xtemp(i,2),i=1,nc)

```

```

!
!-----
!   Show Condenser and Reboiler duties.
!   qc = (- fd_enth(1) - hstream(vars(2*nc+3),vars(3*nc+3),p(2),nc,1)
!   &   + (1.d0+sd_v(1))*hstream(vars(1),vars(nc+1),p(1),nc,kcond-1)
!   &   + (1.d0+sd_l(1))*hstream(vars(nc+3),vars(nc+1),p(1),nc,0))
!   &   /1.d3
!   write(*,*)"Condenser duty(kJ)," ,qc
!   jxr=(ns-1)*(2*nc+2); jxrm1=jxr-(2*nc+2)
!   qr = (- fd_enth(ns)
!   & - hstream(vars(jxrm1+nc+3),vars(jxrm1+nc+1),p(ns-1),nc,0)
!   & + (1.d0+sd_v(1))*hstream(vars(jxr+1),vars(jxr+nc+1),p(ns),nc,1)
!   & + (1.d0+sd_l(1))
!   &   *hstream(vars(jxr+nc+3),vars(jxr+nc+1),p(ns),nc,0))
!   &   /1.d3
!   write(*,*)"Reboiler duty(kJ)," ,qr
!
!-----

!
!   return
!   end
!
!=====
!   subroutine fdjac(x,fvec,df,n,NP)
!   USES funcv
!   implicit real*8 (a-h,o-z)
!   PARAMETER (EPS=1.d-5)
!   dimension df(np,np),fvec(np),x(np),f(np)
!   Computes forward-difference approximation to Jacobian. On input,
!   x(1:n) is the point at which the Jacobian is to be evaluated,
!   fvec(1:n) is the vector of function values at the point, and np
!   is the physical dimension of the Jacobian array df(1:n,1:n) which
!   is output. subroutine funcv(n,x,f) is a fixed-name, user-supplied
!   routine that returns the vector of functions at x.
!   Parameters: EPS is the approximate square root of the machine
!   precision.
!   do j=1,n
!       temp=x(j)
!       h=EPS*abs(temp)
!       if(h .eq. 0.d0)h=EPS
!       x(j)=temp+h           !Trick to reduce finite precision error.
!       h=x(j)-temp
!       call funcv(x, f, n, ierr)
!       x(j)=temp
!       do i=1,n               !Forward difference formula.
!           df(i,j)=(f(i)-fvec(i))/h
!       end do
!   end do
!   return
!   end
!
!=====
!   subroutine funcv(x,f,n,ierr)
!   Calculate discrepancy function values f, for the column
!   variables held in vector x.
!   INPUTS:

```

```

!      x : vector of column variables, as follows for each
!          stage - nc vapor flows, 1 stage temperature, 1 stage
!          reaction extent, and nc liquid flows.
!      n : number of equations to evaluate - not used in this
!          implementation.
!  OUTPUTS:
!      f : vector of calculated discrepancy function values -
!          for each stage 1 energy balance, 1 reaction
!          equilibrium function, nc material balances,
!          and nc equilibrium relationships.
!      ierr: error flag ( >0 if error)
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"
include "cmn_params.f"
include "cmn_cspec.f"
include "cmn_thermo.f"
!
real*8 x(*),f(*)
real*8 xt(ncmax)          !vector of stage l-primes
!
jn=2*nc+2                !no. equations per stage
jfe1=1                    !E function for condenser
jfen=(ns-1)*jn+1         !E function for reboiler
!
do j=1,ns                 !proceed stagewise, 1 to n
  jxv = (j-1)*jn          !pointer to vapor flows
  jxt = jxv+nc+1          !Pointer to stage temp.
  jxx = jxt+1              !Pointer to stage rxn extent
  jxl = jxx                !pointer to liquid flows
  jfe = (j-1)*jn+1        !pointer to energy bal function
  jfr = jfe+1              !pointer to rxn eq function
  jfm = jfr                !pointer to matl bal functions
  jfq = jfm+nc            !pointer to v/l equil functions
!
! calculate total stage flows
tljm1 = 0.d0; tlj = 0.d0; tvj = 0.d0; tvjp1 = 0.d0
xmaxl = 0.d0; imaxl = 0
xtsum = 0.d0; eps = 0.d0
do i=1,nc
  tlj = tlj + x(jxl+i)
  tvj = tvj + x(jxv+i)
  xt(i) = fd_liq(i,j) + fd_vap(i,j) - (1.d0+sd_v(j))*x(jxv+i)
  if (j .ne. 1) then
    tljm1 = tljm1 + x(jxl-jn+i)
    xt(i) = xt(i) + x(jxl-jn+i)
  end if
  if (j .ne. ns) then
    tvjp1 = tvjp1 + x(jxv+jn+i)
    xt(i) = xt(i) + x(jxv+jn+i)
  end if
  if (x(jxl+i) .ge. xmaxl)then
    xmaxl = x(jxl+i)
    imaxl = i
  end if
  xtsum = xtsum + xt(i); eps = eps + rxsto(i)

```

```

end do
!
do i=1,nc
! Material Balance Functions
  f(jfm+i)= -fd_liq(i,j)-fd_vap(i,j)-x(jxx)*rxsto(i)+
&   (1.d0+sd_v(j))*x(jxv+i) + (1.d0+sd_l(j))*x(jxl+i)
  if (j .ne. 1) f(jfm+i) = f(jfm+i)-x(jxl-jn+i)
  if (j .ne. ns) f(jfm+i) = f(jfm+i)-x(jxv+jn+i)
!
! Vapor / Liquid Equilibrium functions
  if (j .eq. 1 .and. kcond .eq. 1)then
    vk = 1.d0      !total condenser
  else
    vk = vler(x(jxl+1),x(jxv+1),x(jxt),p(j),nc,i)  !VLE K
  end if
  f(jfq+i) = stg_mve(j)*vk*x(jxl+i)/tlj -
&   x(jxv+i)/tvj
  if (j .ne. ns) f(jfq+i) = f(jfq+i) +
&   (1.d0-stg_mve(j))*x(jxv+jn+i)/tvjp1
!   f(jfq+i) = f(jfq+i) * 1.d2  !scale Q functions to M's
end do
! Bubble point fn for total condenser
  if (j .eq. 1 .and. kcond .eq. 1)then
    f(jfq+imaxl) = 1.d0
    do i=1,nc
      f(jfq+imaxl)=f(jfq+imaxl)-
&   vler(x(jxl+1),x(jxv+1),x(jxt),p(j),nc,i)*
&   x(jxl+i)/tlj
    end do
!   f(jfq+imaxl) = f(jfq+imaxl) * 1.d2 !scale Q functions to M's
end if
!
! Energy balance function
  f(jfe) = -q(j)-fd_enth(j)
&   +(1.d0+sd_l(j))*hstream(x(jxl+1),x(jxt),p(j),nc,0)
  if (j .eq. 1 .and. kcond .eq. 1)then  !total condenser
    f(jfe) = f(jfe) +
&   (1.d0+sd_v(j))*hstream(x(jxv+1),x(jxt),p(j),nc,0)
  else
    f(jfe) = f(jfe) +
&   (1.d0+sd_v(j))*hstream(x(jxv+1),x(jxt),p(j),nc,1)
  end if
  if (j .ne. 1) f(jfe) = f(jfe) -
&   hstream(x(jxl-jn+1),x(jxt-jn),p(j-1),nc,0)
  if (j .ne. ns) f(jfe) = f(jfe) -
&   hstream(x(jxv+jn+1),x(jxt+jn),p(j+1),nc,1)
!   f(jfe) = f(jfe)/1.d4      !Scale H functions to M's
!
! Reaction equilibrium function
  rxk(j) = rxer(xt,x(jxt),p(j),nc,i,0)
  if ((kinetic .and. holdupl(j) .eq. 0.d0) .or. (.not. kinetic
&   .and. rxeff(j) .eq. 0.d0))then
    f(jfr) = x(jxx) - 0.d0      !no reaction
  else
    if (kinetic) then          !kinetic reaction model
      rxneff = 1.d0; rxntot = xtsum+rxneff*eps*x(jxx)
    end if
  end if
end do

```



```

        f2 = holdupl(j)*rxkf(xt,x(jxt),p(j),nc,i,0)/rxntot
        f1 = rxk(j)*f2; f3 = rxk(j)*x(jxx)/rxntot
    else
        !equilibrium reaction model
        rxneff = 1.d0/rxeff(j); rxntot = xtsum+rxneff*eps*x(jxx)
        f1 = rxk(j); f2 = 1.d0; f3 = 0.d0
    end if
    do i=1,nc
        if (rxsto(i) .lt. 0.d0) then
            f1 = f1 * ((xt(i)+(rxneff*rxsto(i)*x(jxx)))/
& rxntot)**(-rxsto(i))
            else if (rxsto(i) .gt. 0.d0) then
                f2 = f2 * ((xt(i)+(rxneff*rxsto(i)*x(jxx)))/
& rxntot)**rxsto(i)
            end if
        end do
        f(jfr) = f1 - f2 - f3
! f(jfr) = f(jfr) * 1.d2 !Scale to M functions
    end if
end do

!
! Substitute functions due to specifications
! set specification 1
! if (kspec(1) .eq. 2) then !L/D spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
        dst = dst + x(i)
        btm = btm + x(nc+2+i)
    end do
    f(jfe1) = btm/dst - xspec(1)
! f(jfe1) = f(jfe1)*1.d2 !scale to M functions
else if (kspec(1) .eq. 3)then !D/F spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
        dst = dst + x(i)
! btm = btm + x((ns-1)*jn+nc+2+i)
    end do
    do i=1,ns
        btm = btm + fd_totl(i)
    end do
! f(jfe1) = dst/(btm+dst) - xspec(1)
    f(jfe1) = dst/btm - xspec(1)
! f(jfe1) = f(jfe1)*1.d2 !scale to M functions
else if (kspec(1) .eq. 4)then !Di/Fi spec
    dst = x(ispec(1))
    btm = x((ns-1)*jn+nc+2+ispec(1))
    f(jfe1) = dst/(dst+btm) - xspec(1)
! f(jfe1) = f(jfe1)*1.d2 !scale to M functions
else if (kspec(1) .eq. 5)then !Tc spec
    f(jfe1) = x(nc+1) - xspec(1)
! f(jfe1) = f(jfe1)*1.d2 !scale to M functions
else if (kspec(1) .eq. 11)then !L1 spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
        dst = dst + x(nc+2+i)
        btm = btm + x((ns-1)*jn+i)
    end do

```

```

    f(jfe1) = dst - xspec(1)
else if (kspec(1) .eq. 12)then    !Vn spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
        dst = dst + x(nc+2+i)
        btm = btm + x((ns-1)*jn+i)
    end do
    f(jfe1) = btm - xspec(1)
else if (kspec(1) .eq. 6)then    !Tr spec
    f(jfe1) = x((ns-1)*jn+nc+1) - xspec(1)
!   f(jfe1) = f(jfe1)*1.d2    !scale to M functions
else if (kspec(1) .eq. 7)then    !Bi/Fi spec
    dst = x(ispec(1))
    btm = x((ns-1)*jn+nc+2+ispec(1))
    f(jfe1) = btm/(dst+btm) - xspec(1)
!   f(jfe1) = f(jfe1)*1.d2    !scale to M functions
else if (kspec(1) .eq. 8)then    !B/F spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
!       dst = dst + x(i)
        btm = btm + x((ns-1)*jn+nc+2+i)
    end do
    do i=1,ns
        dst = dst + fd_totl(i)
    end do
!   f(jfe1) = btm/(btm+dst) - xspec(1)
    f(jfe1) = btm/dst - xspec(1)
!   f(jfe1) = f(jfe1)*1.d2    !scale to M functions
else if (kspec(1) .eq. 9)then    !V/B spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
        dst = dst + x((ns-1)*jn+i)
        btm = btm + x((ns-1)*jn+nc+2+i)
    end do
    f(jfe1) = dst/btm - xspec(1)
!   f(jfe1) = f(jfe1)*1.d2    !scale to M functions
end if
!
!   set specification 2
if (kspec(2) .eq. 2) then    !L/D spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
        dst = dst + x(i)
        btm = btm + x(nc+2+i)
    end do
    f(jfen) = btm/dst - xspec(2)
!   f(jfen) = f(jfen)*1.d2    !scale to M functions
else if (kspec(2) .eq. 3)then    !D/F spec
    dst = 0.d0; btm = 0.d0
    do i=1,nc
!       dst = dst + x(i)
        btm = btm + x((ns-1)*jn+nc+2+i)
    end do
    do i=1,ns
        btm = btm + fd_totl(i)
    end do

```

```

!   f(jfen) = dst/(btm+dst) - xspec(2)
      f(jfen) = dst/btm - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 4)then   !Di/Fi spec
      dst = x(ispec(2))
      btm = x((ns-1)*jn+nc+2+ispec(2))
      f(jfen) = dst/(dst+btm) - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 5)then   !Tc spec
      f(jfen) = x(nc+1) - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 6)then   !Tr spec
      f(jfen) = x((ns-1)*jn+nc+1) - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 7)then   !Bi/Fi spec
      dst = x(ispec(2))
      btm = x((ns-1)*jn+nc+2+ispec(2))
      f(jfen) = btm/(dst+btm) - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 8)then   !B/F spec
      dst = 0.d0; btm = 0.d0
      do i=1,nc
!         dst = dst + x(i)
           btm = btm + x((ns-1)*jn+nc+2+i)
      end do
      do i=1,ns
           dst = dst + fd_totl(i)
      end do
!   f(jfen) = btm/(btm+dst) - xspec(2)
      f(jfen) = btm/dst - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 9)then   !V/B spec
      dst = 0.d0; btm = 0.d0
      do i=1,nc
           dst = dst + x((ns-1)*jn+i)
           btm = btm + x((ns-1)*jn+nc+2+i)
      end do
      f(jfen) = dst/btm - xspec(2)
!   f(jfen) = f(jfen)*1.d2      !scale to M functions
else if (kspec(2) .eq. 11)then  !L1 spec
      dst = 0.d0; btm = 0.d0
      do i=1,nc
           dst = dst + x(nc+2+i)
           btm = btm + x((ns-1)*jn+i)
      end do
      f(jfen) = dst - xspec(2)
else if (kspec(2) .eq. 12)then  !Vn spec
      dst = 0.d0; btm = 0.d0
      do i=1,nc
           dst = dst + x(nc+2+i)
           btm = btm + x((ns-1)*jn+i)
      end do
      f(jfen) = btm - xspec(2)
end if
!
ierr = 0

```

```

!
  return
  end
!
=====
!   Include subroutine packages
!
  include "altthermo.f"
  include "newton.f"
  include "homotopy.f"

```

ALTHERMO.F

```

  subroutine flash(kf, zf, tf, pf, pstg, xf, yf, hf,ftotal,psi)
!   Computes the flash of stream zf to form streams xf and yf
!   Inputs:
!     kf : flash type
!     zf : vector containing feed compositions or flows
!     tf : flash temperature
!     pf : flash pressure
!     pstg: ?
!   Outputs:
!     xf : vector of output liquid compositions or flows
!     yf : vector of output vapor compositions or flows
!     hf :
!     ftotal:
!     psi : Fraction of feed leaving as vapor
!
!   Specification statements:
  implicit real*8 (a-h,o-z)
!   Set parameter values
  include "pgm_params.f"
  parameter (itmax = 25, xacc = 1.d-6)
!   Define data storage
  include "cmn_params.f"
  real*8 zf(ncmax), xf(ncmax), yf(ncmax), z(ncmax), x(ncmax),
&    y(ncmax), vlek(ncmax), ftotal, psi, tbp, tdp

  fpsi(psi, i) = z(i)*(1.d0-vlek(i))/(1.d0+psi*(vlek(i)-1.d0))
  ftmp(t,i) = z(i)*(1.d0-vler(z,z,t,pstg,nc,i))/
& (1.d0+psi*(vler(z,z,t,pstg,nc,i)-1.d0))
!
!   Normalize feed vector and calculate dew and bubble points
  ftotal = 0.d0
  do i=1,nc
    ftotal = ftotal + zf(i)
  end do
  do i=1,nc
    z(i) = zf(i)/ftotal; x(i) = 0.d0; y(i) = 0.d0
  end do
  tbp = bubpt(z, pstg)
  tdp = dewpt(z, pstg)
  if (kf .eq. 1) then          ! Bubble point liquid feed
    tf = tbp
    hf=hstream(zf,tf,pf,nc,0)

```

```

do i=1,nc
  xf(i) = zf(i); yf(i) = 0.d0
end do
psi = 0.d0
else if (kf .eq. 2) then      ! Dew point vapor feed
  tf = tdp
  hf=hstream(zf,tf,pf,nc,1)
  do i=1,nc
    yf(i) = zf(i); xf(i) = 0.d0
  end do
  psi = 1.d0
else if (kf .eq. 3) then      ! Spec temp flash
  if (tf .ge. tdp) then      !T above dew point
    do i=1,nc
      yf(i) = zf(i); xf(i) = 0.d0
    end do
    psi = 1.d0
    hf=hstream(zf,tf,pf,nc,1)
  else if (tf .le. tbp) then  !T below bubble point
    do i=1,nc
      xf(i) = zf(i); yf(i) = 0.d0
    end do
    psi = 0.d0
    hf=hstream(zf,tf,pf,nc,0)
  else                          !T between dew & bubble pts
    psi1 = 0.d0
    psi2 = 1.d0
    f1 = 0.d0
    f2 = 0.d0
    psi = -1
    do i=1,nc
      vlek(i) = vler(z,z,tf,pstg,nc,i)
      f1 = f1 + fpsi(psi1, i)
      f2 = f2 + fpsi(psi2, i)
    end do
    do n=1,itmax
      psi3 = 0.5d0*(psi1+psi2)
      f3 = 0.d0
      do i=1,nc
        f3 = f3 + fpsi(psi3, i)
      end do
      psi4 = psi3 + (psi3 - psi1)*(sign(1.d0, f1-f2)*f3
&                               /sqrt(f3**2 - f1*f2))
      if (abs(psi4-psi) .le. xacc) then
        exit
      end if
      psi = psi4
      f4 = 0.d0
      do i=1,nc
        f4 = f4 + fpsi(psi4, i)
      end do
      if (f4 .eq. 0.d0) then
        end if
      if (sign(f3, f4) .ne. f3) then
        psi1 = psi3; f1 = f3; psi2 = psi4; f2 = f4
      else if (sign(f1, f4) .ne. f1) then

```

```

        psi2 = psi4; f2 = f4
    else if (sign(f2, f4) .ne. f2) then
        psi1 = psi4; f1 = f4
    end if
end do
do i=1,nc
    x(i) = z(i) / (1.d0+psi*(vlek(i)-1.d0))
    y(i) = x(i)*vlek(i)
    xf(i) = ftotal * (1.d0-psi) * x(i)
    yf(i) = ftotal * psi * y(i)
end do
hf=psi*hstream(zf,tf,pf,nc,1) +
& (1.d0-psi)*hstream(zf,tf,pf,nc,0)
end if
else if (kf .eq. 4) then      !Spec V/F flash
if (psi .le. 0.d0) then      !All liquid
do i=1,nc
    xf(i) = zf(i); yf(i) = 0.d0
end do
tf = tbp
hf = hstream(zf,tf,pf,nc,0)
else if (psi .ge. 1.d0) then  !All vapor
do i=1,nc
    yf(i) = zf(i); xf(i) = 0.d0
end do
tf = tdp
hf = hstream(zf,tf,pf,nc,1)
else
t1 = tbp; f1 = 0.d0
t2 = tdp; f2 = 0.d0
tf = -1.d0
do i=1,nc
    f1 = f1+ftmp(t1,i)
    f2 = f2+ftmp(t2,i)
end do
do n=1,itmax
t3 = 0.5d0*(t1+t2); f3 = 0.d0
do i=1,nc
    f3 = f3+ftmp(t3,i)
end do
t4 = t3 + (t3-t1)*(sign(1.d0,f1-f2)*f3
& /sqrt(f3**2 - f1*f2))
if (abs(t4-tf) .le. xacc) then
    exit
end if
tf = t4; f4 = 0.d0
do i=1,nc
    f4 = f4+ftmp(t4,i)
end do
if (f4 .eq. 0.d0) then
end if
if (sign(f3,f4) .ne. f3)then
t1 = t3; f1 = f3; t2 = t4; f2 = f4
else if (sign(f1,f4) .ne. f1) then
t2 = t4; f2 = f4
else if (sign(f2,f4) .ne. f2) then

```

```

        t1 = t4; f1 = f4
    end if
end do
do i=1,nc
    vlek(i) = vler(z,z,tf,pstg,nc,i)
    x(i) = z(i) / (1.d0+psi*(vlek(i)-1.d0))
    y(i) = x(i) * vlek(i)
    xf(i) = ftotal * (1.d0-psi) * x(i)
    yf(i) = ftotal * psi * y(i)
end do
    hf = psi*hstream(zf,tf,pf,nc,1) +
&      (1.d0-psi)*hstream(zf,tf,pf,nc,0)
    end if
end if
return
end
=====
real*8 function bubpt(x,p)
!   Computes bubblepoint temperature of stream x at pressure p
!
!   Specification statements:
implicit real*8 (a-h,o-z)
!   Set parameter values
include "pgm_params.f"
parameter (itmax = 50, xacc = 1.d-6, factor = 1.6d0)
!   Define data storage
include "cmn_params.f"
include "cmn_thermo.f"
!
!   real*8 x(ncmax),xnorm(ncmax)
!
!   Normalize x
xnormsum=0.d0
do i=1,nc
    xnormsum=xnormsum+x(i)
end do
do i=1,nc
    xnorm(i)=x(i)/xnormsum
end do

! Use component boil points to start
t1 = tboil(1)
t2 = tboil(nc)
f1 = 1.d0
f2 = 1.d0
bubpt = -1.d0
do i=1,nc
    f1 = f1 - xnorm(i) * vler(xnorm,xnorm,t1,p,nc,i)
    f2 = f2 - xnorm(i) * vler(xnorm,xnorm,t2,p,nc,i)
end do
do n=1,itmax          ! make sure point is bracketed
    if (f1*f2 .lt. 0.d0) exit
    if (abs(f1) .lt. abs(f2)) then
        t1 = t1+factor*(t1-t2)
        f1 = 1.d0
    do i=1,nc

```

```

        f1 = f1 - xnorm(i) * vler(xnorm,xnorm,t1,p,nc,i)
    end do
else
    t2 = t2+factor*(t2-t1)
    f2 = 1.d0
    do i=1,nc
        f2 = f2 - xnorm(i) * vler(xnorm,xnorm,t2,p,nc,i)
    end do
end if
end do
if (f1*f2 .ge. 0.d0) write(*,*)"BUBPT: Failed to find range."
do n=1,itmax
    ! search for best value
    t3 = 0.5d0*(t1+t2)
    f3 = 1.d0
    do i=1,nc
        f3 = f3 - xnorm(i) * vler(x,x,t3,p,nc,i)
    end do
    t4 = t3 + (t3 - t1)*(sign(1.d0, f1-f2)*f3/sqrt(f3**2 - f1*f2))
    if (abs(t4-bubpt) .le. xacc) return
    bubpt = t4
    f4 = 1.d0
    do i=1,nc
        f4 = f4 - xnorm(i) * vler(x,x,t4,p,nc,i)
    end do
    if (f4 .eq. 0.d0) return
    if (sign(f3, f4) .ne. f3) then
        t1 = t3; f1 = f3; t2 = t4; f2 = f4
    else if (sign(f1, f4) .ne. f1) then
        t2 = t4; f2 = f4
    else if (sign(f2, f4) .ne. f2) then
        t1 = t4; f1 = f4
    end if
    if (abs(t2 - t1) .le. xacc) return
end do
write (*,*) "BUBPT: fails to converge in ",itmax," iterations"
write(*,*)"BUBPT: Returned value is: ",bubpt
return
end
=====
real*8 function dewpt(x,p)
!   Computes dewpoint temperature of stream x at pressure p
!
!   Specification statements:
implicit real*8 (a-h,o-z)
!   Set parameter values
include "pgm_params.f"
parameter (itmax = 50, xacc = 1.d-6, factor = 1.6d0)
!   Define data storage
include "cmn_params.f"
include "cmn_thermo.f"
!
!   real*8 x(ncmax),xnorm(ncmax)
!
!   Normalize x
xnormsum=0.d0
do i=1,nc

```



```

    xnormsum=xnormsum+x(i)
end do
do i=1,nc
    xnorm(i)=x(i)/xnormsum
end do

! Use component boil points to start
t1 = tboil(1)
t2 = tboil(nc)
f1 = 1.d0
f2 = 1.d0
dewpt = -1.d0
do i=1,nc
    f1 = f1 - xnorm(i) / vler(xnorm,xnorm,t1,p,nc,i)
    f2 = f2 - xnorm(i) / vler(xnorm,xnorm,t2,p,nc,i)
end do
do n=1,itmax          ! make sure point is bracketed
    if (f1*f2 .lt. 0.d0) exit
    if (abs(f1) .lt. abs(f2)) then
        t1 = t1+factor*(t1-t2)
        f1 = 1.d0
        do i=1,nc
            f1 = f1 - xnorm(i) / vler(xnorm,xnorm,t1,p,nc,i)
        end do
    else
        t2 = t2+factor*(t2-t1)
        f2 = 1.d0
        do i=1,nc
            f2 = f2 - xnorm(i) / vler(xnorm,xnorm,t2,p,nc,i)
        end do
    end if
end do
if (f1*f2 .ge. 0.d0) write(*,*)"DEWPT: Failed to find range."
do n=1,itmax          ! search for best value
    t3 = 0.5d0*(t1+t2)
    f3 = 1.d0
    do i=1,nc
        f3 = f3 - xnorm(i) / vler(xnorm,xnorm,t3,p,nc,i)
    end do
    t4 = t3 + (t3 - t1)*(sign(1.d0, f1-f2)*f3/sqrt(f3**2 - f1*f2))
    if (abs(t4-dewpt) .le. xacc) return
    dewpt = t4
    f4 = 1.d0
    do i=1,nc
        f4 = f4 - xnorm(i) / vler(xnorm,xnorm,t4,p,nc,i)
    end do
    if (f4 .eq. 0.d0) return
    if (sign(f3, f4) .ne. f3) then
        t1 = t3; f1 = f3; t2 = t4; f2 = f4
    else if (sign(f1, f4) .ne. f1) then
        t2 = t4; f2 = f4
    else if (sign(f2, f4) .ne. f2) then
        t1 = t4; f1 = f4
    end if
    if (abs(t2 - t1) .le. xacc) return
end do

```

```

write (*,*) "DEWPT: fails to converge in ",itmax," iterations"
write(*,*)"DEWPT: Returned value is: ",dewpt
return
end

=====
real*8 function rxex(x,t,pstg,nc,ic,kst)
!   Compute the equilibrium extent of reaction at t and p
!   Inputs:
!       x :   vector of stream compositions or flows
!       t :   temperature for the calculation, K
!       p :   pressure for the calculation, bar
!       nc :  number of components in x
!       ic :  component index (not used in this calc'n)
!       kst:  Stream state (0=>liquid; 1=>vapor)
!   Outputs:
!       rxex: Calculated extent of reaction
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
parameter (gs = 0.381966011d0) !parm for golden section search
!
rxek = rxer(x,t,pstg,nc,ic,kst) !Get the equilibrium constant
xmax = 1.d20
xmin = -1.d20
xsum = 0.d0
eps = 0.d0
do i=1,nc                !find max fwd and rev extents
  xsum = xsum + x(i)
  eps = eps + rxsto(i)
  if (rxsto(i) .ne. 0.d0) then
    xtemp = - x(i) / rxsto(i)
    if (rxsto(i) .lt. 0.d0 .and. xtemp .lt. xmax) xmax = xtemp
    if (rxsto(i) .gt. 0.d0 .and. xtemp .gt. xmin) xmin = xtemp
  end if
end do
!   Initialize for Brent method search to find the root
a = xmin; b = xmax
fa1 = 1.d0; fa2 = rxek
fb1 = 1.d0; fb2 = rxek
do i=1,nc                !f(x) = product of factor, minus rxek
  if (rxsto(i) .gt. 0.d0) then
    fa1=fa1*((x(i)+rxsto(i)*a)/(xsum+eps*a))**rxsto(i)
    fb1=fb1*((x(i)+rxsto(i)*b)/(xsum+eps*b))**rxsto(i)
  else if (rxsto(i) .lt. 0.d0) then
    fa2=fa2*((x(i)+rxsto(i)*a)/(xsum+eps*a))**(-rxsto(i))
    fb2=fb2*((x(i)+rxsto(i)*b)/(xsum+eps*b))**(-rxsto(i))
  end if
end do
fa=fa1-fa2; fb=fb1-fb2
!   fa=fa-rxek; fb=fb-rxek
c = b; fc = fb
do k=1,100                !search loop
  if (fb*fc .ge. 0.d0) then
!       Rename a,b,&c and adjust bounding interval d

```

```

    c=a; fc=fa; d=b-a; e=d
end if
if (abs(fc) .lt. abs(fb)) then !swap a and c with b
    a=b; b=c; c=a
    fa=fb; fb=fc; fc=fa
end if
tol1 = 2.d0*1.d-8*abs(b) + 0.5d0*1.d-8 !check convergence
xm = 0.5d0*(c-b)
if (abs(xm) .le. tol1 .or. fb .eq. 0.d0) then !Converged
    rxex = b
    return
end if
!
if (abs(e) .gt. tol1 .and. abs(fa) .gt. abs(fb)) then
    Try inverse quadratic interpolation
    s = fb/fa
    if (a .eq. c) then
        p = 2.d0*xm*s
        q = 1.d0 - s
    else
        q = fa/fc
        r = fb/fc
        p = s*(2.d0*xm*q*(q-r)-(b-a)*(r-1.d0))
        q = (q-1.d0)*(r-1.d0)*(s-1.d0)
    end if
    if (p .gt. 0.d0) q = -q !Check whether in bounds
    p = abs(p)
    if (2.d0*p .lt. min(3.d0*xm*q-abs(tol1*q), abs(e*q))) then
        e=d !Accept interpolation
        d=p/q
    else
        d=xm !Interpolation failed, use bisection
        e=d
    end if
else
    d=xm !Bounds decreasing too slowly, use bisection
    e=d
end if
a=b !Move last guess to a
fa=fb
if (abs(d) .gt. tol1) then !Evaluate new trial root
    b=b+d
else
    b=b+sign(tol1,xm)
end if
fb1=1.d0; fb2=rxek !Compute function value for new trial root
do i=1,nc
    if (rxsto(i) .gt. 0.d0) then
        fb1 = fb1*((x(i)+rxsto(i)*b)/(xsum+eps*b))**rxsto(i)
    else if (rxsto(i) .lt. 0.d0) then
        fb2 = fb2*((x(i)+rxsto(i)*b)/(xsum+eps*b))**(-rxsto(i))
    end if
end do
fb=fb1-fb2
end do
rxex = b
write (*,*)"Reaction extent = ",rxex," Excess Iterations"

```

```

return
end
=====
real*8 function vler(x,y,t,p,nc,ic)
! Computes the vapor-liquid equilibrium ratio for
! component ic in the mixture x at t and p
! Inputs:
!   x : vector of liquid stream compositions or flows
!   y : vector of vapor stream compositions or flows
!   t : temperature for the calculation, K
!   p : pressure for the calculation, bar
!   nc : number of components in x
!   ic : index of the component of interest
! Outputs:
!   vler: Calculated value of the property
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*),y(*)
!
vler = exp( vpa(ic) - vpb(ic)/t ) / p
! vler =exp(-((1.d0/t)-(1.d0/tboil(ic)))*delhv/rgas)
return
end
=====
real*8 function hstream(x,t,p,nc,kst)
! Compute the enthalpy of stream x at t and p in state kst,
! relative to tref. Value returned is in units of kJ
! Inputs:
!   x : vector of stream compositions or flows
!   t : temperature for the calculation, K
!   p : pressure for the calculation, bar
!   nc : number of components in x
!   kst: Stream state (0=>liquid; 1=>vapor)
! Outputs:
!   hstream: Calculated enthalpy, kJ
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
!
t0 = tref      !Reference Temp
hstream = 0.d0
xsum = 0.d0
do i=1,nc
  xsum = xsum+x(i)
end do
if (kst .eq. 0) then
  do i=1,nc      !!liquid enthalpy
    hstream = hstream + ((t-t0)*cpa0(i)+delhf(i))*x(i)/xsum
!   hstream = hstream + ((t-t0)*cpa0(i))*x(i)/xsum
  end do
else
!   hstream = delhv/xsum

```

```

do i=1,nc          !vapor enthalpy
  hstream = hstream + ((tboil(i)-t0)*cpa0(i) + (t-tboil(i))
&      *cpa1(i) + delhf(i) + delhv)*x(i)/xsum
!   hstream = hstream + ((tboil(i)-t0)*cpa0(i) + (t-tboil(i))
!   &      *cpa1(i))*x(i)/xsum
  end do
end if
hstream = hstream * xsum      !change molar to total    !kJ
return
end
=====
real*8 function rxer(x,t,p,nc,ic,kst)
!   Compute the reaction equilibrium constant at t and p
!   Inputs:
!     x : vector of stream compositions or flows
!     t : temperature for the calculation, K
!     p : pressure for the calculation, bar
!     nc : number of components in x
!     ic : component index (not used in this calc'n)
!     kst: Stream state (0=>liquid; 1=>vapor)
!   Outputs:
!     rxer: Calculated value of the equilibrium constant
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
rxer = rxnke0*exp(((1.d0/rxntref)-(1.d0/t))*rxeeql/rgas)
!
return
end
=====
real*8 function rxkf(x,t,p,nc,ic,kst)
!   Compute the reaction forward rate constant at t and p
!   Inputs:
!     x : vector of stream compositions or flows
!     t : temperature for the calculation, K
!     p : pressure for the calculation, bar
!     nc : number of components in x
!     ic : component index (not used in this calc'n)
!     kst: Stream state (0=>liquid; 1=>vapor)
!   Outputs:
!     rxkf: Calculated value of the rate constant
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
rxkf = rxkf0*exp(((1.d0/rxntref)-(1.d0/t))*rxefwd/rgas)
!
return
end
=====
real*8 function boiltemp(ic,p)
!   Compute the boiling temperature for component ic at pressure p
!   Inputs:

```

```

!      ic :  component index
!      p  :  pressure for the calculation, bar
!  Outputs:
!      boiltemp:  Calculated value of the boiling temperature
!
!      implicit real*8 (a-h,o-z)
!      include "pgm_params.f"      !Storage allocation parameters
!      include "cmn_thermo.f"     !component thermodynamic data
!      boiltemp = vpb(ic)/(vpa(ic) - log(p))
!
!      return
!      end

```

```

!=====

```

STATE.F

```

      subroutine dumpstate
!Subroutine to dump complete problem specification and state
!
!
!  Include files
!  include "cmn_params.f"      !no. stages & no. components
!  include "cmn_cspect.f"     !Problem specifications
!  include "cmn_thermo.f"     !Thermodynamic properties
!  include "cmn_hsparms.f"    !Homotopy parameters
!
!Open file for output
!  open (20, file = filename(1:lnblnk(filename))//'.dat')
!
!Write ns and nc
!  write(20) ns,nc
!Write homotopy solver parameters
!  write(20) dir, dso, dsmin, dsmax, xmax,
!  & ecorc, ecorb, edet, esol, ebif, etur, esta, easy,
!  & idom, ihom, maxdet, minasy, maxasy
!Write thermodynamic stuff
!  write(20) (cname(i), cmolwt(i), tmelt(i),
!  & tboil(i), tcrit(i), pcrit(i), vcrit(i),
!  & zcrit(i), acfac(i), delhf(i), delgf(i),
!  & tcpmin(i), tcpmax(i), cpa0(i),cpa1(i),
!  & cpa2(i), cpa3(i), cpa4(i),vpa(i), vpb(i),
!  & vpc(i), pvpmin(i), pvpmax(i), tvpmin(i),
!  & tvpmax(i),rxsto(i),fwvl(i),i=1,nc)
!  write(20) acvl, bcvl, zcvl, uvl, wvl, fuwvl,
!  & rgas, alpha, tb1, delhv, delhr, cpl, cpv, tref,
!  & rxnke0, rxeeql, rxkf0, rxefwd, rxntref, kthermo,
!  & kinetic
!Write problem specification
!  write(20) kcond, psname_in, pdname_out, c_desc
!  write(20) (xspect(i), kspect(i), ispect(i), jspect(i),i=1,2)
!  write(20) (fd_temp(i), fd_pres(i), fd_enth(i),
!  & fd_totl(i), fd_psi(i), p(i), q(i),
!  & sd_l(i), sd_v(i), stg_mve(i), rxeff(i),
!  & holdupl(i), totl(i), totv(i), hliq(i),
!  & hvap(i), rxk(i), kfeed(i), i=1,ns)
!  write(20) ((fd_liq(j,i), fd_vap(j,i), fd_ctot(j,i),

```

```

&   vlk(j,i),j=1,nc),i=1,ns)
write(20) (vars(i), vars0(i),i=0,ns*(2*nc+2))
!
close(20)
return
end

```

NEWTON.F

```

subroutine nsolver(x,n,tolx,tolf,ntrial,kstatus,its,errf,ipr1,
&                ipr2)
!
!   Use Newton iteration to improve a root x.
!   Given an initial guess x for a root in n dimensions, take ntrial
!   Newton-Raphson steps to improve the root. Stop if the root
!   converges in either summed absolute variable increments tolx
!   or summed absolute function values tolf.
!
!   Reference: W.H.Press, B.P.Flannery, S.A.Teukolsky, and
!   W.T.Vetterling, Numerical Recipes: The Art of
!   Scientific Computing, Cambridge University Press,
!   New York, NY, 1989.
!
!   uses: nlubksb, nludcmp, ...
!
!   Input Variables
!   x: vector containing initially guessed variable values
!   n: dimension of vector x
!   tolx: lower limit of absolute variable increments
!   tolf: lower limit of absolute function values
!   ntrial: number of iterations allowed
!
!   Output Variables
!   x: vector of improved variable values
!   kstatus: 0 if converged, -1 if not
!   its: number of iterations performed
!   errf: L2 norm of residual vector at completion
!
!   input / output variables:
integer n, ntrial, np
real*8 tolf, tolx, x(n)
!
!   local variables
integer i, j, k, indx(n),imax
real*8 d, errf, errx, fjac(n,n),fjacu(n,n), fvec(n), p(n),p0(n),
&   p1(n),chmax,w(n),v(n,n),sum,ratio,temp,fvecx(n),f,fplus,gs,
&   fminus,xtemp(n),nvecnrm,xa,fxa,xb,xfb,x1,fx1,x2,fx2,fin(30)
real*8 rcmax,rcmin,smlnum,bignum,rowcnd,rscale(n),fmax,fmin
real*8 xlim,xlim1
real*8 bigchg, smlchg, chg, avchg
!
include "cmn_params.f"
parameter (gs = 0.381966011d0) !parm for golden section search
!   big & small numbers
parameter (smlnum = 2.22507386d-308,bignum = 1.d0/smlnum)
!-----

```

```

kstatus = 0           !Status okay unless a problem happens
do k=1,ntrial        !Iteration loop starts here
  its=k
  call funcv(x,fvec,n,ierr)      !Get the function vector
  errf = nvecnorm(fvec,n)      !Compute norm of the residual
  if (errf .le. tolf) return
  do i=1,n
    p(i) = -fvec(i)
  end do
  call fdjac(x,fvec,fjac,n,n) !Get the jacobian of the function
!-----
! Scale the jacobian and the p vector to prevent overflows
rcmax = smlnum
rcmin = bignum
do i=1,n           !Scan rows for largest element
  rscale(i) = 0.d0
  do j=1,n
    rscale(i) = max(rscale(i), abs(fjac(i,j)))
  end do
  rcmax = max(rcmax,rscale(i))
  rcmin = min(rcmin,rscale(i))
  if (rcmin .eq. 0.d0) then      !Bail out if singular
    write (ipr1,*)"SOLVER: Singular Jacobian for function ",i
    kstatus = -1
    return
  end if
  rscale(i) = 1.d0 / min(max(rscale(i),smlnum),bignum)
end do
rowcnd = max(rcmin,smlnum)/min(rcmax,bignum)
do i=1,n           !Scale the system
  p(i) = p(i) * rscale(i)
  do j=1,n
    fjac(i,j) = fjac(i,j) * rscale(i)
  end do
end do
!-----
  call nludcmp(fjac, n, n, indx, d)
  call nlubksb(fjac, n, n, indx, p)
!-----
! Limit temperature changes
xlim = 10.d0
xlim1 = 1.2d0
do j=1,ns
  jl=(j-1)*(2*nc+1)
  jv=(j-1)*(2*nc+1)+nc+1
  jt=(j-1)*(2*nc+1)+nc+1
  p(jt)=sign(xlim*(1.d0-exp(-xlim1*abs(p(jt)/xlim))),p(jt))
  do i=1,nc           !Limit flow changes to stay positive
    if (p(jl+i) .lt. -0.8d0*x(jl+i)) p(jl+i) = -0.8d0*x(jl+i)
    if (p(jv+i) .lt. -0.8d0*x(jv+i)) p(jv+i) = -0.8d0*x(jv+i)
  end do
end do
! limit flow changes here, too ??
!-----
! golden section search for optimum distance along the p vector
xa = 0.15d0

```



```

do i=1,n
  xtemp(i) = x(i) + xa*p(i)
end do
call funcv(xtemp,fvecx,n,ierr)
fxa = nvecnorm(fvecx,n)
xb = 1.25d0
do i=1,n
  xtemp(i) = x(i) + xb*p(i)
end do
call funcv(xtemp,fvecx,n,ierr)
fxb = nvecnorm(fvecx,n)
nfi = 20
x1 = xa + (xb-xa)*gs
do i=1,n
  xtemp(i) = x(i) + x1*p(i)
end do
call funcv(xtemp,fvecx,n,ierr)
fx1 = nvecnorm(fvecx,n)
x2 = xb - (xb-xa)*gs
do i=1,n
  xtemp(i) = x(i) + x2*p(i)
end do
call funcv(xtemp,fvecx,n,ierr)
fx2 = nvecnorm(fvecx,n)
do kfi=1,nfi-1
  !IGS search loop
  if (fx1 .lt. fx2) then
    xb = x2; fxb = fx2
    x2 = x1; fx2 = fx1
    x1 = xa + (xb-xa)*gs
    do i=1,n
      xtemp(i) = x(i) + x1*p(i)
    end do
    call funcv(xtemp,fvecx,n,ierr)
    fx1 = nvecnorm(fvecx,n)
    ratio = x1
  else
    xa = x1; fxa = fx1
    x1 = x2; fx1 = fx2
    x2 = xb - (xb-xa)*gs
    do i=1,n
      xtemp(i) = x(i) + x2*p(i)
    end do
    call funcv(xtemp,fvecx,n,ierr)
    fx2 = nvecnorm(fvecx,n)
    ratio = x2
  end if
end do
do i=1,n
  !Adjust the p(i) to reflect damping
  p(i) = ratio * p(i)
end do
!
!-----
errx = 0.d0
do i=1,n
  errx = errx + abs(p(i))
  x(i) = x(i) + p(i)

```

```

        if (x(i) .le. 1.d-12) x(i) = 1.d-12
    end do
    write (ipr1,*)"Iteration: ",k," Damping factor ",ratio,
&      " Error: ",errx
    if (errx .le. tolx) return
end do
kstatus=-1
return
end

!
!=====
subroutine nludcmp(a,n,np,indx,d)
integer n,np,indx(n),nmax
real*8 d,a(np,np),tiny
parameter (nmax=500,tiny=1.d-20)
!largest expected n, and a small number.
! given a matrix a(1:n,1:n), with physical dimension np by np,
! this routine replaces it by the lu decomposition of a rowwise
! permutation of itself. a and n are input. a is output, arranged
! as in equation (2.3.14) above; indx(1:n) is an output vector
! that records the row permutation effected by the partial
! pivoting; d is output as ±1 depending on whether the number of
! row interchanges was even or odd, respectively. this routine is
! used in combination with nlubksb to solve linear equations or
! invert a matrix.
integer i,imax,j,k
real*8 aamax,dum,sum,vv(nmax)
!vv stores the implicit scaling of each row.
d=1.d0 !no row interchanges yet.
do i=1,n
    !loop over rows to get the implicit scaling information.
    aamax=0.d0
    do j=1,n
        if (abs(a(i,j)).gt.aamax) aamax=abs(a(i,j))
    end do
    if (aamax .eq. 0.d0) then
! pause "singular matrix in nludcmp" !no nonzero largest element.
        d=0.d0
        return
    end if
    vv(i)=1.d0/aamax !save the scaling.
end do
do j=1,n !this is the loop over columns of crout's method.
    do i=1,j-1 !this is equation (2.3.12) except for i = j.
        sum=a(i,j)
        do k=1,i-1
            sum=sum-a(i,k)*a(k,j)
        end do
        a(i,j)=sum
    end do
    aamax=0.d0 !initialize for the search for largest pivot element.
    do i=j,n !this is i = j of equation (2.3.12) and i = j+1. . . n
        !of equation (2.3.13).
        sum=a(i,j)
        do k=1,j-1
            sum=sum-a(i,k)*a(k,j)

```

```

end do
a(i,j)=sum
dum=vv(i)*abs(sum)      !figure of merit for the pivot.
if (dum.ge.aamax) then  !is it better than the best so far?
  imax=i
  aamax=dum
end if
end do
if (j.ne.imax)then      !do we need to interchange rows?
  do k=1,n              !yes, do so...
    dum=a(imax,k)
    a(imax,k)=a(j,k)
    a(j,k)=dum
  end do
  d=-d                  !...and change the parity of d.
  vv(imax)=vv(j)       ! also interchange the scale factor.
end if
indx(j)=imax
if(a(j,j) .eq. 0.d0)a(j,j)=tiny
!   if the pivot element is zero the matrix is singular
!   (at least to the precision of the algorithm). for some
!   applications on singular matrices, it is desirable to
!   substitute tiny for zero.
if(j .ne. n)then      !now, finally, divide by the pivot element.
  dum=1.d0/a(j,j)
  do i=j+1,n
    a(i,j)=a(i,j)*dum
  end do
end if
end do                !go back for the next column in the reduction.
return
end

!
=====
subroutine nlubksb(a,n,np,indx,b)
integer n,np,indx(n)
real*8 a(np,np),b(n)
! solves the set of n linear equations a · x = b. here a is input,
! not as the matrix a but rather as its lu decomposition,
! determined by the routine nludcmp. indx is input as the
! permutation vector returned by nludcmp. b(1:n) is input as the
! right-hand side vector b, and returns with the solution vector x.
! a, n, np, and indx are not modified by this routine and can be
! left in place for successive calls with different right-hand
! sides b. this routine takes into account the possibility that
! b will begin with many zero elements, so it is efficient
! for use in matrix inversion.
integer i,ii,j,ll
real*8 sum
ii=0 !when ii is set to a positive value, it will become the index
! of the first nonvanishing element of b. we now do
! the forward substitution, equation (2.3.6). the only new
! wrinkle is to unscramble the permutation as we go.
do i=1,n
  ll=indx(i)
  sum=b(ll)

```

```

    b(ii)=b(i)
    if (ii.ne.0)then
      do j=ii,i-1
        sum=sum-a(i,j)*b(j)
      end do
    else if (sum .ne. 0.d0) then
      ii=i      ! a nonzero element was encountered, so
                ! from now on we will have to do the sums
                ! in the loop above.
    end if
    b(i)=sum
  end do
do i=n,1,-1  ! now we do the backsubstitution, equation (2.3.7).
  sum=b(i)
  do j=i+1,n
    sum=sum-a(i,j)*b(j)
  end do
  b(i)=sum/a(i,i) ! store a component of the solution vector x.
end do
return      ! all done!
end

!
!=====
SUBROUTINE mprove(a,alud,n,np,indx,b,x)
INTEGER n,np,indx(n),i,j
REAL*8 a(np,np),alud(np,np),b(n),x(n),r(n),sdp
!  USES nlubksb
do i=1,n
  sdp=-b(i)
  do j=1,n
    sdp=sdp+a(i,j)*x(j)
  end do
  r(i)=sdp
end do
call nlubksb(alud,n,np,indx,r)
do i=1,n
  x(i)=x(i)-r(i)
end do
return
END

!
!=====
real*8 function nvecnorm(x,n)
!  Returns Euclidean norm of x => sqrt(sum(xi**2))
implicit real*8 (a-h,o-z)
dimension x(*)
nvecnorm = 0.d0
do i=1,n
  nvecnorm = nvecnorm + x(i)*x(i)
end do
nvecnorm = sqrt(nvecnorm)
return
end

!=====
real*8 function vecnorm1(x,n)
!  Returns 1- norm of x => sum(abs(xi))

```

```

implicit real*8 (a-h,o-z)
dimension x(*)
vecnrm1 = 0.d0
do i=1,n
  vecnrm1 = vecnrm1 + abs(x(i))
end do
return
end

=====
real*8 function vecnrmi(x,n)
! Returns inf norm of x => max(xi)
implicit real*8 (a-h,o-z)
dimension x(*)
vecnrmi = 0.d0
do i=1,n
  temp = abs(x(i))
  if (temp .gt. vecnrmi) vecnrmi = temp
end do
return
end

```

COMMON BLOCK DEFINITIONS

CMN_CSPEC.F

```

character*80 c_desc
character*24 psname_in, pdname_out
integer kspec, ispec, jspec, kcond, kfeed
real*8 fd_liq, fd_vap, fd_ctot, fd_temp, fd_pres, fd_enth,
& fd_totl, fd_psi,
& p, q, sd_l, sd_v, stg_mve, rxeff, totl, totv, hliq, hvap,
& rxk, vlk, vars, vars0, xspec
common /colspec/ fd_liq(ncmax,nsmax), fd_vap(ncmax,nsmax),
& fd_ctot(ncmax,nsmax),
& fd_temp(nsmax), fd_pres(nsmax), fd_enth(nsmax),fd_totl(nsmax),
& fd_psi(nsmax),
& p(nsmax), q(nsmax), sd_l(nsmax), sd_v(nsmax),
& stg_mve(nsmax),rxeff(nsmax),holdupl(nsmax),
& totl(nsmax),totv(nsmax), hliq(nsmax), hvap(nsmax),
& rxk(nsmax), vlk(ncmax,nsmax), vars(0:nvmax), vars0(0:nvmax),
& rxcoord, scinit, xspec(2), kspec(2), ispec(2), jspec(2), kcond,
& kfeed(nsmax), psname_in, pdname_out, c_desc
!
integer in_spc, out_spc, out_log, out_sol, out_pth, in_cdata
common /iochn/in_spc, out_spc, out_log, out_sol, out_pth, in_cdata

```

CMN_HSPARMS.F

```

common /hsparms/ dir, dso, dsmin, dsmax, xmax,
& ecorc, ecorb, edet, esol, ebif, etur, esta, easy,
& idom, ihom, maxdet, minasy, maxasy

```

CMN_PARAMS.F

```

common /params/ns, nc

```

CMN_THERMO.F

```

character*24 cname
logical kinetic
common /thermo/ cname(ncmax), cmolwt(ncmax), tmelt(ncmax),

```

```
& tboil(ncmax), tcrit(ncmax), pcrit(ncmax), vcrit(ncmax),  
& zcrit(ncmax), acfac(ncmax), delhf(ncmax), delgf(ncmax),  
& tcpmin(ncmax), tcpmax(ncmax), cpa0(ncmax),cpa1(ncmax),  
& cpa2(ncmax), cpa3(ncmax), cpa4(ncmax),vpa(ncmax), vpb(ncmax),  
& vpc(ncmax), pvpmin(ncmax), pvpmax(ncmax), tvpmin(ncmax),  
& tvpmax(ncmax),rxsto(ncmax),  
& fwvl(ncmax), acvl, bcvl, zcvl, uvl, wvl, fuwvl,  
& rgas,  
& alpha, tb1, delhv, delhr, cpl, cpv, tref,  
& rxnke0, rxeeql, rxkf0, rxefwd, rxntref,  
& kthermo,  
& kinetic
```

PGM_PARAMS.F

```
parameter (nsmax = 50, ncmax = 10, nvmax = nsmax*(2*ncmax+2))  
parameter (nimax = nvmax, nrmax = 2*nimax)
```

APPENDIX C.
REACTIVE FLASH PROGRAM SOURCE CODE

MAIN PROGRAM

```

    program scflash
!   Distillation computation by simultaneous correction method.
!   Revised main program
!   Written by: T. Mills
!   Date:    04/08/2009
!
!
!   Specification statements:
implicit real*8 (a-h,o-z)
logical c_in, f_in, dflag, quit, first, feasible, rstart
integer ioflag, kthermo, nargs, nc, ns, method
!
!   Set parameter values
include "pgm_params.f"
parameter (dflag = .false.)
!
!   Define local storage areas
integer nnull, nnullv(nvmax)
real*8 tmpdfx(nvmax,nvmax), tmpfx(nvmax), tmpwrk(nvmax), solndet
!
!   Define common storage areas
include "cmn_params.f"
include "cmn_spec.f"
include "cmn_thermo.f"
!
!   Define i/o channels
data in_spc,out_spc,out_log,out_sol,in_cdata/ 10,11,12,13,14/
data out_pth/ 15/
!
!-----
!   Executable statements begin here
!
!   Get the name of the input file, then open the file if
!   it exists, or quit.
!
if (iargc() .ge. 1) then
    call getarg(1,psname_in)
else
    write (*,'(a$)') " Problem Specification file: "
    read (*,*) psname_in
    if ( psname_in .eq. ' ') stop
end if
inquire(file= psname_in, exist= f_in)
if (f_in) then
    open (in_spc, file = psname_in, status = "old" )
    rewind in_spc
else
    write (*,'(a$)') " Specification file doesn't exist... "
    stop
end if
!
first = .true.
do
! while ( .not. quit)
!-----

```



```

!   Get problem specification
call probspec(f_in,method,first,quit)
!   Exit if no new case to solve
if (quit) then
  write (*,*) "Termination signal given"
  stop
end if
!   Open files for log and problem solutions
open (out_log, file = pdname_out(1:LnBlnk(pdname_out))//'.log' )
open (out_sol, file = pdname_out(1:LnBlnk(pdname_out))//'.sol' )
open (out_pth, file = pdname_out(1:LnBlnk(pdname_out))//'.pth' )
!
!-----
!   Set up initial profile guesses
call initprob
!
!-----
!   Initial profiles are set, now time to solve the problem.
write (*,*)
write (*,*)"Case: ",pdname_out
write (*,*)c_desc
write (*,*)
write(out_log,*)"Initial estimates..."
call display(out_log)
do j=1,2*nc+2      !Save initial starting point
  vars0(j) = vars(j)
end do
kstatus = 0
maxits = 5000
nsoln = 0; nturn = 0; nstart = 1; nfeas = 0; nstalls = 3
do while (.true.)
  call solver(vars,2*nc+2,1.d-6,1.d-06,100,
&      kstatus,nits,error,out_log,out_pth)
  write (*,*)"Homotopy parm ",error," after ",nits," steps."
  write (out_log,*)"Homotopy parm ",error," after ",nits,
&      " steps."
  if (kstatus .lt. 100) nstalls = 3
  if (kstatus .eq. 1) then  !Solution point found
    feasible = .true.
    do j=1,2*nc+2
      if (j .ne. (nc+2) .and. vars(j) .lt.
&      -1.d-7) feasible = .false.
    end do
    call funcv(vars(1),tmpfx,2*nc+2,nnull)
    call fdjac(vars(1),tmpfx,tmpdfx,2*nc+2,nvmax)
    call ludcmp(tmpdfx,2*nc+2,nvmax,nnullv,tmpwrk,solndet,
&      nnull)
    nsoln = nsoln + 1
    if (feasible) then
      nfeas = nfeas + 1
      write (*,*) "Feasible solution ",nfeas,":"
      write (out_sol,*) "Feasible solution ",nfeas,":"
      write (out_log,*) "Feasible solution ",nfeas,":"
      write (*,*) "Jacobian Determinant: ",solndet
      write (out_sol,*) "Jacobian Determinant: ",solndet
      write (out_log,*) "Jacobian Determinant: ",solndet

```

```

!       write column profiles to console for excel
        call display2
    else
        write (*,*) "Infeasible solution"
        write (out_sol,*) "Infeasible solution:"
        write (out_log,*) "Infeasible solution:"
        write (*,*) "Jacobian Determinant: ",solndet
        write (out_sol,*) "Jacobian Determinant: ",solndet
        write (out_log,*) "Jacobian Determinant: ",solndet
    end if
    call display(out_sol)
    call display(out_log)
    kstatus = 1
else if (kstatus .eq. 2) then    !Bifurcation found
    write (*,*) "Bifurcation found..."
    kstatus = 1
else if (kstatus .eq. 3) then    !Trifurcation found
    write (*,*) "Trifurcation found..."
    kstatus = 1
else if (kstatus .eq. 4) then    !Turning point found
    nturn = nturn + 1
    write (*,*) "Turning point ",nturn,":"
    kstatus = 1
else if (kstatus .eq. 5) then    !Starting point found
    nstart = nstart + 1
    write (*,*) "Starting point ",nstart,":"
    rstart = .true.    !test for repeated start point
    do j=1,2*nc+2
        if (abs(vars0(j)-vars(j))/abs(vars0(j)) .ge. 1.d-6)
&           rstart = .false.
        end do
    if (rstart) then
        nstart = nstart - 1
        write (*,*) "Path returns to original start point..."
        write (out_log,*) "returns to original start point..."
        exit
    end if
    kstatus = 1
else if (kstatus .eq. 10) then    !Step count exceeded
    kstatus = 1
else if (kstatus .eq. 20 .or. kstatus .eq. 21) then
!           Path goes to infinity
    write (*,*) "Path goes to infinity..."
    write (out_log,*) "Path goes to infinity..."
    exit
else if (kstatus .eq. 101) then    !Step size too small
    write (*,*) "Stopped due to small step size..."
    write (out_log,*) "Stopped due to small step size..."
    nstalls = nstalls - 1
    if (nstalls .eq. 0) exit
    kstatus = 1
else if (kstatus .eq. 102) then    !Process is stagnant
    write (*,*) "Stopped due to stagnation..."
    write (out_log,*) "Stopped due to stagnation..."
    nstalls = nstalls - 1
    if (nstalls .eq. 0) exit

```

```

    kstatus = 1
else if (kstatus .eq. 105) then !Singular homotopy matrix
    write (*,*) "Homotopy matrix is singular..."
    write (out_log,*) "Homotopy matrix is singular..."
    exit
else if (kstatus .eq. 106) then !No tangent vector
    write (*,*) "Tangent vector not obtained..."
    write (out_log,*) "Tangent vector not obtained..."
    exit
else if (kstatus .eq. 201) then !Start point out of bounds
    write (*,*) "Start point out of domain..."
    write (out_log,*) "Start point out of domain..."
    exit
else if (kstatus .eq. 202) then !Base point out of bounds
    write (*,*) "Base point out of domain..."
    write (out_log,*) "Base point out of domain..."
    exit
end if
if (nits .ge. maxits) then
    write (*,*) "Maximum steps exceeded..."
    exit
end if
end do
write (*,*)
write (*,*)"Solutions: ",nsoln," Feasible: ",nfeas
write (*,*)"Start points: ",nstart," Turn points: ",nturn
write (*,*)
write (*,*)
!
close (out_log)
close (out_sol)
close (out_pth)
!
end do ! while ( .not. quit)
stop
end
!
=====
! Include subroutine packages
!
include "probspec.f"
include "initprob.f"
include "display.f"
include "display2.f"
include "fdjac.f"
include "funcv.f"
include "altthermo.f"
include "homotopy.f"

```

PROBSPEC.F

```

subroutine probspec(f_in,method,first,quit)
! Subroutine to get problem specification from console or file
! Parameters:
!   f_in    logical, TRUE if input to be from file
!   in_spc  integer, channel # for input

```

```

!      out_spc  integer, channel # for saving problem spec
!      in_cdata integer, channel # for component props file
!      kstatus  integer, ?
!
!      Specification statements:
implicit real*8 (a-h,o-z)
logical f_in, c_in, dflag, quit, first, cdflag
integer ioflag, kthermo, nargs, nc, ns, method
character*80 ans
character*24 cname_in, formula, casno, cdfile
character*6 command
logical P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,P11,P12,P13,P14,P15,P16,
& P17,P18,P21,P31
save P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,P11,P12,P13,P14,P15,P16,
& P17,P18,P21,P31
!
!      Set parameter values
include "pgm_params.f"
!
!      Define common storage areas
include "cmn_params.f"
include "cmn_spec.f"
include "cmn_thermo.f"
include "cmn_hsparms.f"
!
common /rxn/ sprxk
save /hsparms/
!
quit = .true.
rgas=8.314510d0                !Energy units are joules
!-----
!      Set default values if first call
if (first) then
  P1=.false.;P2=.false.;P3=.false.;P4=.false.;P5=.false.
  P6=.false.;P7=.false.;P8=.false.;P9=.false.;P10=.false.
  P11=.false.;P12=.false.;P13=.false.;P14=.false.;P15=.false.
  P16=.false.;P17=.false.;P18=.false.;P21=.false.;P31=.false.
  nc=0; method=1; kthermo=1
  kspec=0;xspec=0.d0
  pdname_out=' '; c_desc=' '
  do i=1,ncmax
    cname(i)=' ';rxsto(i)=0.d0
  end do
  p=0.d0;fd_pres=0.d0;fd_temp=0.d0
  q=0.d0
  rxeff=0.d0;holdupl=0.d0
  do i=1,ncmax
    fd_ctot(i)=0.d0
  end do
  rxcoord = 0.d0
  scinit = 1.d0
  sprxk = 0.d0
  idom = 0; ihom = 1; dir = 1.d0; dso = 1.d-01
  dsmin = 1.d-20; dsmax = 5.d04; xmax = 1.d05
  ecorc = 1.d-04; ecorb = 1.d-06; edet = 5.d-01
  esol = 1.d-04; ebif = 1.d-04; etur = 1.d-06

```

```

esta = 1.d-04; easy = 1.d-06; maxdet = 5
minasy = 5; maxasy = 20
first = .false.
end if
!-----
pdname_out = ' '; c_desc = ' ' !Clear filename & description
P1 = .false.
do
  read (in_spc,'(a80)',IOSTAT=ioflag) ans
  if (ioflag .ne. 0) exit
  read (ans,*) command
  if (command .eq. "XC") exit
  if (command .eq. "P1") then !Case ID string
    read (ans,*) command, pdname_out
    if (pdname_out(1:1) .eq. "")
&      pdname_out=pdname_out(2:len_trim(pdname_out))
    P1 = .true.
  else if (command .eq. "P2") then !Case Description
    read (ans,*) command, c_desc
    if (c_desc(1:1) .eq. "")
&      c_desc=c_desc(2:len_trim(c_desc))
    P2 = .true.
  else if (command .eq. "P4") then !Case Thermo model
    read (ans,*) command, kthermo
    P4 = .true.
  else if (command .eq. "P5") then !Case Components
    read (ans,*) command, nc, cdfile
    if (cdfile(1:1) .eq. "")
&      cdfile=cdfile(2:len_trim(cdfile))
    inquire (file=cdfile, exist=cdflag)
    if (.not. cdflag) then
      quit=.true.; return
    end if
    open (in_cdata, file=cdfile)
    do i=1,nc
      read (in_spc,*) cname_in
      rewind in_cdata !find component in database
      do
        read (in_cdata,*,IOSTAT=ioflag) icomp, cname(i),
&      formula, casno, cmolwt(i), tmelt(i), tboil(i),
&      tcrit(i), pcrit(i), vcrit(i), zcrit(i),
&      acfac(i), delhf(i), delgf(i), tcpmin(i),
&      tcpmax(i), cpa0(i), cpa1(i), cpa2(i), cpa3(i),
&      cpa4(i), ieq, vpa(i), vpb(i), vpc(i),
&      pvpmin(i), pvpmax(i), tvpmin(i), tvpmax(i)
        if (ioflag .ne. 0) then
          quit=.true.; return
        end if
        if (cname(i) .eq. cname_in) exit
      end do
    end do
    P5 = .true.
  else if (command .eq. "P8") then !Case Top spec
    read (ans,*) command, kspec,xspec,ispec
    if (kspec .ne. 1 .or. kspec .ne. 2) q=xspec
    P8 = .true.
  end if
end do

```

```

else if (command .eq. "P10") then !Case Cond P & stg delta
  read (ans,*) command, p
  P10 = .true.
else if (command .eq. "P11") then !Case Feed spec
  !Clear old spec
  kfeed=0;fd_pres=0.d0;fd_temp=0.d0
  do i=1,nc
    fd_ctot(i)=0.d0
  end do
  read (ans,*) command, nf
  read (in_spc,*)j,kfeed,fd_pres,fd_temp,
&      (fd_ctot(i),i=1,nc)
  P11 = .true.
else if (command .eq. "P15") then !Case Stoich coeffs
  read (ans,*) command, (rxsto(i),i=1,nc)
  P15 = .true.
else if (command .eq. "P16") then !Case Rxn effs
  read (ans,*) command, rxeff
  P16 = .true.
else if (command .eq. "P18") then !Stage molar holdups
  read (ans,*) command, holdupl
  P16 = .true.
else if (command .eq. "P21") then !Spec homo solver parms
  read (ans,*) command, nq
  P18 = .true.
  if (nq .eq. 1) read (ans,*) command, nq, dir
  if (nq .eq. 2) read (ans,*) command, nq, dso
  if (nq .eq. 3) read (ans,*) command, nq, dsmin
  if (nq .eq. 4) read (ans,*) command, nq, dsmax
  if (nq .eq. 5) read (ans,*) command, nq, xmax
  if (nq .eq. 6) read (ans,*) command, nq, ecorc
  if (nq .eq. 7) read (ans,*) command, nq, ecorb
  if (nq .eq. 8) read (ans,*) command, nq, edet
  if (nq .eq. 9) read (ans,*) command, nq, esol
  if (nq .eq. 10) read (ans,*) command, nq, ebif
  if (nq .eq. 11) read (ans,*) command, nq, etur
  if (nq .eq. 12) read (ans,*) command, nq, esta
  if (nq .eq. 13) read (ans,*) command, nq, easy
  if (nq .eq. 14) read (ans,*) command, nq, idom
  if (nq .eq. 15) read (ans,*) command, nq, ihom
  if (nq .eq. 16) read (ans,*) command, nq, maxdet
  if (nq .eq. 17) read (ans,*) command, nq, minasy
  if (nq .eq. 18) read (ans,*) command, nq, maxasy
else if (command .eq. "P31") then !input for simple thermo
&      read (ans,*)command,alpha,tb1,delhv,delhr,cpl,cpv,
      rxntref, rxnke0,rxkf0,rxefwd
  kinetic = .true. !default to kinetic reaction model
  xtemp=0.d0 !set up to allocate delhr
  do i=1,nc
    if (rxsto(i) .gt. 0.d0) xtemp=xtemp+rxsto(i)
  end do
  do i=1,nc
    cpa0(i)=cpl; cpa1(i)=cpv; delhf(i)=0.d0
    if (i .eq. 1) then !set component boiling points
      tboil(i)=tb1
    else

```

```

        tboil(i)=delhv/(delhv/tboil(i-1) - rgas*log(alpha))
    end if
    vpb(i) = delhv / rgas
    vpa(i) = 1.3163d-02 + vpb(i) / tboil(i)
    if (rxsto(i) .gt. 0.d0) delhf(i)=delhr*rxsto(i)/xtemp
end do
rxeeql = delhr !set constants for rxn equilibrium K
if (rxkf0 .eq. 0.d0) kinetic = .false.
else if (command .eq. "P32") then !input for Antoine eq
    read (ans,*)command,i,vpa(i),vpb(i)
    tboil(i) = vpb(i) / ( vpa(i) - 1.3163d-02)
else if (command .eq. "P33") then !rx coord for init
    read (ans,*)command,rxcoord
else if (command .eq. "P34") then !scale factor for init
    read (ans,*)command,scinit
end if
end do
!
! Determine whether or not to run a case
quit = .not. (P1 .and. P5 .and. P8 .and. P10 .and. P11)
!
return
end

```

INITPROB.F

```

subroutine initprob
! Subroutine to set up initial solution estimates
!
!
! Specification statements:
implicit real*8 (a-h,o-z)
logical c_in, dflag, quit, trefset
integer ioflag, kthermo, nargs, nc, ns
character*80 ans
character*24 cname_in, formula, casno
!
! Set parameter values
include "pgm_params.f"
parameter (dflag = .false.)
!
! Define local storage areas
real*8 xnull, fvnull(ncmax),flnull(ncmax)
real*8 zfeed(ncmax), xfeed(ncmax), yfeed(ncmax),fctotal(ncmax),
& rxlim(ncmax),bulk_l(nsmax),bulk_v(nsmax),
& f(nsmax),g(ncmax,nsmax),vlek(ncmax,nsmax),
& fvalues(0:nvmax),fftf,ffvf
!
! Define common storage areas
include "cmn_params.f"
include "cmn_spec.f"
include "cmn_thermo.f"
!
common /rxn/ sprxk
!
!-----
! Clear the feed variables

```

```

ffvf=0.d0; fttf=0.d0
tref=tboil(1)
fd_enth=0.d0; fd_totl=0.d0; fd_psi=0.d0
do i=1,nc
  fd_liq(i)=0.d0; fd_vap(i)=0.d0
  fctotal(i) = 0.d0
end do
!
! Flash the feed, or compute its temperatures
call flash(kfeed,fd_ctot,fd_temp,fd_pres,p,
&         xfeed,yfeed,fd_enth,fd_totl,fd_psi)
do i=1,nc
  fd_liq(i) = xfeed(i)
  fd_vap(i) = yfeed(i)
  ffvf = ffvf + yfeed(i)
  fctotal(i) = fctotal(i) + fd_ctot(i)
  fttf = fttf + fd_ctot(i)
end do
ffvf = ffvf / fttf      !Fraction of total feed as vapor
!
! React composite feed to start
if (rxcoord .ge. 0.d0 .and. rxcoord .le. 1.d0) then
  !Reaction coordinate is specified
  do i=1,nc      !Compute feed over stoich coeff for all cpds
    rxlim(i) = 0.d0
    if(rxsto(i) .ne. 0.d0) rxlim(i) = -fctotal(i)/rxsto(i)
  end do
  rxflim = 0.d0; rxblim = 0.d0
  do i=1,nc      !find limiting extents
    rxblim = min(rxblim,rxlim(i))
    rxflim = max(rxflim,rxlim(i))
  end do
  do i=1,nc
    if (rxsto(i) .gt. 0) rxblim = max(rxblim,rxlim(i))
    if (rxsto(i) .lt. 0) rxflim = min(rxflim,rxlim(i))
  end do
  rxext = rxcoord*(rxflim - rxblim) + rxblim !Reaction extent
else
  !Approach to equilibrium is specified
  if (rxcoord .ge. 1.d0 .or. rxcoord .le. -1.d0) rxcoord = -1.d0
  !limit values to 0>x>=-1
  call flash(4,fctotal,fd_temp,p,p,
&         flnull,fvnull,xnull,xnull,ffvf) !Est avg T
  rxext = rxex(fctotal,fd_temp,p,nc,0,0) !Reaction extent
  rxext = -rxcoord * rxext
end if
fctsum = 0.d0
do i=1,nc
  fctotal(i) = fctotal(i) + rxsto(i)*rxext
  fctsum = fctsum + fctotal(i)      !sum of reacted feed
end do
do i=1,nc
  fctotal(i) = fctotal(i)/fctsum    !convert to mol fractions
end do
!
! Set initial reaction extent estimates

```



```

vars(nc+2) = 0.d0
!
! Set initial temperature estimate
vars(nc+1) = fd_temp
if (kspec .eq. 2) vars(nc+1) = xspec
!
! Approximate D/F and L1/D
fdf = fd_psi           !D/F
if (kspec .eq. 1) fdf = xspec
if (fdf .eq. 0.d0) fdf = 1.d-05 !Need at least some vapor to start
fld = 1.d0 - fdf       !L/D
!
! Tref = avg temperature
tref = vars(nc+1)
!
! Set bulk flow profiles, assuming constant overflow
totv = fdf * fctsum    !D
totl = fld * fctsum    !L
!
! Set component flow profiles
jv=0; jl=jv+nc+2
do i=1,nc
  vars(jv+i) = totv * fcttotal(i) * scinit
  vars(jl+i) = totl * fcttotal(i) * scinit
end do
!
return
end

```

DISPLAY.F

```

subroutine display(kchnl)
! Write distillation problem/solution description to console or
! log file.
!
! INPUTS:
! kchnl: i/o channel to use for output
!
implicit real*8 (a-h,o-z)
include "pgm_params.f" !Program parameters
include "cmn_params.f" !No. stages and No. components
include "cmn_cspec.f" !Column specifications
include "cmn_thermo.f" !Thermodynamic data
!
common /rxn/ sprxk
real*8 xtemp(ncmax)
!
!-----
! Show case ID and Description
write (kchnl,*)
write (kchnl,*)"Case ID: ", pdname_out
write (kchnl,'(a)')c_desc
!
!-----
! Show thermodynamic model used
! write (kchnl,'(a$)')"Thermodynamic model: "
! if (kthermo .eq. 4) then

```

```

!   write (kchnl,'(a)')"Van der Waals"
!   else if (kthermo .eq. 3) then
!     write (kchnl,'(a)')"Redlich-Kwong"
!   else if (kthermo .eq. 2) then
!     write (kchnl,'(a)')"Soave-Redlich-Kwong"
!   else
!     write (kchnl,'(a)')"Peng-Robinson"
!   end if
!
!-----
!   Show no. stages, no. components, and condenser type
write (kchnl,'(a,i3)')" Components: ",nc
!   if (kcond .eq. 2) then
!     write (kchnl,'(a)')"Partial"
!   else
!     write (kchnl,'(a)')"Total"
!   end if
!
!-----
!   Show component data (simplified system)
write(kchnl,'(a)')"Component information:"
write(kchnl,'(a)')"      alpha   Hv   Hr//"
&"   CpL   CpV   Krx"
write(kchnl,'(8x,6f10.2)')alpha,delhv,delhr,cpl,cpv,rxnke0
write(kchnl,'(a)')"      nu   Tb   CpL//"
&"   CpV   Hr"
do i=1,nc
  write(kchnl,'(2x,a6,5f10.2)')cname(i),rxsto(i),tboil(i),cpa0(i),
&   cpa1(i),delhf(i)
end do
!
!-----
!   Show material balance and energy balance specifications
if (kspec .eq. 1) then           !Spec V/F
write(kchnl,'(a,f10.3)')"Specified Vapor Fraction:",xspec
else if (kspec .eq. 2) then     !Spec T
write(kchnl,'(a,f10.3)')"Specified Temperature:",xspec
end if
!
!-----
!   Show column feeds
write(kchnl,*)"Feed:"
write(kchnl,1010)"Temp(K): ",fd_temp,
&   " Press(bar): ",fd_pres,
&   " Enthalpy(J): ",fd_enth
1010 format(a,f9.4,a,f9.4,a,f9.2)
write(kchnl,*)"      ", " Liquid   Vapor"
do i=1,nc
  write(kchnl,'(a12,2f10.4)')cname(i),fd_liq(i), fd_vap(i)
end do
!
!-----
!   Show Heat duty.
qc = (- fd_enth
&   + hstream(vars(1),vars(nc+1),p,nc,1)
&   + hstream(vars(nc+3),vars(nc+1),p,nc,0))

```

```

& /1.d3
write(kchnl,*)"Heat duty(kJ): ",qc
!
!-----
! Show pressure, temperature, heat duty, side draw, and
! efficiency profiles
write(kchnl,'(a)') " Q(kJ)  //"
& "Rxn eff  Rx(mol)  Rx(kJ)"
do i=1,nc
  xtemp(i)=fd_liq(i)+fd_vap(i)-vars(i)
end do
rxex = rxex(xtemp,vars(nc+1),p,nc,0,0)* rxeff
write (kchnl,1000)q,rxeff,rxex,rxex*delhr/1.d3
1000 format(2x,7f11.4)
!
!-----
! Show Pressure, Temperature, Heat duty, and Bulk flow profiles.
write(kchnl,'(a)') " P(bar)  T(K)  //"
& "L(mol)  V(mol)  H err  L(kJ)  V(kJ)"
jstg = 0
totv = 0.d0
totl = 0.d0
do i=1,nc
  totv = totv + vars(jstg+i)
  totl = totl + vars(jstg+nc+2+i)
  vlk(i) = vler(vars(jstg+nc+3),vars(jstg+1),
& vars(jstg+nc+1),p,nc,i)
end do
hvap = hstream(vars(jstg+1),vars(jstg+nc+1),p,nc,1)/ 1.d3
hliq = hstream(vars(jstg+nc+2+1),vars(jstg+nc+1),p,nc,0)/ 1.d3
rxk = rxer(vars(jstg+nc+3),vars(jstg+nc+1),p,nc,0,0)
herr = fd_enth+q-hliq-hvap
if (q .eq. 0.d0) herr = herr + qc
write (kchnl,1000)p,vars(jstg+nc+1),totl,totv, herr,hliq,hvap
write (kchnl,'(57x,2f11.4)')hliq/totl,hvap/totv
!
!-----
! Show Vapor flow profiles
write(kchnl,*)"Vapor flows/compositions:"
do ii=1,nc,5
  ij=ii+4
  if (ij .ge. nc) ij=nc
  write(kchnl,'(6x,5a12)')(cname(i),i=ii,ij)
  jj=0
  write(kchnl,'(2x,5f12.4)')(vars(jj+i),i=ii,ij)
  write(kchnl,'(2x,5f12.6)')(vars(jj+i)/totv,i=ii,ij)
end do
!
!-----
! Show Liquid flow profiles
write(kchnl,*)"Liquid flows/compositions:"
do ii=1,nc,5
  ij=ii+4
  if (ij .ge. nc) ij=nc
  write(kchnl,'(6x,5a12)')(cname(i),i=ii,ij)
  jj=nc+2
  write(kchnl,'(2x,5f12.4)')(vars(jj+i),i=ii,ij)

```

```

        write(kchnl,'(2x,5f12.6)')(vars(jj+i)/totl,i=ii,ij)
    end do
!
!-----
! Show component creation/consumption
write(kchnl,*)"Component creation & consumption:"
do i=1,nc
    xtemp(i)=vars(i)+vars(nc+2+i)
    xtemp(i)=xtemp(i)-fd_liq(i)-fd_vap(i)
end do
do ii=1,nc,5
    ij=ii+4
    if (ij .ge. nc) ij=nc
    write(kchnl,'(6x,5a12)')(cname(i),i=ii,ij)
    write(kchnl,'(2x,5f12.4)')(xtemp(i),i=ii,ij)
end do
!
!-----
! Show VLE equilibrium ratios
write(kchnl,*)"Vapor/Liquid equilibrium ratios:"
do ii=1,nc,5
    ij=ii+4
    if (ij .ge. nc) ij=nc
    write(kchnl,'(9x,5a12)')(cname(i),i=ii,ij)
    jv=0
    jl=jv+nc+2
    write(kchnl,'(2x,5e12.4)')(vlk(i),i=ii,ij)
    write(kchnl,'(5x,5e12.4)')(((vars(jv+i)*totl)/
&      (vars(jl+i)*totv)),i=ii,ij)
end do
!
!-----
! Show Reaction equilibrium ratios
write(kchnl,*)"Reaction equilibrium ratios:"
write(kchnl,'(3x,a,2x,a)')"From thermo", "From flows"
rktemp = 1.d0
do i=1,nc
    if (rxsto(i) .ne. 0.d0) rktemp=rktemp*
&      ((vars(nc+2+i)/totl)**rxsto(i))
end do
    write(kchnl,'(2x,2e12.4)')rxk,rktemp
!
!-----
! Show Stream bubble and dew points
write (kchnl,*)"Stream bubble/dew points:"
write (kchnl,*)"  L bubble   V dew"
jstg=0
dbub=bubpt(vars(jstg+nc+3),p)
ddew=dewpt(vars(jstg+1),p)
write(kchnl,'(2x,2f10.4)')dbub,ddew

return
end
DISPLAY2.F

subroutine display2

```

```

!   Write solution description to console for excel
!
implicit real*8 (a-h,o-z)
include "pgm_params.f" !Program parameters
include "cmn_params.f" !No. stages and No. components
include "cmn_cspect.f" !Column specifications
include "cmn_thermo.f" !Thermodynamic data
!
real*8 xtemp(ncmax)
!
!-----
!   Show case ID
write (*,*)
write (*,*)"Case ID,", pdname_out
!
!-----
!   Show Temperature and Bulk flow profiles.
write(*,*)"j,T,L,V,L/V"
jstg = 0
totv = 0.d0
totl = 0.d0
do i=1,nc
  totv = totv + vars(jstg+i)
  totl = totl + vars(jstg+nc+2+i)
end do
jstg = 0
write (*,(f12.6,3(" ",f12.6)))vars(jstg+nc+1),totl,
&          totv,totl/totv
!-----
!   Show Vapor composition profiles
write(*,*)"y's"
jstg = 0
write(*,(f12.6,9(" ",f12.6)))(vars(jstg+i)/totv,i=1,nc)
!
!-----
!   Show Liquid composition profiles
write(*,*)"x's"
jstg = nc+2
write(*,(f12.6,9(" ",f12.6)))(vars(jstg+i)/totl,i=1,nc)
!
!-----
!   Show component overall conversion
write(*,*)"Overall conversion"
do i=1,nc
  xtemp(i)=fd_ctot(i)
  if (xtemp(i) .ne. 0.d0) xtemp(i)=1.d0-
&          ((vars(i)+vars(nc+2+i))/xtemp(i))
end do
write(*,(f12.6,9(" ",f12.6)))(xtemp(i),i=1,nc)
!
!-----
!   Show Condenser and Reboiler duties.
qc = (- fd_enth
&    + hstream(vars(1),vars(nc+1),p,nc,1)
&    + hstream(vars(nc+3),vars(nc+1),p,nc,0))
&    /1.d3

```

```

write(*,*)"Heat duty(kJ)," ,qc
!
!-----

return
end
FDJAC.F

subroutine fdjac(x,fvec,df,n,NP)
!   USES funcv
implicit real*8 (a-h,o-z)
PARAMETER (EPS=1.d-5)
dimension df(np,np),fvec(np),x(np),f(np)
!   Computes forward-difference approximation to Jacobian. On input,
!   x(1:n) is the point at which the Jacobian is to be evaluated,
!   fvec(1:n) is the vector of function values at the point, and np
!   is the physical dimension of the Jacobian array df(1:n,1:n) which
!   is output. subroutine funcv(n,x,f) is a fixed-name, user-supplied
!   routine that returns the vector of functions at x.
!   Parameters: EPS is the approximate square root of the machine
!   precision.
do j=1,n
  temp=x(j)
  h=EPS*abs(temp)
  if(h .eq. 0.d0)h=EPS
  x(j)=temp+h      !Trick to reduce finite precision error.
  h=x(j)-temp
  call funcv(x, f, n, ierr)
  x(j)=temp
  do i=1,n          !Forward difference formula.
    df(i,j)=(f(i)-fvec(i))/h
  end do
end do
return
end

FUNCV.F

subroutine funcv(x,f,n,ierr)
!   Calculate discrepancy function values f, for the column
!   variables held in vector x.
!   REVISED: 4/8/09    Changed column to flash drum
!   INPUTS:
!     x : vector of column variables, as follows for each
!         stage - nc vapor flows, 1 stage temperature, 1 stage
!         reaction extent, and nc liquid flows.
!     n : number of equations to evaluate - not used in this
!         implementation.
!   OUTPUTS:
!     f : vector of calculated discrepancy function values -
!         for each stage 1 energy balance, 1 reaction
!         equilibrium function, nc material balances,
!         and nc equilibrium relationships.
!     ierr: error flag ( >0 if error)
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"

```

```

include "cmn_params.f"
include "cmn_cspec.f"
include "cmn_thermo.f"
!
real*8 x(*),f(*)
real*8 xt(ncmax)          !vector of stage l-primes
!
  jxv = 0                  !pointer to vapor flows
  jxt = jxv+nc+1          !Pointer to temperature
  jxx = jxt+1              !Pointer to rxn extent
  jxl = jxx                !pointer to liquid flows
  jfe = 1                  !pointer to energy bal function
  jfr = jfe+1              !pointer to rxn eq function
  jfm = jfr                !pointer to matl bal functions
  jfq = jfm+nc            !pointer to v/l equil functions
!
! calculate total stage flows
  tlj = 0.d0; tvj = 0.d0
  xmaxl = 0.d0; imaxl = 0
  xtsum = 0.d0; eps = 0.d0
  do i=1,nc
    tlj = tlj + x(jxl+i)
    tvj = tvj + x(jxv+i)
    xt(i) = fd_liq(i) + fd_vap(i) - x(jxv+i)
    if (x(jxl+i) .ge. xmaxl)then
      xmaxl = x(jxl+i)
      imaxl = i
    end if
    xtsum = xtsum + xt(i); eps = eps + rxsto(i)
  end do
!
  do i=1,nc
! Material Balance Functions
    f(jfm+i) = -fd_ctot(i) - x(jxx)*rxsto(i) + x(jxv+i) + x(jxl+i)
!
! Vapor / Liquid Equilibrium functions
    vk = vler(x(jxl+1),x(jxv+1),x(jxt),p,nc,i) !VLE K
    f(jfq+i) = vk*x(jxl+i)/tlj - x(jxv+i)/tvj
!    f(jfq+i) = f(jfq+i)*(tlj+tvj)/2.d0 !Scale to M functions
  end do
!
! Energy balance function
  f(jfe) = -q - fd_enth
&      +hstream(x(jxl+1),x(jxt),p,nc,0)
&      +hstream(x(jxv+1),x(jxt),p,nc,1)
!                               !Scale H functions to M's
  f(jfe) = f(jfe)/((hstream(x(jxl+1),x(jxt),p,nc,0)/tlj+
! &      hstream(x(jxv+1),x(jxt),p,nc,1)/tvj)/2)
!
! Reaction equilibrium function
  rxk = rxer(xt,x(jxt),p,nc,i,0)
  if ((kinetic .and. holdupl .eq. 0.d0) .or. (.not. kinetic
&      .and. rxeff .eq. 0.d0))then
    f(jfr) = x(jxx) - 0.d0      !no reaction
  else
    if (kinetic) then          !kinetic reaction model

```

```

    rxneff = 1.d0; rxntot = xtsum+rxneff*eps*x(jxx)
    f2 = holdupl*rxkf(xt,x(jxt),p,nc,i,0)/rxntot
    f1 = rxk*f2; f3 = rxk*x(jxx)/rxntot
else
    !equilibrium reaction model
    rxneff = 1.d0/rxeff; rxntot = xtsum+rxneff*eps*x(jxx)
    f1 = rxk; f2 = 1.d0; f3 = 0.d0
end if
do i=1,nc
    if (rxsto(i) .lt. 0.d0) then
        f1 = f1 * ((xt(i)+(rxneff*rxsto(i)*x(jxx)))/
& rxntot)**(-rxsto(i))
    else if (rxsto(i) .gt. 0.d0) then
        f2 = f2 * ((xt(i)+(rxneff*rxsto(i)*x(jxx)))/
& rxntot)**rxsto(i)
    end if
end do
f(jfr) = f1 - f2 - f3
end if

!
! Substitute functions due to specifications
!
if (kspec .eq. 1) then
    !Spec V/F
    dst = 0.d0
    do i=1,nc
        dst = dst + x(jxv+i)
    end do
    f(jfe) = dst - xspec*fd_totl
else if (kspec .eq. 2) then
    !Spec T
    f(jfe) = x(jxt) - xspec
end if
ierr = 0
!
return
end

```

ALTTHERMO.F

```

subroutine flash(kf, zf, tf, pf, pstg, xf, yf, hf,ftotal,psi)
! Computes the flash of stream zf to form streams xf and yf
! Inputs:
!   kf : flash type
!   zf : vector containing feed compositions or flows
!   tf : flash temperature
!   pf : flash pressure
!   pstg: ?
! Outputs:
!   xf : vector of output liquid compositions or flows
!   yf : vector of output vapor compositions or flows
!   hf :
!   ftotal:
!   psi : Fraction of feed leaving as vapor
!
! Specification statements:
implicit real*8 (a-h,o-z)
! Set parameter values
include "pgm_params.f"

```



```

parameter (itmax = 25, xacc = 1.d-6)
!   Define data storage
include "cmn_params.f"
real*8 zf(ncmax), xf(ncmax), yf(ncmax), z(ncmax), x(ncmax),
&   y(ncmax), vlek(ncmax), ftotal, psi, tbp, tdp

fpsi(psi, i) = z(i)*(1.d0-vlek(i))/(1.d0+psi*(vlek(i)-1.d0))
ftmp(t,i) = z(i)*(1.d0-vler(z,z,t,pstg,nc,i)/
& (1.d0+psi*(vler(z,z,t,pstg,nc,i)-1.d0))
!
!   Normalize feed vector and calculate dew and bubble points
ftotal = 0.d0
do i=1,nc
    ftotal = ftotal + zf(i)
end do
do i=1,nc
    z(i) = zf(i)/ftotal; x(i) = 0.d0; y(i) = 0.d0
end do
tbp = bubpt(z, pstg)
tdp = dewpt(z, pstg)
if (kf .eq. 1) then          ! Bubble point liquid feed
    tf = tbp
    hf=hstream(zf,tf,pf,nc,0)
    do i=1,nc
        xf(i) = zf(i); yf(i) = 0.d0
    end do
    psi = 0.d0
else if (kf .eq. 2) then    ! Dew point vapor feed
    tf = tdp
    hf=hstream(zf,tf,pf,nc,1)
    do i=1,nc
        yf(i) = zf(i); xf(i) = 0.d0
    end do
    psi = 1.d0
else if (kf .eq. 3) then    ! Spec temp flash
    if (tf .ge. tdp) then    ! T above dew point
        do i=1,nc
            yf(i) = zf(i); xf(i) = 0.d0
        end do
        psi = 1.d0
        hf=hstream(zf,tf,pf,nc,1)
    else if (tf .le. tbp) then ! T below bubble point
        do i=1,nc
            xf(i) = zf(i); yf(i) = 0.d0
        end do
        psi = 0.d0
        hf=hstream(zf,tf,pf,nc,0)
    else                    ! T between dew & bubble pts
        psi1 = 0.d0
        psi2 = 1.d0
        f1 = 0.d0
        f2 = 0.d0
        psi = -1
        do i=1,nc
            vlek(i) = vler(z,z,tf,pstg,nc,i)
            f1 = f1 + fpsi(psi1, i)

```

```

    f2 = f2 + fpsi(psi2, i)
end do
do n=1,itmax
  psi3 = 0.5d0*(psi1+psi2)
  f3 = 0.d0
  do i=1,nc
    f3 = f3 + fpsi(psi3, i)
  end do
  psi4 = psi3 + (psi3 - psi1)*(sign(1.d0, f1-f2)*f3
&      /sqrt(f3**2 - f1*f2))
  if (abs(psi4-psi) .le. xacc) then
    exit
  end if
  psi = psi4
  f4 = 0.d0
  do i=1,nc
    f4 = f4 + fpsi(psi4, i)
  end do
  if (f4 .eq. 0.d0) then
    end if
  if (sign(f3, f4) .ne. f3) then
    psi1 = psi3; f1 = f3; psi2 = psi4; f2 = f4
  else if (sign(f1, f4) .ne. f1) then
    psi2 = psi4; f2 = f4
  else if (sign(f2, f4) .ne. f2) then
    psi1 = psi4; f1 = f4
  end if
end do
do i=1,nc
  x(i) = z(i) / (1.d0+psi*(vlek(i)-1.d0))
  y(i) = x(i)*vlek(i)
  xf(i) = ftotal * (1.d0-psi) * x(i)
  yf(i) = ftotal * psi * y(i)
end do
hf=psi*hstream(zf,tf,pf,nc,1) +
& (1.d0-psi)*hstream(zf,tf,pf,nc,0)
end if
else if (kf .eq. 4) then      !Spec V/F flash
  if (psi .le. 0.d0) then    !All liquid
    do i=1,nc
      xf(i) = zf(i); yf(i) = 0.d0
    end do
    tf = tbp
    hf = hstream(zf,tf,pf,nc,0)
  else if (psi .ge. 1.d0) then !All vapor
    do i=1,nc
      yf(i) = zf(i); xf(i) = 0.d0
    end do
    tf = tdp
    hf = hstream(zf,tf,pf,nc,1)
  else
    t1 = tbp; f1 = 0.d0
    t2 = tdp; f2 = 0.d0
    tf = -1.d0
    do i=1,nc
      f1 = f1+ftmp(t1,i)

```

```

        f2 = f2+ftmp(t2,i)
    end do
    do n=1,itmax
        t3 = 0.5d0*(t1+t2); f3 = 0.d0
        do i=1,nc
            f3 = f3+ftmp(t3,i)
        end do
        t4 = t3 + (t3-t1)*(sign(1.d0,f1-f2)*f3
&          /sqrt(f3**2 - f1*f2))
        if (abs(t4-tf) .le. xacc) then
            exit
        end if
        tf = t4; f4 = 0.d0
        do i=1,nc
            f4 = f4+ftmp(t4,i)
        end do
        if (f4 .eq. 0.d0) then
            end if
        if (sign(f3,f4) .ne. f3)then
            t1 = t3; f1 = f3; t2 = t4; f2 = f4
        else if (sign(f1,f4) .ne. f1) then
            t2 = t4; f2 = f4
        else if (sign(f2,f4) .ne. f2) then
            t1 = t4; f1 = f4
        end if
    end do
    do i=1,nc
        vlek(i) = vler(z,z,tf,pstg,nc,i)
        x(i) = z(i) / (1.d0+psi*(vlek(i)-1.d0))
        y(i) = x(i) * vlek(i)
        xf(i) = ftotal * (1.d0-psi) * x(i)
        yf(i) = ftotal * psi * y(i)
    end do
    hf = psi*hstream(zf,tf,pf,nc,1) +
&      (1.d0-psi)*hstream(zf,tf,pf,nc,0)
    end if
end if
return
end

```

```

=====
real*8 function bubpt(x,p)
!   Computes bubblepoint temperature of stream x at pressure p
!
!   Specification statements:
implicit real*8 (a-h,o-z)
!   Set parameter values
include "pgm_params.f"
parameter (itmax = 50, xacc = 1.d-6, factor = 1.6d0)
!   Define data storage
include "cmn_params.f"
include "cmn_thermo.f"
!
!   real*8 x(ncmax),xnorm(ncmax)
!
!   Normalize x
xnormsum=0.d0

```

```

do i=1,nc
  xnormsum=xnormsum+x(i)
end do
do i=1,nc
  xnorm(i)=x(i)/xnormsum
end do

! Use component boil points to start
t1 = tboil(1)
t2 = tboil(nc)
f1 = 1.d0
f2 = 1.d0
bubpt = -1.d0
do i=1,nc
  f1 = f1 - xnorm(i) * vler(xnorm,xnorm,t1,p,nc,i)
  f2 = f2 - xnorm(i) * vler(xnorm,xnorm,t2,p,nc,i)
end do
do n=1,itmax          ! make sure point is bracketed
  if (f1*f2 .lt. 0.d0) exit
  if (abs(f1) .lt. abs(f2)) then
    t1 = t1+factor*(t1-t2)
    f1 = 1.d0
    do i=1,nc
      f1 = f1 - xnorm(i) * vler(xnorm,xnorm,t1,p,nc,i)
    end do
  else
    t2 = t2+factor*(t2-t1)
    f2 = 1.d0
    do i=1,nc
      f2 = f2 - xnorm(i) * vler(xnorm,xnorm,t2,p,nc,i)
    end do
  end if
end do
if (f1*f2 .ge. 0.d0) write(*,*)"BUBPT: Failed to find range."
do n=1,itmax          ! search for best value
  t3 = 0.5d0*(t1+t2)
  f3 = 1.d0
  do i=1,nc
    f3 = f3 - xnorm(i) * vler(x,x,t3,p,nc,i)
  end do
  t4 = t3 + (t3 - t1)*(sign(1.d0, f1-f2)*f3/sqrt(f3**2 - f1*f2))
  if (abs(t4-bubpt) .le. xacc) return
  bubpt = t4
  f4 = 1.d0
  do i=1,nc
    f4 = f4 - xnorm(i) * vler(x,x,t4,p,nc,i)
  end do
  if (f4 .eq. 0.d0) return
  if (sign(f3, f4) .ne. f3) then
    t1 = t3; f1 = f3; t2 = t4; f2 = f4
  else if (sign(f1, f4) .ne. f1) then
    t2 = t4; f2 = f4
  else if (sign(f2, f4) .ne. f2) then
    t1 = t4; f1 = f4
  end if
  if (abs(t2 - t1) .le. xacc) return

```

```

end do
write (*,*) "BUBPT: fails to converge in ",itmax," iterations"
write(*,*)"BUBPT: Returned value is: ",bubpt
return
end
=====
real*8 function dewpt(x,p)
!   Computes dewpoint temperature of stream x at pressure p
!
!   Specification statements:
implicit real*8 (a-h,o-z)
!   Set parameter values
include "pgm_params.f"
parameter (itmax = 50, xacc = 1.d-6, factor = 1.6d0)
!   Define data storage
include "cmn_params.f"
include "cmn_thermo.f"
!
real*8 x(ncmax),xnorm(ncmax)
!
!   Normalize x
xnormsum=0.d0
do i=1,nc
  xnormsum=xnormsum+x(i)
end do
do i=1,nc
  xnorm(i)=x(i)/xnormsum
end do

! Use component boil points to start
t1 = tboil(1)
t2 = tboil(nc)
f1 = 1.d0
f2 = 1.d0
dewpt = -1.d0
do i=1,nc
  f1 = f1 - xnorm(i) / vler(xnorm,xnorm,t1,p,nc,i)
  f2 = f2 - xnorm(i) / vler(xnorm,xnorm,t2,p,nc,i)
end do
do n=1,itmax
  ! make sure point is bracketed
  if (f1*f2 .lt. 0.d0) exit
  if (abs(f1) .lt. abs(f2)) then
    t1 = t1+factor*(t1-t2)
    f1 = 1.d0
    do i=1,nc
      f1 = f1 - xnorm(i) / vler(xnorm,xnorm,t1,p,nc,i)
    end do
  else
    t2 = t2+factor*(t2-t1)
    f2 = 1.d0
    do i=1,nc
      f2 = f2 - xnorm(i) / vler(xnorm,xnorm,t2,p,nc,i)
    end do
  end if
end do
if (f1*f2 .ge. 0.d0) write(*,*)"DEWPT: Failed to find range."

```

```

do n=1,itmax          ! search for best value
  t3 = 0.5d0*(t1+t2)
  f3 = 1.d0
  do i=1,nc
    f3 = f3 - xnorm(i) / vler(xnorm,xnorm,t3,p,nc,i)
  end do
  t4 = t3 + (t3 - t1)*(sign(1.d0, f1-f2)*f3/sqrt(f3**2 - f1*f2))
  if (abs(t4-dewpt) .le. xacc) return
  dewpt = t4
  f4 = 1.d0
  do i=1,nc
    f4 = f4 - xnorm(i) / vler(xnorm,xnorm,t4,p,nc,i)
  end do
  if (f4 .eq. 0.d0) return
  if (sign(f3, f4) .ne. f3) then
    t1 = t3; f1 = f3; t2 = t4; f2 = f4
  else if (sign(f1, f4) .ne. f1) then
    t2 = t4; f2 = f4
  else if (sign(f2, f4) .ne. f2) then
    t1 = t4; f1 = f4
  end if
  if (abs(t2 - t1) .le. xacc) return
end do
write (*,*) "DEWPT: fails to converge in ",itmax," iterations"
write(*,*)"DEWPT: Returned value is: ",dewpt
return
end
=====
real*8 function rxex(x,t,pstg,nc,ic,kst)
!   Compute the equilibrium extent of reaction at t and p
!   Inputs:
!     x :   vector of stream compositions or flows
!     t :   temperature for the calculation, K
!     p :   pressure for the calculation, bar
!     nc :  number of components in x
!     ic :  component index (not used in this calc'n)
!     kst:  Stream state (0=>liquid; 1=>vapor)
!   Outputs:
!     rxex: Calculated extent of reaction
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
parameter (gs = 0.381966011d0) !parm for golden section search
!
rxek = rxer(x,t,pstg,nc,ic,kst) !Get the equilibrium constant
xmax = 1.d20
xmin = -1.d20
xsum = 0.d0
eps = 0.d0
do i=1,nc                !find max fwd and rev extents
  xsum = xsum + x(i)
  eps = eps + rxsto(i)
  if (rxsto(i) .ne. 0.d0) then
    xtemp = - x(i) / rxsto(i)

```

```

        if (rxsto(i) .lt. 0.d0 .and. xtemp .lt. xmax) xmax = xtemp
        if (rxsto(i) .gt. 0.d0 .and. xtemp .gt. xmin) xmin = xtemp
    end if
end do
! Initialize for Brent method search to find the root
a = xmin; b = xmax
fa1 = 1.d0; fa2 = rxek
fb1 = 1.d0; fb2 = rxek
do i=1,nc          !f(x) = product of factor, minus rxek
    if (rxsto(i) .gt. 0.d0) then
        fa1=fa1*((x(i)+rxsto(i)*a)/(xsum+eps*a))**rxsto(i)
        fb1=fb1*((x(i)+rxsto(i)*b)/(xsum+eps*b))**rxsto(i)
    else if (rxsto(i) .lt. 0.d0) then
        fa2=fa2*((x(i)+rxsto(i)*a)/(xsum+eps*a))**(-rxsto(i))
        fb2=fb2*((x(i)+rxsto(i)*b)/(xsum+eps*b))**(-rxsto(i))
    end if
end do
fa=fa1-fa2; fb=fb1-fb2
! fa=fa-rxek; fb=fb-rxek
c = b; fc = fb
do k=1,100          !search loop
    if (fb*fc .ge. 0.d0) then
!       Rename a,b,&c and adjust bounding interval d
        c=a; fc=fa; d=b-a; e=d
    end if
    if (abs(fc) .lt. abs(fb)) then !swap a and c with b
        a=b; b=c; c=a
        fa=fb; fb=fc; fc=fa
    end if
    tol1 = 2.d0*1.d-8*abs(b) + 0.5d0*1.d-8 !check convergence
    xm = 0.5d0*(c-b)
    if (abs(xm) .le. tol1 .or. fb .eq. 0.d0) then !Converged
        rxex = b
        return
    end if
    if (abs(e) .gt. tol1 .and. abs(fa) .gt. abs(fb)) then
!       Try inverse quadratic interpolation
        s = fb/fa
        if (a .eq. c) then
            p = 2.d0*xm*s
            q = 1.d0 - s
        else
            q = fa/fc
            r = fb/fc
            p = s*(2.d0*xm*q*(q-r)-(b-a)*(r-1.d0))
            q = (q-1.d0)*(r-1.d0)*(s-1.d0)
        end if
        if (p .gt. 0.d0) q = -q !Check whether in bounds
        p = abs(p)
        if (2.d0*p .lt. min(3.d0*xm*q-abs(tol1*q), abs(e*q))) then
            e=d          !Accept interpolation
            d=p/q
        else
            d=xm          !Interpolation failed, use bisection
            e=d
        end if
    end if
end do

```

```

else
  d=xm      !Bounds decreasing too slowly, use bisection
  e=d
end if
a=b        !Move last guess to a
fa=fb
if (abs(d) .gt. tol1) then      !Evaluate new trial root
  b=b+d
else
  b=b+sign(tol1,xm)
end if
fb1=1.d0; fb2=rxek  !Compute function value for new trial root
do i=1,nc
  if (rxsto(i) .gt. 0.d0) then
    fb1 = fb1*((x(i)+rxsto(i)*b)/(xsum+eps*b))**rxsto(i)
  else if (rxsto(i) .lt. 0.d0) then
    fb2 = fb2*((x(i)+rxsto(i)*b)/(xsum+eps*b))**(-rxsto(i))
  end if
end do
fb=fb1-fb2
end do
rxex = b
write (*,*)"Reaction extent = ",rxex," Excess Iterations"
return
end
=====
real*8 function vler(x,y,t,p,nc,ic)
! Computes the vapor-liquid equilibrium ratio for
! component ic in the mixture x at t and p
! Inputs:
!   x : vector of liquid stream compositions or flows
!   y : vector of vapor stream compositions or flows
!   t : temperature for the calculation, K
!   p : pressure for the calculation, bar
!   nc : number of components in x
!   ic : index of the component of interest
! Outputs:
!   vler: Calculated value of the property
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*),y(*)
!
vler = exp( vpa(ic) - vpb(ic)/t ) / p
! vler =exp(-((1.d0/t)-(1.d0/tboil(ic)))*delhv/rgas)
return
end
=====
real*8 function hstream(x,t,p,nc,kst)
! Compute the enthalpy of stream x at t and p in state kst,
! relative to tref. Value returned is in units of kJ
! Inputs:
!   x : vector of stream compositions or flows
!   t : temperature for the calculation, K
!   p : pressure for the calculation, bar

```



```

!      nc :   number of components in x
!      kst:   Stream state (0=>liquid; 1=>vapor)
!  Outputs:
!      hstream:  Calculated enthalpy, kJ
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
!
t0 = tref          !Reference Temp
hstream = 0.d0
xsum = 0.d0
do i=1,nc
  xsum = xsum+x(i)
end do
if (kst .eq. 0) then
  do i=1,nc          !liquid enthalpy
    hstream = hstream + ((t-t0)*cpa0(i)+delhf(i))*x(i)/xsum
!    hstream = hstream + ((t-t0)*cpa0(i))*x(i)/xsum
  end do
else
!  hstream = delhv/xsum
  do i=1,nc          !vapor enthalpy
    hstream = hstream + ((tboil(i)-t0)*cpa0(i) + (t-tboil(i))
&      *cpa1(i) + delhf(i) + delhv)*x(i)/xsum
!    hstream = hstream + ((tboil(i)-t0)*cpa0(i) + (t-tboil(i))
!    &      *cpa1(i))*x(i)/xsum
  end do
end if
hstream = hstream * xsum      !change molar to total   !kJ
return
end
=====
real*8 function rxer(x,t,p,nc,ic,kst)
!  Compute the reaction equilibrium constant at t and p
!  Inputs:
!      x :   vector of stream compositions or flows
!      t :   temperature for the calculation, K
!      p :   pressure for the calculation, bar
!      nc :  number of components in x
!      ic :  component index (not used in this calc'n)
!      kst:  Stream state (0=>liquid; 1=>vapor)
!  Outputs:
!      rxer:  Calculated value of the equilibrium constant
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"     !component thermodynamic data
dimension x(*)
rxer = rxnke0*exp(((1.d0/rxntref)-(1.d0/t))*rxeeql/rgas)
!
return
end
=====
real*8 function rxkf(x,t,p,nc,ic,kst)

```

```

! Compute the reaction forward rate constant at t and p
! Inputs:
!   x : vector of stream compositions or flows
!   t : temperature for the calculation, K
!   p : pressure for the calculation, bar
!   nc : number of components in x
!   ic : component index (not used in this calc'n)
!   kst: Stream state (0=>liquid; 1=>vapor)
! Outputs:
!   rxkf: Calculated value of the rate constant
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"    !component thermodynamic data
dimension x(*)
rxkf = rxkf0*exp(((1.d0/rxntref)-(1.d0/t))*rxefwd/rgas)
!
return
end

```

```

=====
real*8 function boiltemp(ic,p)
! Compute the boiling temperature for component ic at pressure p
! Inputs:
!   ic : component index
!   p : pressure for the calculation, bar
! Outputs:
!   boiltemp: Calculated value of the boiling temperature
!
implicit real*8 (a-h,o-z)
include "pgm_params.f"      !Storage allocation parameters
include "cmn_thermo.f"    !component thermodynamic data
boiltemp = vpb(ic)/(vpa(ic) - log(p))
!
return
end
=====

```

COMMON BLOCK DEFINITIONS

CMN_CSPEC.F

```

character*80 c_desc
character*24 piname_in, pdname_out
integer kspec, ispec, jspec, kcond, kfeed
real*8 fd_liq, fd_vap, fd_ctot, fd_temp, fd_pres, fd_enth,
& fd_totl, fd_psi,
& p, q, sd_l, sd_v, stg_mve, rxeff, totl, totv, hliq, hvap,
& rxk, vlk, vars, vars0, xspec
common /colspec/ fd_liq(ncmax,nsmax), fd_vap(ncmax,nsmax),
& fd_ctot(ncmax,nsmax),
& fd_temp(nsmax), fd_pres(nsmax), fd_enth(nsmax),fd_totl(nsmax),
& fd_psi(nsmax),
& p(nsmax), q(nsmax), sd_l(nsmax), sd_v(nsmax),
& stg_mve(nsmax),rxeff(nsmax),holdupl(nsmax),
& totl(nsmax),totv(nsmax), hliq(nsmax), hvap(nsmax),
& rxk(nsmax), vlk(ncmax,nsmax), vars(0:nvmax), vars0(0:nvmax),

```

```
& rxcoord, scinit, xspec(2), kspec(2), ispec(2), jspec(2), kcond,
& kfeed(nsmx), psmx_in, pdname_out, c_desc
```

```
!
```

```
integer in_spc, out_spc, out_log, out_sol, out_pth, in_cdata
common /iochn/in_spc, out_spc, out_log, out_sol, out_pth, in_cdata
```

CMN_HSPARMS.F

```
common /hsparms/ dir, dso, dsmin, dsmax, xmax,
& ecorc, ecorb, edet, esol, ebif, etur, esta, easy,
& idom, ihom, maxdet, minasy, maxasy
```

CMN_PARAMS.F

```
common /params/ns, nc
```

CMN_THERMO.F

```
character*24 cname
logical kinetic
common /thermo/ cname(ncmax), cmolwt(ncmax), tmelt(ncmax),
& tboil(ncmax), tcrit(ncmax), pcrit(ncmax), vcrit(ncmax),
& zcrit(ncmax), acfac(ncmax), delhf(ncmax), delgf(ncmax),
& tcpmin(ncmax), tcpmax(ncmax), cpa0(ncmax),cpa1(ncmax),
& cpa2(ncmax), cpa3(ncmax), cpa4(ncmax),vpa(ncmax), vpb(ncmax),
& vpc(ncmax), pvpmin(ncmax), pvpmax(ncmax), tvpmin(ncmax),
& tvpmax(ncmax),rxsto(ncmax),
& fwvl(ncmax), acvl, bcvl, zcvl, uvl, wvl, fuwvl,
& rgas,
& alpha, tb1, delhv, delhr, cpl, cpv, tref,
& rxnke0, rxeeql, rxkf0, rxefwd, rxntref,
& kthermo,
& kinetic
```

PGM_PARAMS.F

```
parameter (nsmx = 50, ncmax = 10, nvmax = nsmx*(2*ncmax+2))
parameter (nimax = nvmax, nrmax = 2*nimax)
```

APPENDIX D.
HOMOTOPY CONTINUATION SOLVER SOURCE CODE
From Choi (1990)

HOMOTOPY.F

```

subroutine solver(x,n,tolx,tolf,ntrial,kstatus,its,errf,
&               ipr1,ipr2)
!
! Use homotopy continuation to find multiple roots of a function
! f(x), given a vector of starting guesses. This subroutine is
! an interface between the scdist main and the homcon homotopy
! subroutine.
implicit real*8 (a-h,o-z)
! Parameter specifications
include "pgm_params.f"
include "cmn_hsparms.f"
! Input Variable declarations:
real*8    x(0:n),tolx,tolf,errf
integer   n,ntrial,kstatus,its
! Homcon Variable Declarations:
complex*16 z(nimax), u(nimax), v(nimax)
complex*16 dudz(nimax,nimax), dvdz(nimax,nimax)
real*8    xo(0:nrmax), xa(0:nrmax), xb(0:nrmax)
real*8    xi(0:nrmax), xn(0:nrmax)
real*8    fo(nrmax), f(nrmax), g(nrmax), h(nrmax)
real*8    dfdxo(nrmax,nrmax), dfdx(nrmax,nrmax)
real*8    dgdx(nrmax,nrmax), dhdx(0:nrmax,0:nrmax)
real*8    dxdsa(0:nrmax), dxdsb(0:nrmax), dxdsn(0:nrmax)
real*8    dx(0:nrmax), work(0:nrmax)
integer   indx(0:nrmax)
save
!
!               Set values to pass to homcon
nc=n           !number of equations
job=kstatus    !Command passed in thru status var
maxcon=ntrial !Max no. continuation steps
if (kstatus .eq. 0) then
  do i=1,n
    xo(i)=x(i) !starting vector
  end do
end if
! nimax=n           !max dimension of complex
! nrmax=n*2        !max dimension of real
! idom=0           !domain is real (1 for complex)
! ihom=1           !homotopy type - Newton
! dir=1.d0         !direction => increasing t
! dso=1.0d-01      !initial step size
! dsmin=1.0d-20    !minimum step size
! dsmax=5.0d+04    !maximum step size
! xmax=1.0d+05     !Continuation space boundary
! ecorc=1.0d-04    !tolerance for continuation point
! ecorb=1.0d-06    !tolerance for bisection search
! edet=5.0d-01     !max relative determinant change
! esol=1.0d-04     !tolerance for solution
! ebif=1.0d-04     !tolerance for bifurcation point
! etur=1.0d-06     !tolerance for turn point
! esta=1.0d-04     !tolerance for starting point
! easy=1.0d-06     !tolerance for asymptotic behavior
! maxdet=5         !Max no. determinant evaluations

```

```

!   minasy=5           !Min no. asymptotic steps
!   maxasy=20         !Max no. asymptotic steps
!   ipr1=             output channel for history (log)
!   ipr2=             output channel for path data
!
      call homcon(z,u,v,dudz,dvdz,nc,nimax,xo,xa,
&   xb,xi,xn,fo,f,g,h,dfdxo,dfdx,
&   dgdx,dhdx,dxdsa,dxdsb,dxdsn,dx,
&   indx,work,nr,nrmax,idom,ihom,job,
&   dir,dso,dsa,dsb,dsn,dsmn,dsmx,
&   xmax,ecorc,ecorb,edet,esol,ebif,
&   etur,esta,easy,resa,resb,resn,
&   deto,deta,detb,detn,maxcon,maxdet,
&   minasy,maxasy,ncon,ncor,nbis,ndet,
&   nasy,nlud,ipr1,ipr2,istat)

      do i=0,n
        x(i)=xi(i)           !solution vector
      end do
      kstatus=istat         !Solver status code
      its=ncon              !No continuation steps
      errf = 1.d0 - xi(0)   !Homotopy parameter at last step
!
      return
      end
=====
!
      subroutine reqn(x,f,g,n,nmax,ierr)
!   Evaluate discrepancy functions for vector x
      real*8 x(0:n),f(n),g(n)
      call funcv(x(1),f,n,ierr)      !Evaluate functions at x
      return
      end

      subroutine rjac(x,dfdx,dgdx,n,nmax,ierr)
      real*8 x(0:nmax),dfdx(nmax,nmax),dgdx(nmax,nmax),f(nmax)
      call funcv(x(1),f,n,ierr)      !evaluate functions at x
      call fdjac(x(1),f,dfdx,n,nmax) !evaluate the jacobian
!   ierr=0
      return
      end

      subroutine ceqn(x,f,g,n,nmax,ierr)
      complex*16 x(n),f(n),g(n)
      real*8 xr(n),fr(n)
      do i=1,n
        xr(i)=dreal(x(i))
      end do
      call funcv(xr(1),fr,n,ierr)      !Evaluate functions at x
      do i=1,n
        f(i)=dcmplx(fr(i),0.d0)
      end do
      ierr=0
      return
      end

```

```

subroutine cjac(x,dfdx,dgdx,n,nmax,ierr)
complex*16 x(n),dfdx(n,n),dgdx(n,n)
real*8   xr(n),dfdxr(n,n),fr(n)
do i=1,n
  xr(i)=dreal(x(i))
end do
call funcv(xr(1),fr,n,ierr)      !Evaluate functions at x
call fdjac(xr(1),fr,dfdxr,n,n)  !evaluate the jacobian
do i=1,n
  do j=1,n
    dfdx(i,j)=dcmplx(dfdxr(i,j),0.d0)
  end do
end do
!   ierr=0
return
end

```

```

=====
!
subroutine homcon(z,u,v,dudz,dvdz,nc,ncmax,xo,xa,
& xb,xi,xn,fo,f,g,h,dfdxo,dfdx,
& dgdx,dhdx,dxdsa,dxdsb,dxdsn,dx,
& indx,work,nr,nrmax,idom,ihom,job,
& dir,dso,dsa,dsb,dsn,dsmin,dsmx,
& xmax,ecorc,ecorb,edet,esol,ebif,
& etur,esta,easy,resa,resb,resn,
& deto,deta,detb,detn,maxcon,maxdet,
& minasy,maxasy,ncon,ncor,nbis,ndet,
& nasy,nlud,ipr1,ipr2,istat)
*   traces a homotopy path using the two rules algorithm with
*   determinant monitoring.
*   Input Variables:
*     nc: number of original equations
*     ncmax: maximum dimension of complex equations
*     nrmax: maximum dimension of real equations
*     idom =0: compute in the real domain
*           =1: compute in the complex domain
*     ihom =0: use user-specified g(x)
*           1: use Newton homotopy
*           2: use fixed point homotopy
*           3: use affine homotopy
*           4: use second order homotopy
*     job =0: start path tracking
*           1: continue path tracking
*           2: reverse path tracking direction
*           3: trace a bifurcating branch
*           4: jump on a user-specified base point
*           5: reflect the path
*     <0: do more continuations
*     For job=0 or 4,
*     dir >0: track in increasing t direction
*           =0: use user-specified initial tangent vector
*           <0: track in decreasing t direction
*     For job=3,
*     dir =0: use user-specified tangent vector
*           <>0: bifurcation angle,deg(-180 to +180)

```

```

*   dso: initial step size for job=0,3 or 4(1.0d-02)
*   dsmin: minimum step size(1.0d-20)
*   dsmax: maximum step size(5.0d+04)
*   xmax: continuation space boundary(1.0d+05)
*   ecorc: tolerance for continuation point(1.0d-04)
*   ecorb: tolerance for bisection search point(1.0d-06)
*   edet: maximum relative change in determinant(5.0d-01)
*   esol: tolerance for solution(1.0d-04)
*   ebif: tolerance for bifurcation point(1.0d-04)
*   etur: tolerance for turning point(1.0d-06)
*   esta: tolerance for starting point(1.0d-04)
*   easy: tolerance for asymptotic behavior(1.0d-06)
* Output Variables:
*   dsa: step size at first base point
*   dsb: step size at last base point
*   dsn: step size at new point
*   ncon: continuation count
*   ncor: correction count
*   nbis: bisection search count
*   ndet: determinant control count
*   nasy: asymptotic step count
*   nlud: LU-decomposition count
*   xa(0:nr): first base point
*   xb(0:nr): last base point
*   xi(0:nr): solution vector
*   xn(0:nr): new point
*   istat = 1: solution found
*           2: bifurcation point found
*           3:(near)trifurcation point found
*           4: turning point found
*           5: starting point found
*          10: maximum number of continuations tried
*          20: homotopy path goes to infinity
*              without asymptotic behavior
*          21: homotopy path goes to infinity
*              with asymptotic behavior
*          101: step size is smaller than lower bound
*          102: continuation process is stagnant
*          105: homotopy matrix is singular
*          106: tangent vector is not obtained
*          201: starting point is out of domain
*          202: base point is out of domain
* Local Variables:
*   dsp: previous step size
*   idet: increment in determinant control count
*   cont: .true. if path tracking continued
*   tang: .true. if tangent vector determined
implicit real*8 (a-h,o-z)
integer mincor, maxcor
real*8 zero, half, one, two, deg
! parameter (mincor=1,maxcor=4)
parameter (mincor=10,maxcor=25)
parameter (zero=0.0d+00, half=0.5d+00)
parameter (one=1.0d+00, two=2.0d+00)
parameter (deg=1.745329251994329d-02)
complex*16 z(ncmax), u(ncmax), v(ncmax)

```



```

complex*16 dudz(ncmax,ncmax), dvdz(ncmax,ncmax)
integer idom, ihom, indx(0:nrmax), ipr1, ipr2, istat, job, maxasy,
& maxcon, maxdet, minasy, nasy, nbis, nc, ncmax, ncon, ncor,
& ndet, nlud, nr, nrmax
real*8 xo(0:nrmax), xa(0:nrmax), xb(0:nrmax)
real*8 xi(0:nrmax), xn(0:nrmax)
real*8 fo(nrmax), f(nrmax), g(nrmax), h(nrmax)
real*8 dfdxo(nrmax,nrmax), dfdx(nrmax,nrmax)
real*8 dgdx(nrmax,nrmax), dhdx(0:nrmax,0:nrmax)
real*8 dxdsa(0:nrmax), dxdsb(0:nrmax), dxdsn(0:nrmax)
real*8 dx(0:nrmax), work(0:nrmax)
real*8 deta, detb, detn, deto, dir, dsa, dsb, dsmax, dsmin, dsn,
& dso, easy, ebif, ecorb, ecorc, edet, esol, esta, etur, resa,
& resb, resn, xmax
logical ldet,lsol,lbif,ltur,lsta,cont,tang
logical accel,conv,newpt,regul,bifur,short,curv,asym
integer i, ibif, ibis, icon, icor, idet, ierr, isol, ista, itur,
& kcon, nc2, ncp1, nrmp1, nrp1
real*8 bound, cs, ddxds, denom, detp, dsp, ecor, nrn, secb, secn,
& sn, ta, tb, theta, ti, tn, to, vnrm, xanrm, xbnrm, xnnrm,
& xnnrm2
save
if(job.ge.0)then
*
*                               Set constants
ncp1=nc+1
nc2=2*nc
*
*                               Clear memories for the first base point
do i=0,nc2
  xa(i)=zero
  dxdsa(i)=zero
end do
resa=zero
deta=zero
dsa=zero
*
*                               Reset dimension
if(idom .eq. 0)then
*
*                               Compute in the real domain
nr=nc
*
*                               Clear imaginary parts
do i=ncp1,nc2
  xo(i)=zero
  xb(i)=zero
  xi(i)=zero
  xn(i)=zero
  fo(i)=zero
  f(i)=zero
  g(i)=zero
  h(i)=zero
end do
if(job .ne. 3)then
  do i=ncp1,nc2
    dxdsb(i)=zero
    dxdsn(i)=zero
  end do
end if
else

```

```

*
      Compute in the complex domain
      nr=nc2
      end if
      nrp1=nr+1
      nr=one/nr
*
      Clear counters
      icon=0
      idet=0
      ibis=0
      isol=0
      ibif=0
      itur=0
      ista=0
      end if
      if(job .eq. 0)then
*
      Start path tracking
      Set objects
*
      ldet=.false.
      lsol=.false.
      ltur=.false.
      lbif=.false.
      lsta=.false.
      if(edet .gt. zero)ldet=.true.
      if(esol .gt. zero)lsol=.true.
      if(ebif .gt. zero)lbif=.true.
      if(etur .gt. zero)ltur=.true.
      if(esta .gt. zero)lsta=.true.
*
      Set constants
      nrmp1=nrmax+1
      bound=xmax
*
      Clear memories
      dsb=zero
      dsn=zero
      resb=zero
      resn=zero
      deto=zero
      detb=zero
      detn=zero
      do i=0,nc2
        xb(i)=zero
        xi(i)=zero
        xn(i)=zero
        fo(i)=zero
        f(i)=zero
        g(i)=zero
        h(i)=zero
        dxdsn(i)=zero
      end do
*
      Set initial values
      ncon=0
      ncor=0
      nbis=0
      ndet=0
      nlud=0
      xo(0)=one
      to=zero

```

```

*                                     Print initial values
write(ipr1,500)
write(ipr1,520)to,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
*                                     Evaluate equation functions at the starting point
call eqnfun(z,u,v,nc,ncmax,xo,fo,g,nrmax,idom,
&         ihom,ierr)
*                                     Determine Jacobian matrix at the starting point
call jacmat(z,dudz,dvdz,nc,ncmax,xo,dfdxo,dgdx,
&         nrmax,idom,ihom,ierr)
*                                     Check feasibility of the starting point
if(ierr .gt. 0)then
  istat=201
  write(ipr1,850)
  write(ipr1,580)
  write(ipr1,520)to,idom,ihom,nlud
  write(ipr1,530)ncon,icon,ncor,ndet
  write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
  return          !if starting point infeasible
end if
*                                     Set the base point
do i=0,nr
  xa(i)=xo(i)
end do
ta=one-xa(0)
xanrm=vecnorm(xa,nrp1)
icor=0
*                                     Set the step size
dsa=dso
*                                     Describe the current status
cont=.false.
tang=.false.
else if(job .eq. 1)then
*                                     Continue path tracking
do i=0,nr
  xa(i)=xn(i)
  dxdsa(i)=dxdsn(i)
end do
ta=tn
xanrm=xnnrm
resa=resn
deta=detn
dsa=max(dso,dsn)
cont=.true.
tang=.true.
else if(job .eq. 2)then
*                                     Reverse path tracking direction
do i=0,nr
  xa(i)=xb(i)
  dxdsa(i)=-dxdsb(i)
end do
ta=tb
xanrm=xbnrm
resa=resb
deta=-detb

```

```

    dsa=max(dso,dsn)
    cont=.false.
    tang=.true.
else if(job .eq. 3)then
*           Trace a bifurcating branch
    do i=0,nr
      xa(i)=xi(i)
    end do
    ta=one-xa(0)
    xanrm=vecnrm(xa,nrp1)
    icor=0
    resa=zero
    deta=zero
*           Set the tangent vector
    if(dir .ne. zero)then
      theta=dir*deg
      cs=cos(theta)
      sn=sin(theta)
      do i=1,nc
        dxdsa(i)=cs*dxdsn(i)-sn*dxdsn(nc+i)
        dxdsa(nc+i)=cs*dxdsn(nc+i)+sn*dxdsn(i)
      end do
      dxdsa(0)=zero
    end if
    if(idom .eq. 0)then
*           Clear imaginary parts
      do i=ncp1,nc2
        dxdsa(i)=zero
        dxdsn(i)=zero
      end do
    end if
*           Set the step size
    dsa=dso
*           Describe the current status
    cont=.false.
    tang=.true.
else if(job .eq. 4)then
*           Jump on a user-specified base point
    do i=0,nr
      xa(i)=xb(i)
      dxdsa(i)=dxdsb(i)
    end do
    ta=one-xa(0)
    xanrm=vecnrm(xa,nrp1)
    icor=0
    resa=zero
    deta=zero
    dsa=dso
    cont=.false.
    tang=.false.
else if(job .eq. 5)then
*           Reflect the path
    xnnrm2=two*vecnrm(xn,nrp1)
    do i=0,nr
      xn(i)=xn(i)-xnnrm2*dxdsn(i)
    end do

```

```

*           Refine the reflected point near the homotopy path
  icor=0
  conv=.false.
  do while( .not. conv .and. icor .lt. maxcor)
    call newcor(z,u,v,dudz,dvdz,nc,ncmax,xo,xn,
&           fo,f,g,h,dfdxo,dfdx,dgdx,dhdx,
&           dxdsn,dx,indx,work,nr,nrmax,idom,
&           ihom,icor,resn,detn,nlud,ierr)
    tn=one-xn(0)
*           Check feasibility of the base point
    if(ierr .gt. 0)then
      istat=202
      write(ipr1,860)
      write(ipr1,580)
      write(ipr1,520)tn,idom,ihom,nlud
      write(ipr1,530)ncon,icon,ncor,ndet
      write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
      return
    end if
    icor=icor+1
    ncor=ncor+1
*           Check convergence of correction
    if(resb .lt. ecorc*abs(detb)**nr)conv=.true.
  end do
*           Set the base point and the tangent vector
  do i=0,nr
    xa(i)=xn(i)
    dxdsa(i)=dxdsn(i)
  end do
  ta=tn
  xanrm=vecnrm(xa,nrp1)
  resa=resn
  deta=detn
*           Set the step size
  dsa=max(dso,dsb)
*           Describe the current status
  cont=.false.
  tang=.true.
end if
if(job.ge.0)then
*           Reset variables
  ecor=ecorc
  newpt=.true.
  accel=.true.
  if( .not. cont)then
    nasy=0
    asym=.false.
    detb=zero
    dsb=zero
  end if
  if( .not. tang)then
*           Tangent vector at base point not determined yet
*           Evaluate equation functions at base point
    call eqnfun(z,u,v,nc,ncmax,xa,f,g,nrmax,idom,
&           ihom,ierr)
*           Determine Jacobian matrix at base point

```

```

call jacmat(z,dudz,dvdz,nc,ncmax,xa,dfdx,dgdx,
*      &      nrmx,idom,ihom,ierr)
*      Check feasibility of the base point
if(ierr .gt. 0)then
  istat=202
  write(ipr1,860)
  write(ipr1,580)
  write(ipr1,520)ta,idom,ihom,nlud
  write(ipr1,530)ncon,icon,ncor,ndet
  write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
  return
end if
*      Initialize tangent vector if not specified
if(dir .ne. zero)then
  dxdsa(0)=-sign(one,dir)
  do i=1,nr
    dxdsa(i)=zero
  end do
end if
*      Evaluate homotopy functions
call homfun(xo,xa,fo,f,g,h,dfdxo,nr,nrmx,ihom)
*      Set homotopy matrix(augmented Jacobian)
call hommat(xo,xa,fo,f,g,h,dfdxo,dfdx,dgdx,
*      &      dhdx,dxdsa,nr,nrmx,ihom)
*      LU-decompose homotopy matrix
call ludcmp(dhdx,nrp1,nrmp1,indx,work,deta,nlud)
*      Check regularity of homotopy matrix at base point
if(deta .eq. zero)then
  istat=105
  write(ipr1,880)
  write(ipr1,580)
  write(ipr1,520)to,idom,ihom,nlud
  write(ipr1,530)ncon,icon,ncor,ndet
  write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
  return
end if
*      Determine tangent vector at base point
dxdsa(0)=one
do i=1,nr
  dxdsa(i)=zero
end do
call lubksb(dhdx,nrp1,nrmp1,indx,dxdsa)
*      Normalize the tangent vector
vnorm=vecnorm(dxdsa,nrp1)
if(vnorm .eq. zero)then
  istat=106
  write(ipr1,890)
  write(ipr1,580)
  write(ipr1,520)ta,idom,ihom,nlud
  write(ipr1,530)ncon,icon,ncor,ndet
  write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
  return
end if
do i=0,nr
  dxdsa(i)=dxdsa(i)/vnorm
end do

```

```

*           Determine homotopy eqn residual at base point
  resa=vecnorm(h,nr)
*           Set homotopy matrix at base point
  call hommat(xo,xa,fo,f,g,h,dfdxo,dfdx,dgdx,
&           dhdx,dxdsa,nr,nrmax,ihom)
*           Calculate determinant of homotopy matrix
  call ludcmp(dhdx,nrp1,nrmp1,indx,work,deta,nlud)
*           Store determinant at starting point
  if(job .eq. 0)deto=deta
  end if
*           Copy first base point
  do i=0,nr
    xb(i)=xa(i)
    dxdsb(i)=dxdsa(i)
  end do
  tb=ta
  xbnrm=xanrm
  resb=resa
  detp=detb
  detb=deta
  dsp=dsb
  dsb=dsa
  end if
*           Enter prediction-correction loop
  kcon=0
  do while(kcon .lt. maxcon)
    if(newpt)then
*           New base point has been determined
*           Check regularity of homotopy matrix at base point
      regul=.false.
      if(abs(detb) .gt. ebif*abs(deto))regul=.true.
*           Record base point data as continuation history
      if(ipr1 .gt. 0)then
        write(ipr1,100)ncon,dsp,icor,resb,detb
        write(ipr1,120)(xb(i),i=1,nc)
!       write(ipr1,120)(xb(i),i=ncp1,nc2)
        write(ipr1,130)tb,xb(0),asym
      end if
      if(ipr2 .gt. 0)then
        if (ncon .eq. 0)then
          write(ipr2,*)'ncon,t,detb,resb,ddxds,dxdsb(0),dsb'
        end if
        write(ipr2,'(i5,1000(" ",e10.4:))')ncon,1.d0-xb(0),detb,
&       resb,ddxds,dxdsb(0),dsb,(xb(i),i=1,nc)
!       write(ipr2,130)xb(0)
!       write(ipr2,200)(xb(i),i=1,nc)
      end if
    end if
*           Perform Euler prediction and Newton correction
    newpt=.false.
    do while( .not. newpt)
*           Check the continuation step size
      if(dsb .lt. dsmin)then
        istat=101
        write(ipr1,810)
        write(ipr1,580)

```

```

write(ipr1,520)tb,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
return
end if
short=.false.
if(dsb .lt. dso)short=.true.
if(dsb .gt. dsmax)dsb=dsmax
dsn=dsb
*
                                Perform Euler prediction
do i=0,nr
xi(i)=xb(i)+dxdsb(i)*dsb
if(xi(i) .ne. xb(i))newpt=.true.
xn(i)=xi(i)
end do
*
                                Check movement
if( .not. newpt)then
istat=102
write(ipr1,830)
write(ipr1,580)
write(ipr1,520)tb,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
return
end if
*
                                Perform Newton correction
icor=0
conv=.false.
do while(newpt .and. .not. conv .and. icor .lt. maxcor)
call newcor(z,u,v,dudz,dvdz,nc,nmax,xo,xn,
&          fo,f,g,h,dfdxo,dfdx,dgdxdhdx,
&          dxdsb,dx,indx,work,nr,nrmax,idom,
&          ihom,icor,resn,detn,nlud,ierr)
*
                                Check feasibility of intermediate point
if(ierr .gt. 0)then
newpt=.false.
write(ipr1,950)
write(ipr1,920)ncon
else
icor=icor+1
ncor=ncor+1
*
                                Check convergence of correction
if(resn .lt. ecor*abs(detn)**nr)conv=.true.
end if
end do
if(conv)then
if(icor .le. mincor)then
*
                                Step size too small. Double next step size
if(accel)dsn=dsb*two
end if
else
*
                                Step size too large. Discard current point
newpt=.false.
end if
if(newpt)then
*
                                Check bifurcation

```



```

    bifur=.false.
    if(lbif .and. isgn(detb)*isgn(detn) .lt. 0)
&       bifur=.true.
    if(lidet .and. .not. bifur .and. .not. asym .and. regul)
&       then
*       Check relative change in the determinant of the homotopy matrix
    if(abs(detn-detb) .gt. edet*abs(detb))then
*       Change too large. Discard current point
        newpt=.false.
        idet=idet+1
        ndet=ndet+1
        if(idet .gt. maxdet)then
*           Step size halved too many times
*           Accept current point as new point
            write(ipr1,930)
            write(ipr1,920)ncon
            newpt=.true.
        end if
    end if
    end if
    end if
    if(newpt)then
*           Accept current point as new point
        idet=0
    else
*           Apply step-halving
        dsb=dsb*half
    end if
    end do
*           New point determined
    kcon=kcon+1
    icon=icon+1
    ncon=ncon+1
    tn=one-xn(0)
*           Determine tangent vector at new point
    dxdsn(0)=one
    do i=1,nr
        dxdsn(i)=zero
    end do
    call lubksb(dhdx,nrp1,nrmp1,indx,dxdsn)
*           Normalize tangent vector
    vnrm=vecnorm(dxdsn,nrp1)
    do i=0,nr
        dxdsn(i)=dxdsn(i)/vnrm
    end do
*           Calculate curvature times step size
    do i=0,nr
        dx(i)=dxdsn(i)-dxdsb(i)
    end do
    ddxds=vecnorm(dx,nrp1)
*           Check curvature
    curv=.false.
    if(ddxds .gt. esol)curv=.true.
*           Check direction of continuation
    xnnrm=vecnorm(xn,nrp1)
    if(xnnrm .gt. xbnrm)then

```

```

*                               Continuation goes outward
if(accel)then
*                               Check asymptotic behavior
  asym=.false.
  if(ddxds .lt. easy)then
    nasy=nasy+1
    if(nasy .ge. minasy)asym=.true.
  else
    nasy=0
  end if
end if
*                               Check position of new point
if(xnnrm .gt. bound .or. nasy .ge. maxasy)then
*                               Homotopy path goes to infinity
  istat=20
  if(asym)istat=21
  write(ipr1,720)
  write(ipr1,730)xnnrm,nasy
  write(ipr1,580)
  write(ipr1,520)tn,idom,ihom,nlud
  write(ipr1,530)ncon,icon,ncor,ndet
  write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
  return
end if
*                               Check for a solution
if(Isol .and. isgn(xb(0))*isgn(xn(0)) .lt. 0)then
*                               Solution located on curve between xb and xn
  if(short .and. .not. curv .and. abs(xn(0)) .lt. esol)then
*                               Solution found
    denom=xn(0)-xb(0)
    secb=xb(0)/denom
    secn=xn(0)/denom
    do i=0,nr
      xi(i)=secn*xb(i)-secb*xn(i)
    end do
    ti=one
    istat=1
    write(ipr1,610)
    write(ipr1,520)ti,idom,ihom,nlud
    write(ipr1,530)ncon,icon,ncor,ndet
    write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
    return
  end if
  isol=isol+1
  newpt=.false.
*                               Check for bifurcation point
else if(lbif .and. bifur)then
*                               Bifurcation point located on curve between xb and xn
  if(short .and. abs(detn) .lt. ebif*abs(deto))then
*                               Bifurcation point found
    denom=detn-detb
    secb=detb/denom
    secn=detn/denom
    do i=0,nr
      xi(i)=secn*xb(i)-secb*xn(i)

```

```

end do
ti=one-xi(0)
istat=2
write(ipr1,620)
write(ipr1,520)ti,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
return
end if
ibif=ibif+1
newpt=.false.
else if(lbif .and. .not. regul .and.
&      isgn(detb)*isgn(detp) .gt. 0 .and.
&      abs(detb) .lt. abs(detp) .and.
&      abs(detb) .lt. abs(detn))then
*      Even number of bifurcation points may be located near xb
do i=0,nr
xi(i)=xb(i)
end do
ti=one-xi(0)
istat=3
write(ipr1,630)
write(ipr1,520)ti,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
return
*
*      Check for turning point
else if(ltur .and. isgn(dxdsb(0))*isgn(dxdsn(0)) .lt. 0)
&      then
*      Turning point located on curve between xb and xn
if(short .and. abs(dxdsn(0))*dsb .lt. etur)then
*      Turning point found
denom=dxdsn(0)-dxdsb(0)
secb=dxdsb(0)/denom
secn=dxdsn(0)/denom
do i=0,nr
xi(i)=secn*xb(i)-secb*xn(i)
end do
ti=one-xi(0)
istat=4
write(ipr1,640)
write(ipr1,520)ti,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
return
end if
itur=itur+1
newpt=.false.
*
*      Check for starting point
else if(ista .and. isgn(tb)*isgn(tn) .lt. 0)then
*      Starting point located on curve between xb and xn
if(short .and. .not. curv .and. abs(tn) .lt. esol)then
*      Starting point found
denom=tn-tb
secb=tb/denom
secn=tn/denom

```

```

do i=0,nr
  xi(i)=secn*xb(i)-secb*xn(i)
end do
ti=zero
istat=5
write(ipr1,650)
write(ipr1,520)ti,idom,ihom,nlud
write(ipr1,530)ncon,icon,ncor,ndet
write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
return
end if
ista=ista+1
newpt=.false.
else
*           Accept new point as next base point
do i=0,nr
  xb(i)=xn(i)
  dxdsb(i)=dxdsn(i)
end do
tb=tn
xbnrm=xnnrm
resb=resn
detp=detb
detb=detn
dsp=dsb
dsb=dsn
cont=.true.
tang=.true.
accel=.true.
end if
*           if( .not. newpt)then
*           Activate bisection search
  accel=.false.
  ecor=ecorb
  dsb=dsb*half
  ibis=ibis+1
  nbis=nbis+1
end if
end do
*           Maximum number of continuations tried
  istat=10
  write(ipr1,710)
  write(ipr1,580)
  write(ipr1,520)tb,idom,ihom,nlud
  write(ipr1,530)ncon,icon,ncor,ndet
  write(ipr1,540)nbis,ibis,isol,ibif,itur,ista
  return
*   Output formats:
100 format(/1x,i5,1p,e13.5,i3,1x,2e13.5)
120 format(4x,1p,5e15.7)
130 format(4x,1p,2e15.7,i3)
200 format(1p,6e13.5)
500 format('/Continuation Started')
520 format('Homotopy parameter:',1p,e13.5,
  & ' Dom:',i4,' Hom:',i4,' LUd:',i4)
530 format('Cont and search: ',i7,'      Net:',i4,

```

```

    & ' Cor:',i4,' Det:',i4)
540 format('Bisection search: ',i7,'      Net:',i3,
    & ' Sol:',i4,' Bif:',i4/34x,
    & ' T:',i4,' St:',i4)
580 format('/Continuation Terminated')
610 format('/Solution Found')
620 format('/Bifurcation Point Found')
630 format('/(Near)Trifurcation Point Found')
640 format('/Turning Point Found')
650 format('/Starting Point Found')
710 format('/Maximum number of continuations tried')
720 format('/Homotopy path goes to infinity')
730 format('Norm of pos vector:',1p,e13.5,
    & ' Asymptotic step count:',i9)
810 format('/Step size is smaller than lower bound')
830 format('/Continuation process is stagnant')
850 format('/Starting point is out of domain')
860 format('/Base point is out of domain')
880 format('/Homotopy matrix is singular')
890 format('/Tangent vector is not obtained')
920 format('after continuation',i6)
930 format('Warning: Relative change in determinant of',
    & ' homotopy matrix is large')
950 format('Warning: Intermediate point is out of domain')
    end

```

```

!=====
!
    subroutine newcor(z,u,v,dudz,dvdz,nc,ncmax,xo,x,
    & fo,f,g,h,dfdxo,dfdx,dgdx,dhdx,
    & dxds,dx,indx,work,nr,nrmax,idom,
    & ihom,icor,res,det,nlud,ierr)
*   corrects a point x(s+ds) in direction perpendicular to
*   dx/ds(s) onto the homotopy path.
*   Input Variables
*   x(0:nr): point to be corrected (oldpoint)
*   dxds(0:nr): unit tangent vector at base point
*   nc: dimension of original equations
*   nr: dimension of real equations
*   ncmax: maximum dimension of complex equations
*   nrmax: maximum dimension of real equations
*   icor: correction count
*   Output Variables
*   x(0:nr): corrected point (newpoint)
*   res: homotopy equation residual at new point
*   det: determinant of homotopy matrix
*   at new point, if icor=0
*   at old point, if icor>0
*   ierr: errorcode
    implicit real*8 (a-h,o-z)
    parameter(zero=0.0d+00)
    complex*16 z(ncmax), u(ncmax), v(ncmax)
    complex*16 dudz(ncmax,ncmax), dvdz(ncmax,ncmax)
    dimension xo(0:nrmax),x(0:nrmax)
    dimension fo(nrmax),f(nrmax)

```

```

dimension g(nrmax),h(nrmax)
dimension dfdxo(nrmax,nrmax)
dimension dfdx(nrmax,nrmax)
dimension dgdx(nrmax,nrmax)
dimension dhdx(0:nrmax,0:nrmax)
dimension dxds(0:nrmax),dx(0:nrmax)
dimension indx(0:nrmax),work(0:nrmax)
*   Set constants
nrp1=nr+1
nrmp1=nrmax+1
if(icor .eq. 0)then
*   Evaluate equation functions.
  call eqnfun(z,u,v,nc,ncmax,x,f,g,nrmax,idom,
&           ihom,ierr)
  if(ierr .gt. 0)return
*   Evaluate homotopy functions.
  call homfun(xo,x,fo,f,g,h,dfdxo,nr,nrmax,ihom)
  end if
  if(icor .ne. 1)then
*   Determine the Jacobian matrix.
  call jacmat(z,dudz,dvdz,nc,ncmax,x,dfdx,dgdx,
&           nrmax,idom,ihom,ierr)
  if(ierr .gt. 0)return
*   Set the homotopy matrix.
  call hommat(xo,x,fo,f,g,h,dfdxo,dfdx,dgdx,dhdx,
&           dxds,nr,nrmax,ihom)
*   LU-decompose the homotopy matrix.
  call ludcmp(dhdx,nrp1,nrmp1,indx,work,det,nlud)
  end if
*   Determine the Newton corrector.
  dx(0)=zero
  do i=1,nr
    dx(i)=-h(i)
  end do
  call lubksb(dhdx,nrp1,nrmp1,indx,dx)
*   Update the continuation point.
  do i=0,nr
    x(i)=x(i)+dx(i)
  end do
*   Evaluate equation functions.
  call eqnfun(z,u,v,nc,ncmax,x,f,g,nrmax,idom,
&           ihom,ierr)
  if(ierr .gt. 0)return
*   Evaluate homotopy functions.
  call homfun(xo,x,fo,f,g,h,dfdxo,nr,nrmax,ihom)
*   Determine the homotopy equation residual.
  res=vecnorm(h,nr)
  if(icor .eq. 0)then
*   Determine the Jacobian matrix.
  call jacmat(z,dudz,dvdz,nc,ncmax,x,dfdx,dgdx,
&           nrmax,idom,ihom,ierr)
  if(ierr .gt. 0)return
*   Set the homotopy matrix.
  call hommat(xo,x,fo,f,g,h,dfdxo,dfdx,dgdx,dhdx,
&           dxds,nr,nrmax,ihom)
*   LU-decompose the homotopy matrix.

```

```

    call ludcmp(dhdx,nrp1,nrmp1,indx,work,det,nlud)
end if
return
end

```

```

=====
!
  subroutine eqnfun(z,u,v,n,ncmax,x,f,g,nrmax,idom,
    & ihom,ierr)
  *
  * evaluates equation functions.
  * Input Variables
  * x(1:n): real parts of current point
  * x(n+1:2n): imaginary parts of current point
  * n: dimension of original equations
  * ncmax: maximum dimension of complex equations
  * nrmax: maximum dimension of real equations
  * idom: domain(0:real 1:complex)
  * ihom: homotopy type(0: user-specified g(x))
  * Output Variables
  * f(1:n): equation functions at current point
  * g(1:n): starting functions at current point
  implicit real*8 (a-h,o-z)
  complex*16 z(ncmax), u(ncmax), v(ncmax)
  dimension x(0:nrmax),f(nrmax),g(nrmax)
  if(idom .eq. 0)then
  * Evaluate real equation functions.
    call reqn(x,f,g,n,nrmax,ierr)
  else
  * Evaluate complex equation functions.
    do i=1,n
      z(i)=dcmplx(x(i),x(n+i))
    end do
    call ceqn(z,u,v,n,ncmax,ierr)
    do i=1,n
      f(i)=dreal(u(i))
      f(n+i)=dimag(u(i))
    end do
    if(ihom .eq. 0)then
  * Evaluate user-specified starting functions.
      do i=1,n
        g(i)=dreal(v(i))
        g(n+i)=dimag(v(i))
      end do
    end if
  end if
end

```

```

=====
!
  subroutine jacmat(z,dudz,dvdz,n,ncmax,x,dfdx,dgdx,
    & nrmax,idom,ihom,ierr)
  *
  * determines the Jacobian matrix for the equation functions.
  * Input Variables
  * x(1:n): real parts of current point

```

```

*   x(n+1:2n): imaginary parts of current point
*   n: dimension of original equations
*   ncmx: maximum dimension of complex equations
*   nrmax: maximum dimension of real equations
*   idom: domain(0:real 1:complex)
*   ihom: homotopytype(0:user-specified g(x))
*   Output Variables
*   dfdx(n,n): Jacobian matrix for equation functions
*   dgdx(n,n): Jacobian matrix for starting functions
implicit real*8 (a-h,o-z)
complex*16 z(ncmx),dudz(ncmx,ncmx),dvdz(ncmx,ncmx)
dimension x(0:nrmax),dfdx(nrmax,nrmax),dgdx(nrmax,nrmax)
if(idom .eq. 0)then
*   Determine real Jacobian matrix
  call rjac(x,dfdx,dgdx,n,nrmax,ierr)
else
*   Set complex array z which corresponds to real array x.
  do i=1,n
    z(i)=dcmplx(x(i),x(n+i))
  end do
*   Determine complex Jacobian matrix.
  call cjac(z,dudz,dvdz,n,ncmx,ierr)
  do i=1,n
    do j=1,n
      dre=dreal(dudz(i,j))
      dim=dimag(dudz(i,j))
      dfdx(i,j)=dre
      dfdx(i,n+j)=-dim
      dfdx(n+i,j)=dim
      dfdx(n+i,n+j)=dre
    end do
  end do
  if(ihom .eq. 0)then
*   Determine Jacobian matrix for user-specified starting functions.
    do i=1,n
      do j=1,n
        dre=dreal(dvdz(i,j))
        dim=dimag(dvdz(i,j))
        dgdx(i,j)=dre
        dgdx(i,n+j)=-dim
        dgdx(n+i,j)=dim
        dgdx(n+i,n+j)=dre
      end do
    end do
  end if
end if
return
end

```

```

!=====
!
subroutine homfun(xo,x,fo,f,g,h,dfdxo,n,nmax,ihom)
*   evaluates the homotopy functions.
*   InputVariables
*   xo(0:n): starting point

```



```

*   x(0:n): current point (t=1-x(0))
*   fo(1:n): equation functions at starting point
*   f(1:n): equation functions at current point
*   dfdxo(n,n): Jacobian matrix at starting point
*   n: dimension of real equations
*   nmax: maximum dimension of real equations
*   ihom: homotopy function type
*   Output Variables
*   g(l:n>): starting functions at current point
*   h(l:n): homotopy functions at current point
implicit real*8 (a-h,o-z)
parameter(zero=0.0d+00,one=1.0d+00)
dimension xo(0:nmax),x(0:nmax)
dimension fo(nmax),f(nmax)
dimension g(nmax),h(nmax)
dimension dfdxo(nmax,nmax)
*   Evaluate the homotopy parameter
omt=x(0)
t=one-omt
*   Evaluate the homotopy functions.
if(ihom .eq. 1)then
*   Use Newton homotopy.
do i=1,n
  h(i)=f(i)-omt*fo(i)
end do
else if(ihom .eq. 2)then
*   Use fixed point homotopy.
do i=1,n
  g(i)=x(i)-xo(i)
  h(i)=t*f(i)+omt*g(i)
end do
else if(ihom .eq. 3)then
*   Use scale-invariant affine homotopy.
do i=1,n
  sum=zero
  do j=1,n
    sum=sum+dfdxo(i,j)*(x(j)-xo(j))
  end do
  g(i)=sum
  h(i)=t*f(i)+omt*g(i)
end do
else if(ihom .eq. 4)then
*   Use second order homotopy.
do i=1,n
  sum=zero
  do j=1,n
    sum=sum+dfdxo(i,j)*(x(j)-xo(j))
  end do
  g(i)=sum
  h(i)=t*(f(i)-omt*fo(i))+omt*g(i)
end do
else
*   Use user-specified starting functions.
do i=1,n
  h(i)=t*f(i)+omt*g(i)
end do

```

```

end if
return
end

```

```

=====
!
  subroutine hommat(xo,x,fo,f,g,h,dfdxo,dfdx,dgdx,dhdx,
& dxds,n,nmax,ihom)
*   determines the Jacobian matrix for the homotopy functions,
*   and sets the augmented Jacobian matrix (homotopy matrix).
*   Input Variables
*   xo(0:n): starting point
*   x(0:n): current point(t=1-x(0))
*   fo(1:n): equation functions at starting point
*   f(1:n): equation functions at current point
*   s(l:n): starting functions at current point
*   dfdxo(n,n): Jacobian matrix at starting point
*   dfdx(n,n): Jacobian matrix at current point
*   dgdx(n,n): Jacobian matrix for starting functions
*   dxds(0:n): unit tangent vector at current point
*   n: dimension of real equations
*   nmax: maximum dimension of real equations
*   ihom: homotopy function type
*   Output Variables
*   dhdx(0:n,0:n): homotopy matrix at current point
implicit real*8 (a-h,o-z)
parameter(zero=0.0d+00,one=1.0d+00,two=2.0d+00)
dimension xo(0:nmax),x(0:nmax)
dimension fo(nmax),f(nmax)
dimension g(nmax),h(nmax)
dimension dfdxo(nmax,nmax)
dimension dfdx(nmax,nmax)
dimension dgdx(nmax,nmax)
dimension dhdx(0:nmax,0:nmax)
dimension dxds(0:nmax)
*   Evaluate the homotopy parameter.
omt=x(0)
t=one-omt
*   Set the first row (augmented row).
do j=0,n
  dhdx(0,j)=dxds(j)
end do
*   Determine the Jacobian matrix for the homotopy functions.
if(ihom .eq. 1)then
*   Use Newton homotopy.
do i=1,n
  do j=1,n
    dhdx(i,j)=dfdx(i,j)
  end do
  dhdx(i,0)=-fo(i)
end do
else if(ihom .eq. 2)then
*   Use fixed point homotopy.
do i=1,n
  do j=1,n

```

```

    dhdx(i,j)=t*dfdx(i,j)
  end do
  dhdx(i,i)=dhdx(i,i)+omt
  dhdx(i,0)=g(i)-f(i)
  end do
else if(ihom .eq. 3)then
* Use scale-invariant affine homotopy.
  do i=1,n
    do j=1,n
      dhdx(i,j)=t*dfdx(i,j)+omt*dfdxo(i,j)
    end do
    dhdx(i,0)=g(i)-f(i)
  end do
else if(ihom .eq. 4)then
* Use second order homotopy.
  c=two*omt-one
  do i=1,n
    do j=1,n
      dhdx(i,j)=t*dfdx(i,j)+omt*dfdxo(i,j)
    end do
    dhdx(i,0)=g(i)-f(i)+c*fo(i)
  end do
else
* Use user-specified starting functions.
  do i=1,n
    do j=1,n
      dhdx(i,j)=t*dfdx(i,j)+omt*dgdx(i,j)
    end do
    dhdx(i,0)=g(i)-f(i)
  end do
end if
return
end

```

```

!=====
!
```

```

subroutine ludcmp(a,n,np,indx,work,det,nlud)
* LU-decomposes an n x n matrix, a.
* Reference: W.H.Press, B.P.Flannery, S.A.Teukolsky, and
* W.T.Vetterling, Numerical Recipes: The Art of
* Scientific Computing, Cambridge University Press,
* New York, NY, 1989.
* Input Variables
* a: matrix to be LU-decomposed
* n: dimension of matrix a
* nP: physical dimension of matrix a
* nlud: LU-decomposition count
* Output Variables
* a: LU-decomposed matrix
* indx: row permutation by partial pivoting
* det: determinant of matrix a
* nlud: LU-decomposition count
implicit real*8 (a-h,o-z)
parameter(tiny=1.0d-20)
parameter(zero=0.0d+00,one=1.0d+00)

```

```

dimension a(np,*),indx(*),work(*)
det=zero
do i=1,n
  aamax=zero
  do j=1,n
    if(abs(a(i,j)) .gt. aamax)aamax=abs(a(i,j))
  end do
  if(aamax .eq. zero)return
  work(i)=one/aamax
end do
det=one
do j=1,n
  do i=1,j-1
    sum=a(i,j)
    do k=1,i-1
      sum=sum-a(i,k)*a(k,j)
    end do
    a(i,j)=sum
  end do
  aamax=zero
  do i=j,n
    sum=a(i,j)
    do k=1,j-1
      sum=sum-a(i,k)*a(k,j)
    end do
    a(i,j)=sum
    dum=work(i)*abs(sum)
    if(dum .ge. aamax)then
      imax=i
      aamax=dum
    end if
  end do
  if(j .ne. imax)then
    do k=1,n
      dum=a(imax,k)
      a(imax,k)=a(j,k)
      a(j,k)=dum
    end do
    det=-det
    work(imax)=work(j)
  end if
  indx(j)=imax
  if(j .ne. n)then
    if(a(j,j) .eq. zero)a(j,j)=tiny
    dum=one/a(j,j)
    do i=j+1,n
      a(i,j)=a(i,j)*dum
    end do
  end if
end do
if(a(n,n) .eq. zero)a(n,n)=tiny
do j=1,n
  det=det*a(j,j)
end do
nlud=nlud+1
return

```

end

```

=====
!
subroutine lubksb(a,n,np,indx,b)
* solves equation LUx=b.
* Reference: W.H.Press, B.P.Flannery, S.A.Teukolsky, and
* W.T.Vetterling, Numerical Recipes: The Art of
* Scientific Computing, Cambridge University Press,
* New York, NY, 1989.
* Input Variables
* a: LU-decomposed matrix
* n: dimension of matrix a
* nP: physical dimension of matrix a
* indx: row permutation vector
* b: right-hand side vector
* Output Variables
* b: solution vector
implicit real*8 (a-h,o-z)
dimension a(np,*),indx(*),b(*)
ii=0
do i=1,n
  ll=indx(i)
  sum=b(ll)
  b(ll)=b(i)
  if(ii .ne. 0)then
    do j=ii,i-1
      sum=sum-a(i,j)*b(j)
    end do
  else if(sum .ne. 0)then
    ii=i
  end if
  b(i)=sum
end do
do i=n,1,-1
  sum=b(i)
  do j=i+1,n
    sum=sum-a(i,j)*b(j)
  end do
  b(i)=sum/a(i,i)
end do
return
end

```

```

=====
!
function vecnorm(x,n)
* returns Euclidean norm of x(1:n).
implicit real*8 (a-h,o-z)
dimension x(*)
sum=0.0d+00
do i=1,n
  sum=sum+x(i)**2
end do

```

```
vecnorm=sqrt(sum)
return
end
```

```
!=====
!  
function isgn(x)  
* returns sign of x.  
  real*8 x  
  if(x)10,20,30  
10 isgn=-1  
  return  
20 isgn=0  
  return  
30 isgn=1  
  end
```

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