Computing Multiple Solutions to Systems of Interlinked Separation Columns

Globally convergent homotopy continuation methods have been used successfully to find multiple solutions to systems of nonlinear equations used to model multicomponent, multistage separation processes. However, the solutions were achieved by using a multitude of different starting points. This paper describes a procedure for finding all or some solutions of the nonlinear equation system from just one starting point. A reliable algorithm, which utilizes a deflated decomposition technique to overcome the turning-point problem, an efficient procedure to estimate step sizes, and variable mapping functions to prevent failure when computing physical properties, is developed to follow the homotopy path. The Jacobian matrix is retained as a special structure in all calculation steps. The algorithm has found, from one starting point, all the real roots of the interlinked separation system studied by Chavez et al. (1986). Two additional examples, including one optimization problem and one constrained nonlinear equation system, are presented to illustrate other applications of the algorithm.

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Introduction

Conventional methods—e.g., Newton's method, quasi-Newton methods, Broyden's method—have been applied for many years to solve the nonlinear equations used to model chemical engineering problems. However, these methods are not guaranteed to converge to a solution and at best can only find one solution from a given starting guess. Recently, a new globally convergent continuation method has attracted great interest among mathematicians, scientists, engineers, and economists. This new method goes back at least to the work of Lahaye (1934), who used the classical theorem of Leray and Schauder (1934). Modern homotopy continuation algorithms, such as those of Kubicek (1976), Keller (1977, 1978), Hirsch and Smale (1979), Li and York (1980), Chow et al. (1978), Rheinboldt (1980), Rheinboldt and Burkardt (1983a, b), Allgower and Georg (1980a), and Watson et al. (1987) are based on ideas of Davidenko (1953) and Klopfenstein (1961), who differentiated the homotopy equation to obtain an initial-value ordinary differential equation problem. However, upon tracing the homotopy path by solving that problem, the Jacobian matrix may become singular at some points, causing failure of the calculation of the linearized system. Fortunately, Keller (1983), Chan (1984a, b, c), and Griewank (1985) have developed algorithms to overcome this problem. The comprehensive book by Garcia and Zangwill (1981) covers most basic ideas of continuation methods.

Although continuation methods have been known for several decades, it is only recently that chemical engineers have reported applications and developments of these methods for solving mathematical models comprised of systems of nonlinear equations. Important works include: Salgovic et al. (1981), Bhargava and Hlavacek (1984), Wayburn (1983), Wayburn and Seader (1983, 1984, 1987), Chavez (1985), Chavez et al. (1986), Hlavacek (1985), Byrne and Baird (1985), and Vickery and Taylor (1986a, b).

By using modern continuation methods, problems can be solved that are not amenable to solution by locally convergent Newton-type methods. For example, important multiple real solutions have been found, using different starting guesses, for systems of interlinked separation columns by Chavez et al. (1986). However, there are many disadvantages to guessing different starting points in order to find multiple solutions. One is that unless the nonlinear equations are polynomials we cannot predetermine the number of roots. When the nonlinear equations are polynomials, continuation methods such as those of Garcia and Zangwill (1979), Kojima and Mizuno (1983), Wright (1985), Pasquini and Trigiante (1985), and Watson et

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al. (1987) can be applied to systematically determine all solutions, real and complex. For these methods, n starting points are needed to create n homotopy paths leading to the n roots. For other types of nonlinear equation systems that include transcendental functions, no homotopy function is guaranteed to find all solutions. Allgower and Georg (1980b, 1983) suggested a d-trick homotopy function that may find all solutions to the system of nonlinear equations under specific conditions. Unfortunately these conditions are not satisfied for most general nonlinear equation systems.

Garcia and Zangwill (1981) proposed an all-solutions homotopy whose paths can lead to each of the different solutions by starting from many different points. However, because we do not know how many roots exist for general systems of nonlinear equations, the construction of the all-solutions homotopy is uncertain. Conventional numerical methods (e.g., Newton's method) can be used with a deflation technique, as described by Brown and Gearhart (1971), to obtain further solutions. But this technique depends strongly on the type of deflation and numerical method used. It is restricted to solving relatively simple numerical problems. Up to now, as far as we know, the method proposed here is a unique way to find further solutions of the large nonlinear equations system for modeling chemical engineering separation problems by using the continuation method from only one initial point.

Instead of trying to find homotopy functions that can be guaranteed to find all roots, this paper proposes an algorithm to follow the differential Newton-type homotopy path to find some or all solutions of a system of nonlinear equations that model an interlinked separation system. Features of the algorithm include:

1. The Euler-predictor and Newton-corrector method is used to follow the path.
2. The deflated decomposition technique developed by Stewart (1981) and Chan (1984a, b, c) is used to follow the homotopy path around turning points.
3. The den Heijer and Rheinboldt (1981) step-length algorithm is used to efficiently estimate step sizes along the path.
4. Variable mapping functions are used to prevent the occurrence, along the path, of unacceptable negative values of variables that could cause failure of correlations for computing thermodynamic properties. For example, negative mole fractions or flow rates must be avoided.

Two applications to interlinked separation systems are presented. For each example, all solutions are found from just one starting guess. The proposed algorithm may have application to other computational problems where it is desirable to find all solutions to systems of nonlinear equations. Two additional examples illustrate the application of the algorithm to optimization and a constrained nonlinear equations system.

Development of the Algorithm

Differential homotopy continuation function

For computing a solution $x^* \in R^n$ of a given equation system

$$f(x) = 0 \tag{1}$$

where f: $R^n \rightarrow R^n$, the homotopy function $H(x, t)$ is chosen such that

$$H(x, t) = tf(x) + (1 - t)g(x) = 0 \tag{2}$$

where $t \in [0, 1]$, and H: $R^n \times R^1 \rightarrow R^n$.

Let $\lambda = 1 - t$. Then, Eq. 2 can be expressed as

$$H(x, \lambda) = (1 - \lambda)f(x) + \lambda g(x) = 0 \tag{3}$$

When $\lambda = 1$, the solution is x^o, which is assumed known or easily calculated. When $\lambda = 0$, the solution is x^*, which is the desired root of the original system of equations, $f(x)$. Without losing generality, the Newton homotopy function is used here, where $g(x) = f(x) - f(x^o)$. To prevent some disadvantages of classical continuation methods, the variables x and λ are determined as functions of the parameter p, the arc length of the homotopy path. Thus, Eq. 3 is differentiated with respect to p to give:

$$f'(x)\frac{dx}{dp} - \frac{d\lambda}{dp}f(x^o) = 0 \tag{4}$$

where $[(dx/dp)^T, d\lambda/dp]^T$ is chosen to satisfy the following relation:

$$(dx/dp)^T(dx/dp) + (d\lambda/dp)^2 = 1 \tag{5}$$

This converts the problem to an initial-value problem (IVP) in ordinary differential equations as follows:

$$[f'(x)\,|\,-f(x^o)]\begin{bmatrix}\dot{x}\\ \dot{\lambda}\end{bmatrix} = 0$$
$$\dot{x}^T\dot{x} + \dot{\lambda}^2 = 1 \tag{6}$$

with $x(0) = x^o$, $\lambda(0) = 1$, and where $\lambda \in [0, 1]$.

However, as used extensively in this study, if λ is not restricted to the interval [0, 1], additional roots may be obtained each time the path crosses $\lambda = 0$. Furthermore, the Newton homotopy path can be followed by either decreasing or increasing λ, starting from a value of one.

Solving the initial-value problem

The predictor-corrector method is a convenient method for solving an IVP in ordinary differential equations. Although a high-order predictor is more effective for convergence of the corrector step, the simple Euler predictor step is adequate if the step size is estimated suitably. The tangent vector, v, of the Euler step can be calculated by solving

$$\begin{bmatrix}f'(x)\,|\,-f(x^o)\\ (e^{n+1})^T\end{bmatrix}v = e^{n+1} \tag{7}$$

where e^{n+1} is the $(n + 1)$th unit coordinate vector. The corresponding unit tangent vector is defined as

$$u = \pm v/\|v\| \tag{8}$$

The sign is chosen to maintain an acute angle with the previous tangent vector on the homotopy path. Then the new variables

are calculated by

$$\begin{bmatrix} x \\ \lambda \end{bmatrix}_N = \begin{bmatrix} x \\ \lambda \end{bmatrix}_o + \sigma u \tag{9}$$

The estimation of the step size, σ, will be discussed later. For the corrector step, the Newton correction vector $[\Delta x^T, \Delta\lambda]^T$ is calculated in the hyperplane orthogonal to the unit tangent vector u with

$$\begin{bmatrix} f'(x) & -f(x^o) \\ u^T & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \end{bmatrix} = \begin{bmatrix} \lambda f(x^o) & -f(x) \\ 0 & \end{bmatrix} \tag{10}$$

This equation can be expressed in the following general form:

$$M \begin{bmatrix} x \\ h \end{bmatrix} = \begin{bmatrix} A & b \\ c^T & d \end{bmatrix} \begin{bmatrix} x \\ h \end{bmatrix} = \begin{bmatrix} f \\ q \end{bmatrix} \tag{11}$$

Keller (1977) suggested using a block-elimination (BE) algorithm to solve for Eq. 11 for x and h. The procedure is as follows:

1. Solve

$$Ar = b \text{ for } r$$

$$As = f \text{ for } s$$

2. Compute

$$h = (q - c^T s)/(d - c^T r)$$

3. Compute

$$x = s - h\,r$$

Keller proved that M will not be singular at the turning point even though A is a singular matrix. Two advantages of this algorithm are:

1. If matrix A has some special structure (e.g., band, sparse, special solver, etc.), other algorithms may destroy the structure. The BE algorithm preserves the structure.

2. Matrix A only needs to be factored once.

Chan and Keller (1982), and Chan (1984c) showed that the BE algorithm may become unstable in the region of turning points when matrix A is singular or nearly singular and may produce completely inaccurate solutions, $[x^T, h]^T$. This is due to an inaccurate calculation of r and s in step 1. Thus, when tracking the differential arc length homotopy path, if the Jacobian matrix becomes nearly singular or exactly singular, the calculation of the linear system will fail. The techniques available to overcome this problem include:

1. *Reparameterization.* With this technique, the last column of the Jacobian matrix is permuted with another column so that the final coefficient matrix becomes nonsingular at the turning point. Reparameterization algorithms include those of Kubicek (1976), Rheinboldt (1980, 1981), and Rheinboldt and Burkardt (1983a, b). Rheinboldt (1981) used the Sherman-Morrison formula to solve the linear system when the Jacobian matrix is banded.

2. *Jumping.* From Sard's theorem, the turning point can be jumped by controlling the step size in the predictor-corrector step. Keller (1977) suggested that this method can be applied under mild smoothness conditions. This technique can be unreliable when the curvature of the homotopy path is too great.

3. *Least-squares Solution.* A system of linear equations, say $Ar = b$, may have no solution when the path reaches a turning point. However, instead of attempting to make an exact calculation at the turning point, an approximate calculation may suffice because the path only needs to be followed loosely unless a zero occurs at the turning point. Watson (1979) and Watson et al. (1987) used the Householder transformation as described by Businger and Golub (1965) to solve the linear system. Alternatively, a deflated decomposition technique as described by Chan (1984a, b, c) and Stewart (1981) may be used, and was selected for use in our study because of its ease of implementation and reliable stability.

Step-size algorithm

A reliable step-size estimation method that predicts the step length of the Euler predictor can reduce the computation time tremendously. Georg (1981), den Heijer and Rheinboldt (1981), Li and York (1980), Deuflhard (1979), Menzel and Schwetlick (1978), and Wacker (1978), have proposed different procedures to estimate step size. From our experience, the optimum choice of algorithm depends on the nature and size of the problem being solved.

In our early studies, the step-size algorithm of Georg (1981) was applied, as discussed in detail by Wayburn and Seader (1983). The step size in this algorithm is governed by the length of the first Newton corrector, the ratio of the lengths of the second and first Newton correctors, and the angle between successive unit tangents of the predictor. For the first, third, and fourth examples presented below, the Georg algorithm with only two Newton correctors was efficient. For the difficult second example, application of the Georg algorithm led to excessive computing time. Therefore, the more complex step-size algorithm of den Heijer and Rheinboldt (1981) was applied. Their algorithm is based on *a posteriori* estimates of the convergence behavior of a sequence of corrector iterates. In our case, up to eight corrector iterates were employed. The use of the algorithm of den Heijer and Rheinboldt with the second example below dramatically reduced computing time. Therefore, that algorithm was adopted here.

Mapping function

Most problems in chemical engineering that involve nonlinear equations are constrained. An example stressed in this paper is the nonlinear equations derived from modeling multicomponent, multistage separation problems. It is possible that while the homotopy path is being tracked, some variables may acquire unacceptable values, e.g., negative mole fractions or flow rates. When this happens, most thermodynamic property packages, which are treated as black boxes, fail to compute the required properties. To eliminate this possibility, variable mapping functions were used.

Consider the problem of finding solutions to the following system of n equations:

$$f(x) = 0 \quad \text{with } x_i \geq 0, i = 1, \ldots, n \tag{12}$$

Naphtali and Sandholm (1971) recommended the following mapping function to prevent negative variables:

$$x^{(l+1)} = x^{(l)} \exp\left(\omega \Delta x^{(l)} / x^{(l)}\right) \tag{13}$$

Another strategy is to convert a negative value to an arbitrary small positive value, say 1.E-8.

Wayburn and Seader (1987) suggested the introduction of an absolute-value function into the function $f(x)$, where the absolute value is regarded as part of the function and not part of x. For example, if $f(|x|) = |x|^{0.5} - 2$ and $x = -4, f(|x|) = 0$, but x still equals -4. If these equations are differentiated with respect to x_i at $x_i = 0$, one obtains

$$\frac{d|x_i|}{dx_i} = \begin{cases} +1, x_i \to 0^+ \\ -1, x_i \to 0^- \end{cases} \tag{14}$$

Unfortunately, Eq. 14 is undifferentiable at $x_i = 0$ and, as they showed, the Newton homotopy path is disconnected at $x_i = 0$.

In this work, we used the following mapping function:

$$y_i^2 = x_i \quad \text{for } i = 1, \ldots, n \tag{15}$$

The original equations then become $f(y) = 0$ without any constraints and the problem can be solved in the y domain instead of in the x domain. The functions are differentiable anywhere with respect to y. Some examples of the use of this mapping function are shown later.

Algorithm for solving the nonlinear equations systems

When the above techniques are combined, the following algorithm results for solving a system of nonlinear equations for a specified number of roots from one starting point:

Algorithm:

1. Enter the following data:

x^o = the starting point
σ^o = the initial stepsize

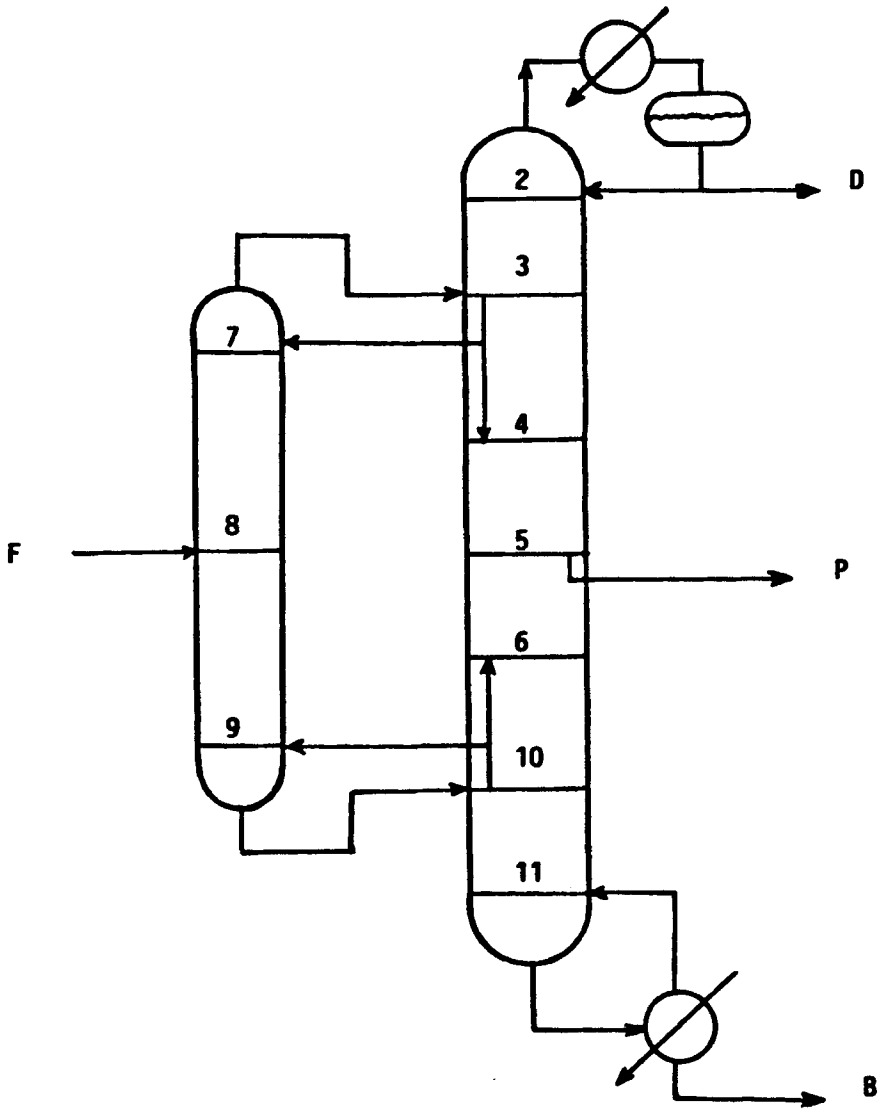

Figure 1. Petlyuk system with 12 stages.

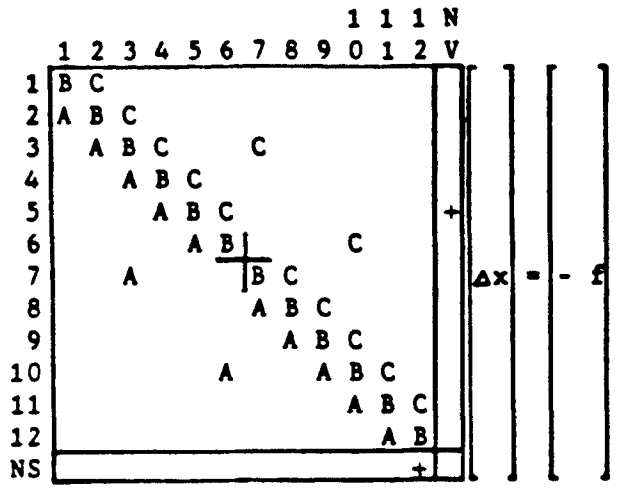

Figure 2. Block tridiagonal matrix with disperse elements.

σ_{max} = maximum allowable stepsize
σ_{min} = minimum allowable stepsize
$MROOTS$ = number of roots to be computed
K_{max} = maximum number of predictor-corrector points along the homotopy path

and other required data for the den Heijer and Rheinboldt step-size algorithm (1981).

2. $x = x^o$, $K = 0$, $\sigma = \sigma^o$, and $MR = 0$, where MR is the number of roots already computed.

3. $K = K + 1$

If $K > K_{max}$, go to 9.

4. Apply the Euler predictor by computing u, the unit tangent vector, from Eqs. 7 and 8 with the deflated decomposition technique, if needed.

5. If $K > 1$, estimate step size σ by the den Heijer and Rheinboldt step-size algorithm.

6. If $\sigma \geq \sigma_{max}$, $\sigma = \sigma_{max}$
If $\sigma \leq \sigma_{min}$, $\sigma = \sigma_{min}$

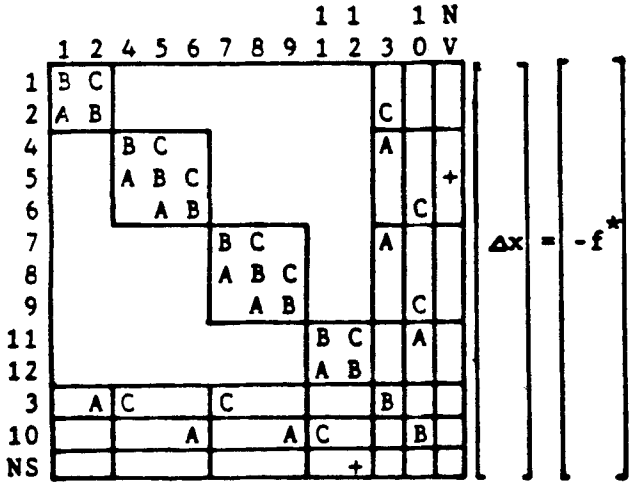

Figure 3. Permuted matrix.

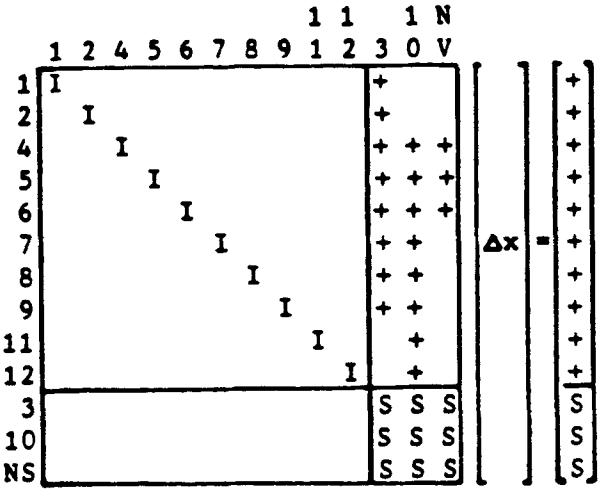

Figure 4. Reduced identity matrix.

Calculate: $\begin{bmatrix} x \\ \lambda \end{bmatrix}_N = \begin{bmatrix} x \\ \lambda \end{bmatrix}_o + \sigma u$

If $\lambda_o \cdot \lambda_N < 0$, go to 8.
If $|\lambda_N|$ > some specified very large value, go to 9.

7. Apply the Newton corrector step to solve Eq. 10 by the BE algorithm with the deflated decomposition technique, or use the deflated BE alogrithm (Chan, 1984c). If the Newton corrector is not converging to the chosen tolerance after a few iterations, then halve the step size and go to 6. Otherwise, if λ goes from positive to negative or negative to positive, go to 8. Otherwise go to 3.

8. Calculate the solution at $\lambda = 0$ by Newton's method. Let $MR = MR + 1$. If $MR \geq MROOTS$, go to 9. Otherwise, go to 3.

9. Stop

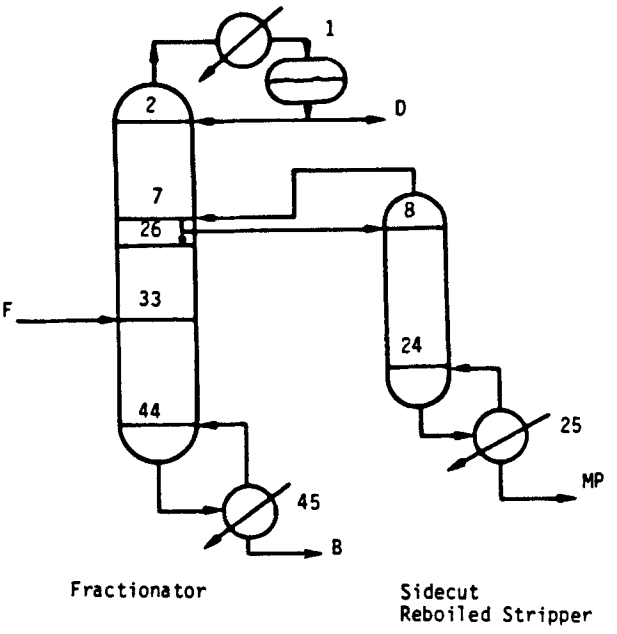

Figure 5. Interlinked system of example 1.

Table 1. Specifications for Example 1

Feed to Prefractionator, *F*
Saturated liquid at 101.3 KPa
Flow rate = 0.126 kmol/s
Molar composition:
benzene = 20%
toluene = 40%
o-xylene = 40%
Products from Fractionator
Distillate, *D*
Saturated liquid
Purity: benzene = 95 mol %
Middle product, *MP*
Saturated liquid
Purity: toluene = 90 mol %
Bottoms, *B*
Saturated liquid
Purity: *o*-xylene = 95 mol %

Examples of the Algorithm

Interlinked separation problems

A detailed mathematical model and procedure for solving interlinked multicomponent, multistage separation systems is described by Wayburn (1983), and Wayburn and Seader (1983). Using that procedure, Chavez (1985) and Chavez et al. (1986) found multiple solutions for three different interlinked systems by using different starting points. In this work we obtained, for each system, all solutions from just one starting point. To prevent failure of the thermodynamic property subroutines, mapping functions were used to constrain temperature, flow rates, and mole fractions to the positive domain at all points along the homotopy path.

As shown by Wayburn (1983) and Chavez (1985), the matrix for interlinked separation systems has a special structure. For example, for a Petlyuk system of the type shown in Figure 1, the Jacobian matrix, as shown in Figure 2, is sparse and mostly block tridiagonal, but contains some disperse submatrix elements. A bordered, block-bordered, block-diagonal, block-tridiagonal form, shown in Figure 3, can be obtained by permuting the disperse elements to the borders, as suggested by Stadtherr and Malachowski (1982). Wayburn (1983) shows how to reduce the Jacobian matrix to the identity matrix shown in Figure 4, by using the routines SGECO and SGESL in LINPACK. Unfortunately, when the Jacobian matrix is ill-conditioned, the method fails. To prevent this the deflated decomposition technique was used to replace the SGESL routine. If LU-factorization is used to handle the entire matrix, the matrix loses its special-structure properties. So this special solver with the deflation technique was applied and was found to be reliable.

Example 1. The interlinked separation system shown in Figure 5 consists of a 27-theoretical-stage fractionator coupled to an 18-theoretical-stage sidecut reboiled stripper to separate a ternary mixture. The pressure of each stage is assumed constant within the system at 101.3 KPa. Specifications for this example are given in Table 1. The external reflux ratio for the fractionator is specified as 7 and the reflux is saturated liquid. Chavez (1985), and Chavez et al. (1986) found two real positive solutions for this interlinked system by using a number of different starting guesses. In this work, one arbitrary starting guess was used to obtain both solutions. The results are shown in Figures 6 and 7, where S is the starting point and A and B are the two solutions in terms of the total vapor returning to the fractionator in Figure 6 and the flow rate of benzene in the vapor leaving stage 17 of the stripper in Figure 7. For these results, the physical properties could not be computed without the proposed variable mapping functions. In Figure 7 the vapor flow rate of benzene is defined by the following equations:

$$v_{1,17} = \begin{cases} y_{1,17}^2 & \text{if } y_{1,17} \geq 0 \\ -y_{1,17}^2 & \text{if } y_{1,17} < 0 \end{cases} \tag{16}$$

The closed loop in Figure 7 was obtained by following the homotopy path in the domain y. The path was started from point S. Then two real roots, first A and then B, were found. When the

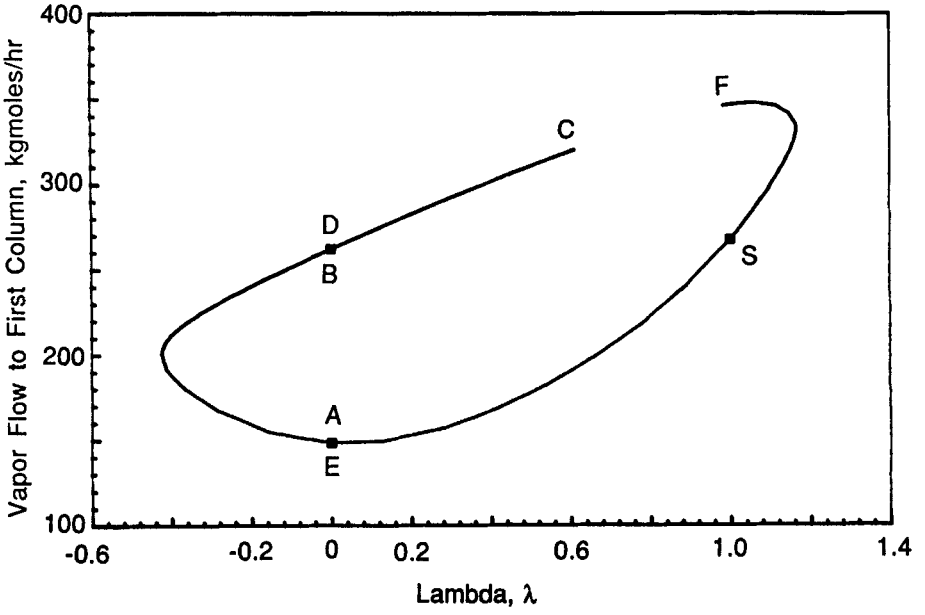

Figure 6. Two solutions for vapor interlink flow in example 1.

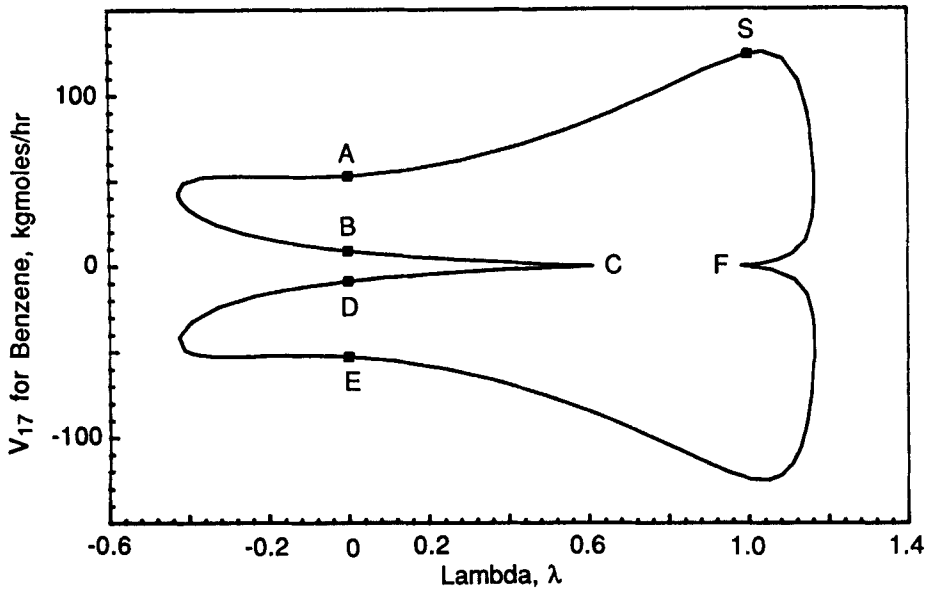

Figure 7. Two solutions for benzene vapor flow in example 1.

path reached point *C*, a negative region was encountered, which produced two negative roots at *D* and then *E*. At point *F*, the path reached the positive domain and then returned to the initial point, *S*. Although not obvious, the path in Figure 6 is also closed, proceeding in the order *S*, *A*, *B*, *C*, *D*, *E*, *F*, *S*. As shown clearly in Figure 7, four turning points occur in the closed path.

Example 2. A Petlyuk interlinked system, as shown in Figure 8, consists of a 20-theoretical-stage prefractionator and a 32-theoretical-stage fractionator. Again, pressure is assumed at 101.3 KPa throughout the system. The specifications are given in Table 2. The external reflux ratio in the fractionator is specified as 5 and the reflux is saturated liquid.

The results are shown in Figures 9 and 10. Chavez (1985) and Chavez et al. (1986) report four different solutions in the positive domain. Solution *A* was found starting from *S* in the direction of decreasing λ. No turning points were encountered along the *S*, *A* path. Now, we also follow the path from *S* in the direction of increasing λ and encounter three more solutions (*B*, *C*, and *D*). If we continue tracing the path from *C*, the path remains in the negative region. Solutions *A*, *B*, *C*, and *D* are precisely the solutions of Chavez (1985) using many different starting points. Here, all real solutions are found from one arbitrary starting point.

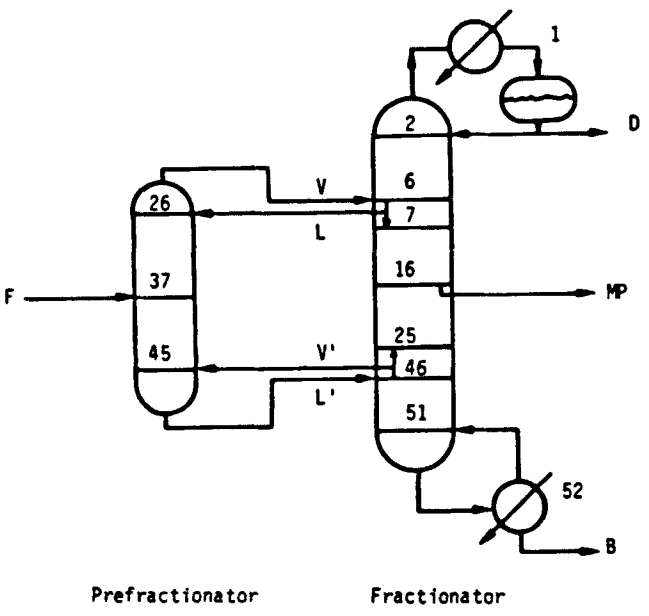

Figure 8. Petlyuk system of example 2.

Optimization and constrained problems

Example 3. Consider an unconstrained optimization problem. We desire to find all stationary points of Himmelblau's function, which, as described by Reklaitis et al. (1983) is:

$$f(x) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \qquad (17)$$

At the desired points, the following equations must be satisfied:

$$g_1(x_1, x_2) = \frac{\partial f(x)}{\partial x_1} = 0 \qquad (18)$$

Table 2. Specifications for Example 2

Feed to Prefractionator
Same as example 1
Products from Fractionator
Distillate, *D*
Saturated liquid
Purity: benzene = 95 mol %
Middle product, *MP*
Saturated liquid
Purity: toluene = 90 mol %
Bottoms, *B*
Saturated liquid
Flow rate = 0.04788 kmol/s
Purity: *o*-xylene = 95 mol %

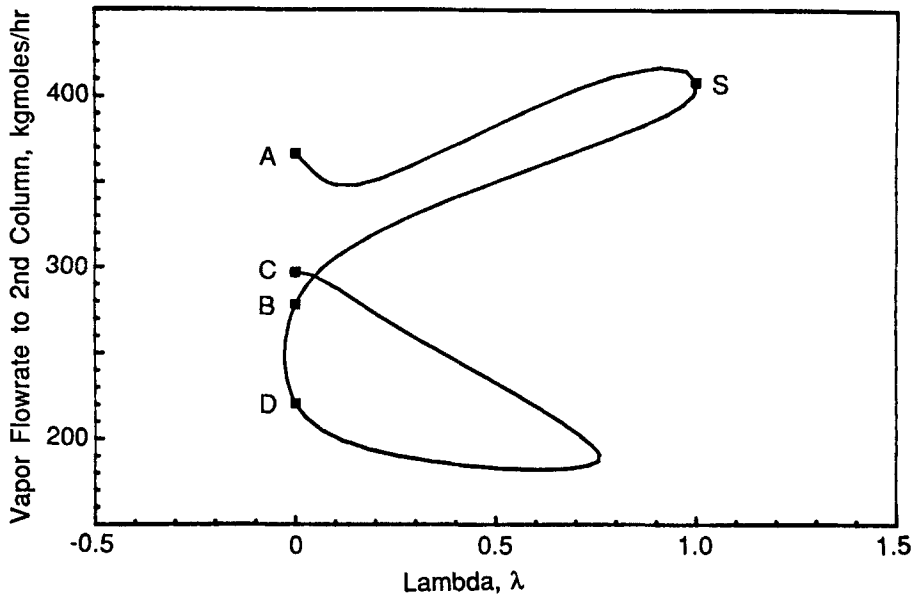

Figure 9. Four solutions for vapor interlink flow in example 2.

$$g_2(x_1, x_2) = \frac{\partial f(x)}{\partial x_2} = 0 \tag{19}$$

If we solve g_1 and g_2 simultaneously by using the Newton homotopy from a starting point of $(x_1, x_2)^o = (0.4, 0.4)$, nine roots of g_1 and g_2 are obtained from a single path by allowing λ to take on values <0 and >1, Table 3. The homotopy path covering the four global minima, one local maximum and four saddle points in Table 3 is plotted in Figure 11 for x_1 and in Figure 12 for x_2. The solutions are the points at $\lambda = 0$. Turning points, totaling eight, occur whenever λ changes direction. The deflated decomposition technique was used to continue the path around these turning points.

Example 4. Consider the following nonlinear system, as described by Wayburn and Seader (1986), with constrained conditions:

$$f_1 = x_2 - 1 = 0$$
$$f_2 = 1.613 - 4(x_1 - 0.3125)^2 - 4(x_2 - 1.625)^2 = 0 \tag{20}$$

with $x_1 \geq 0$, and $x_2 \geq 0$. If the Newton homotopy function is chosen, then as shown in Figure 13, starting from the point $S = (0.2, 2)$ an unclosed curve *A-S-D* can be generated that includes the only two solutions at points E and F. However, because x_1 is constrained to the positive domain, solutions E and F cannot be

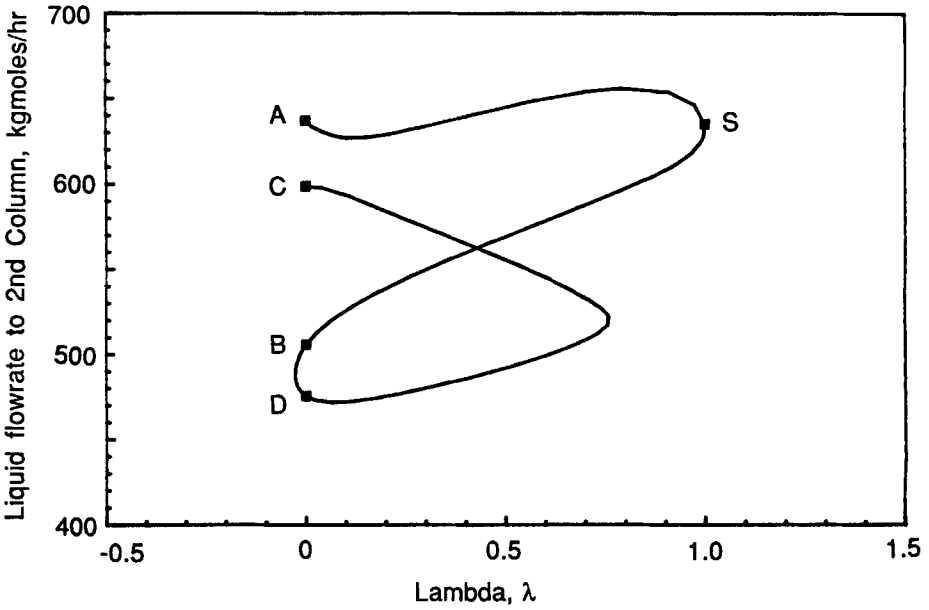

Figure 10. Four solutions for liquid interlink flow in example 2.

Table 3. Solutions for Example 3

x_1^*	x_2^*	f
−0.2709	−0.9230	181.62 (LM)
−0.1279	−1.9538	178.34 (SP)
3.5844	−1.8481	0 (GM)
3.3852	0.0739	13.31 (SP)
3.0	2.0	0 (GM)
0.0867	2.8843	67.72 (SP)
−2.8051	3.1313	0 (GM)
−3.0730	−0.0814	104.02 (SP)
−3.7793	−3.2832	0 (GM)

LM, local maximum
SP, saddle point
GM, global minimum

reached by moving from A in the direction of decreasing λ. If mapping functions are used, the equations become

$$f_1 = y_2^2 - 1 = 0$$
$$f_2 = 1.613 - 4(y_1^2 - 0.3125)^2 - 4(y_2^2 - 1.625)^2 = 0 \quad (21)$$

When these equations are solved in the y domain with a Newton homotopy, starting from the initial point $S = (y_1, y_2)^o = (0.2^{0.5}, 2^{0.5})$, a closed loop, which produces two more roots at B and C, is obtained from the direction of either decreasing or increasing λ starting at $\lambda = 1$. This result is included in Figure 13. The closed-loop path is generated from the following map-

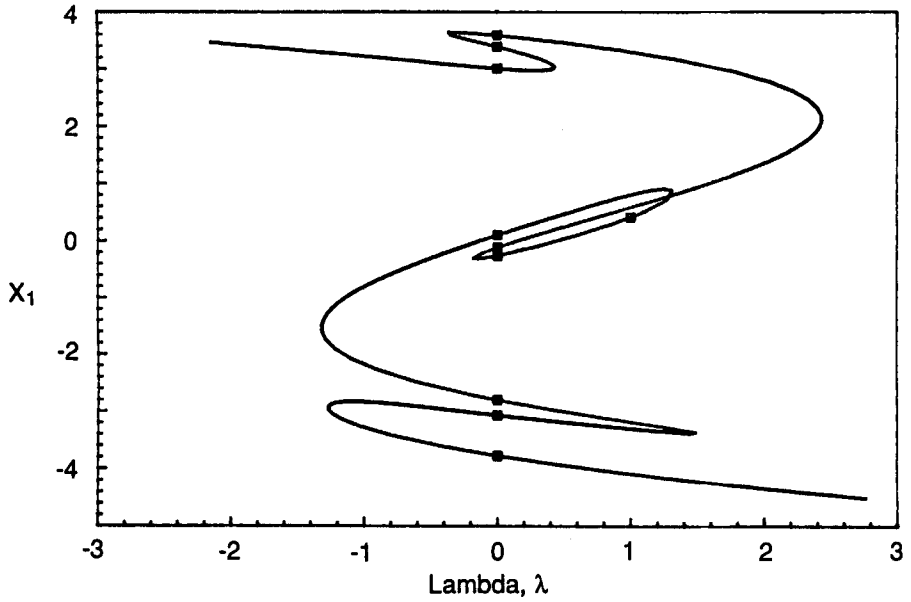

Figure 11. All solutions for x_1 in example 3, Himmelblau's optimization function.

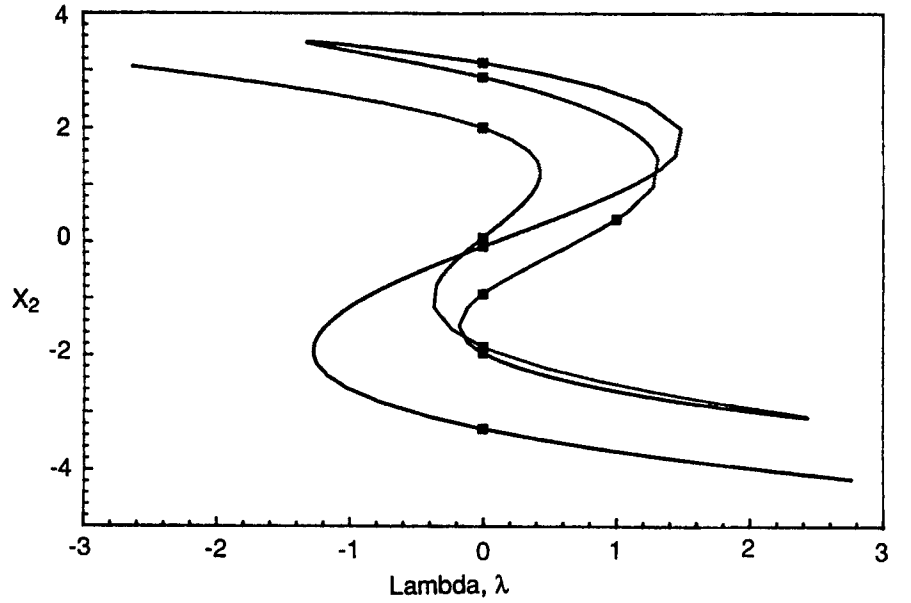

Figure 12. All solutions for x_2 in example 3, Himmelblau's optimization function.

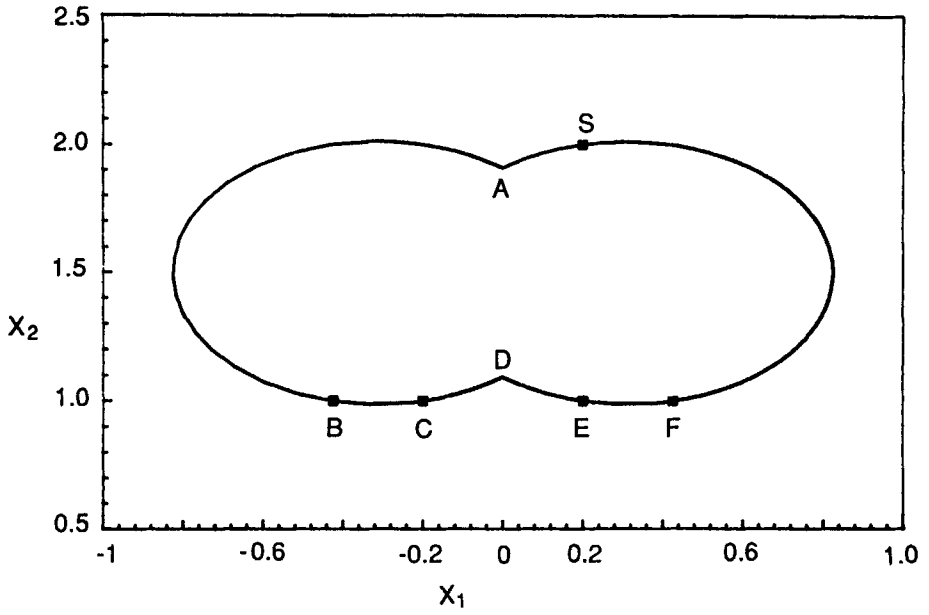

Figure 13. All solutions to example 4.

ping functions:

$$x_i = y_i^2, \quad y_i \geq 0$$
$$x_i = -y_i^2, \quad y_i < 0 \tag{22}$$

This simple example shows that the mapping function technique proposed here can be used to solve constrained problems.

Discussion

It is currently impossible to make *a priori* estimates of the number of roots that exist for large systems of general nonlinear equations that contain transcendental functions. However, from the studies reported here it appears that homotopy continuation methods not only have a globally convergent nature, but also have the potential, for some problems, to find all solutions to the nonlinear system. For the four examples reported above, all desired solutions were found by tracking a Newton homotopy path from only one starting guess. Although the path must inevitably encounter turning points if more than one solution exists, the deflated decomposition technique can be applied to successfully continue following the path without having to alter the structure of the Jacobian matrix. Furthermore, it also appears that mapping functions can be used to handle variable constraints. This may be necessary when calling external subroutines such as those used to provide thermodynamic properties.

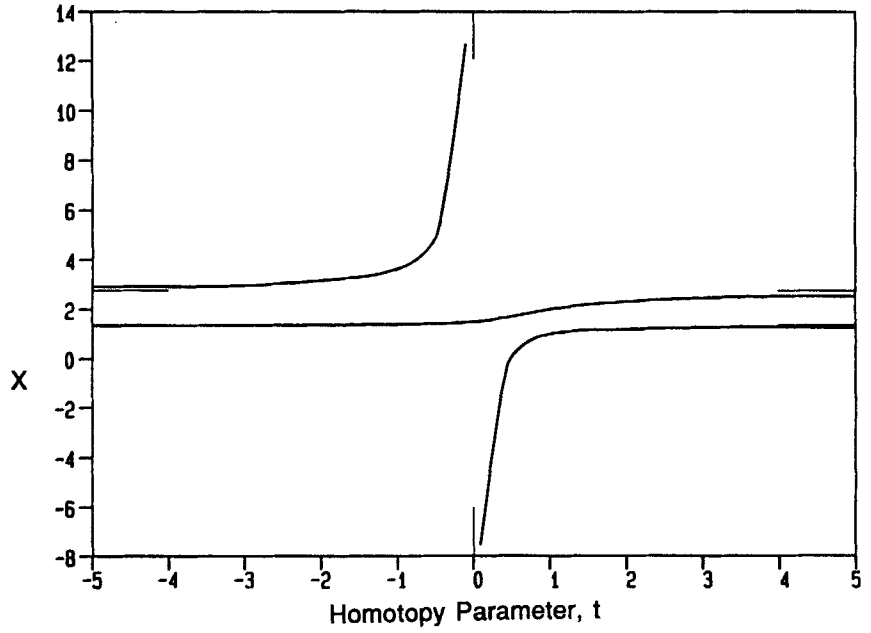

Figure 14. Branches of homotopy path.

The homotopy path, which depends on the initial guess, may encounter some or all roots of the original problem. Therefore, all values that satisfy $f(x) = f(x^o)$ need to be determined initially, so as to attempt to create all paths to all roots of the equations $f(x)$. Unfortunately, it is sometimes difficult to do this for the Newton homotopy function when the system contains many equations. The fixed-point homotopy function, $H = tf(x) + (1 - t)(x - x^o)$, and affine homotopy function, $H = tf(x) + (1 - t)f'(x^o)(x - x^o)$, have only starting point x^o that satisfies $x = x^o$ and, therefore, may be better suited for obtaining all solutions from a single starting function. Owing to the scaling problem of the fixed-point homotopy function, the affine homotopy may be the more desirable of the two and will be used for further research. As far as we know, there is no single homotopy function that can guarantee that all roots for an arbitrary system of nonlinear equations can be generated from a single $f(x^o) = 0$ starting condition. For example, consider the simple case of $f(x) = x^2 - 3x + 2 = 0$, for which the roots are easily seen to be (1, 2). If we construct a fixed-point homotopy, we obtain $H(x, t) = t(x^2 - 3x + 2) + (1 - t)(x - x^o) = 0$. If we let $x^o = 1.5$, the homotopy path consists of the three branches shown in Figure 14. Although these branches are connected at infinity, the path is not of finite length and some sort of branch jumping technique would be required to obtain both solutions from a single starting point.

Finally, it must be mentioned that the proposed variable mapping functions may create a large number of additional solutions that are not of interest. For example, consider the equations $f(x) = 0$, where $x^T = (x_1, \ldots, x_n)^T$, with $x_i \geq 0$, $i = 1, \ldots, n$, where only one positive solution exists. In the attempt to find all positive solutions, 2^n solutions will be created in the domain y.

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Notation

$A = n \times n$ matrix
$b = n \times 1$ vector
$c = n \times 1$ vector
d = scalar
$e^{n+1} = (n + 1)$th unit coordinate vector
f = vector function
f' = Jacobian matrix
g = vector function
h = scalar
H = vector homotopy function
K = iteration number
l = iteration number
M = bordered matrix, Eq. 11
n = number of equations; number of variables
p = arc length parameter
q = scalar
$r = n \times 1$ vector
$s = n \times 1$ vector
t = homotopy parameter
$u = (n + 1) \times 1$ vector
$v = (n + 1) \times 1$ vector; vapor flow rate
$x = n \times 1$ vector
x^o = initial guess vector
x^* = desired solution of equation system
x_i = ith component of vector x
$y = n \times 1$ vector
y_i = defined in Eq. 15

Greek letters

ϵ = belongs to
$\lambda = 1 - t$, homotopy parameter
σ = step length
ω = nonnegative scalar step factor

Subscripts

i = ith component
N = new value
O = old value

Superscripts

T = transpose
o = starting guess
$*$ = desired point

Other

$|\ |$ = absolute value
$\|\ \|$ = Euclidean norm

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