Process Analysis in the Complex Domain

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Analytical support for recent numerical work in process simulation in the complex domain is discussed. In particular, the observation that nondegenerate singular points are saddle points of the two-norm on the complex domain is proved rigorously and its numerical implications are discussed. The isothermal isobaric flash problem admits only real-valued two-phase solutions, provided that the feed conditions are real. Both single- and multivariable chemical process examples illustrate the theoretical results.

Introduction

In recent years there has been active interest in process simulation in the complex domain. Lucia and Xu (1992), Lucia and Taylor (1992), and Lucia et al. (1993) have demonstrated both the feasibility and value of complex domain process simulation since Newton's method and traditional dogleg strategies often exhibit periodic/chaotic behavior or converge to singular points, respectively. This article provides analytical support for iterative calculations in the complex domain using a couple of short proofs. First, nondegenerate singular points (which are not turning or bifurcation points) in the real domain correspond to saddle points in the complex domain as observed initially by Lucia and Xu (1992); therefore, there exists at least one eigendirection at any such singular point that can be used to construct a path to a solution. Secondly, the eigenvalues and eigenvectors of the Hessian matrix of the Rachford-Rice function at all singular points are always real, and thus all solutions to the TP flash problem are always real.

Analytic Functions and Singular Points

Definition 1. Any function, say $f(z)$, for $z \in C^n$ is said to be *analytic* if it is Cauchy-Riemann-differentiable over some neighborhood of z (Greenberg, p. 239, 1978). For this purpose, $f(z)$ is usually written in the form

$$f_j(z) = u_j(x_1, \ldots, x_n, y_1, y_2, \ldots, y_n) + iv_j(x_1, \ldots, x_n, y_1, \ldots, y_n), \quad j = 1, 2, \ldots, n \quad (1)$$

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where x_i and y_i are the real and imaginary ith components of the complex vector z, and u and v are vector functions in R^n.

Definition 2. A *singular point* of $f(z)$ is any point at which the Jacobian matrix of f, $[\partial f_i/\partial z_j]$, is not invertible (or singular). Since each of n components of f and z, that is, f_i and z_j, respectively, is complex, they can be expressed as the sum of real and imaginary parts: thus, $f_i = u_i + iv_i$ and $z_j = x_j + iy_j$. Alternately, at any singular point each of the complex-valued gradient vectors, $\partial f_i/\partial x_j$ and $\partial f_i/\partial y_j$, where

$$\frac{\partial f_i}{\partial x_j} = \frac{\partial[u_i(x, y) + iv_i(x, y)]}{\partial x_j} = \frac{\partial u_i}{\partial x_j} + i\frac{\partial v_i}{\partial x_j} \quad (2)$$

and

$$\frac{\partial f_i}{\partial y_j} = \frac{\partial u_i}{\partial y_j} + i\frac{\partial v_i}{\partial y_j} \quad (3)$$

must vanish $[\partial f_i/\partial x_j = \partial f_i/\partial y_j = 0 + 0i]$ for all i and j (Fleming, 1977). This implies that *all* first partial derivatives of u_i and v_i with respect to x_j and y_j vanish for all i and j at any singular point. Singular points can also be further classified as either degenerate or nondegenerate.

Definition 3. A *degenerate singular point* is any singular point that coincides with a solution of $f(z) = 0$. Otherwise, the singular point is said to be *nondegenerate*. At any degenerate singular point the Hessian matrix of the function f, $[(\partial^2 f_i)/(\partial z_j \partial z_k)]$ has a determinant of zero (Fleming, 1977).

Degenerate singular points can be further classified as turning or bifurcation points.

Definition 4. A turning point is any degenerate singular point at which the Jacobian matrix, $[\partial f_i/\partial z_j]$, has rank $n-1$ and through which passes a single parametric solution curve that folds back on itself. A *bifurcation point*, on the other hand, is any degenerate singular point at which the Jacobian matrix of f has rank $n-2$ and through which passes two distinct branches of a parametric solution curve.

Theorem 1. Nondegenerate singular points of any analytic function, say f, correspond to saddle points *of the real-valued function* $\|f\|^2 = f^T\bar{f}$.

Proof. Recall that any n-dimensional analytic function $f(z)$ for $z \in C^n$ can be written in the form of Eq. 1. Furthermore, the square of the norm of $f(z)$ can be represented as

$$\|f\|^2 = f^T\bar{f} = \sum_j (u_j + iv_j)(u_j - iv_j), \tag{4}$$

the gradient of $\|f\|^2$ is given by

$$\nabla\|f\|^2 = \left[\frac{\partial\|f\|^2}{\partial x_1}, \frac{\partial\|f\|^2}{\partial y_1}, \frac{\partial\|f\|^2}{\partial x_2}, \ldots, \frac{\partial\|f\|^2}{\partial x_n}, \frac{\partial\|f\|^2}{\partial y_n}\right]^T$$
$$= 2\left\{\left[\sum_{j=1}^n u_j\frac{\partial u_j}{\partial x_1} + \sum_{j=1}^n v_j\frac{\partial v_j}{\partial x_1}\right], \left[\sum_{j=1}^n u_j\frac{\partial u_j}{\partial y_1} + \sum_{j=1}^n v_j\frac{\partial v_j}{\partial y_1}\right],\right.$$
$$\left[\sum_{j=1}^n u_j\frac{\partial u_j}{\partial x_2} + \sum_{j=1}^n v_j\frac{\partial v_j}{\partial x_2}\right], \left[\sum_{j=1}^n u_j\frac{\partial u_j}{\partial y_2} + \sum_{j=1}^n v_j\frac{\partial v_j}{\partial y_2}\right], \ldots,$$
$$\left.\left[\sum_{j=1}^n u_j\frac{\partial u_j}{\partial x_n} + \sum_{j=1}^n v_j\frac{\partial v_j}{\partial x_n}\right], \left[\sum_{j=1}^n u_j\frac{\partial u_j}{\partial y_n} + \sum_{j=1}^n v_j\frac{\partial v_j}{\partial y_n}\right]\right\}^T, \tag{5}$$

and the Hessian matrix of $\|f\|^2$, which contains the second partial derivatives of $\|f\|^2$ with respect to x_i and y_i, has the form

$$\nabla^2\|f\|^2 = \begin{bmatrix} \frac{\partial^2\|f\|^2}{\partial x_1^2} & \frac{\partial^2\|f\|^2}{\partial x_1\partial y_1} & \frac{\partial^2\|f\|^2}{\partial x_1\partial x_2} & \cdot & \cdot & \cdot & \cdot \\ \frac{\partial^2\|f\|^2}{\partial y_1\partial x_1} & \frac{\partial^2\|f\|^2}{\partial y_1^2} & \frac{\partial^2\|f\|^2}{\partial y_1\partial x_2} & \cdot & \cdot & \cdot & \cdot \\ \frac{\partial^2\|f\|^2}{\partial x_2\partial x_1} & \frac{\partial^2\|f\|^2}{\partial x_2\partial y_1} & \frac{\partial^2\|f\|^2}{\partial x_2^2} & \cdot & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{\partial^2\|f\|^2}{\partial x_n\partial y_n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{\partial^2\|f\|^2}{\partial y_n\partial x_n} & \frac{\partial^2\|f\|^2}{\partial y_n^2} \end{bmatrix} \tag{6}$$

Note that Eqs. 5 and 6 are a consequence of the isomorphism between C^n and R^{2n}. Note also that $\nabla\|f\|^2$ in Eq. 5 equals zero if

(i) $f(z) = u(x, y) + iv(x, y) = 0 + 0i$ and/or

(ii) the Jacobian matrix of f is singular (see Definition 2).

Because f is analytic, functions u and v are harmonic and satisfy the (Laplacian) equations (Greenberg, p. 239, 1978).

$$\left(\frac{\partial^2 u_j}{\partial x_i^2} + \frac{\partial^2 u_j}{\partial y_i^2}\right) = 0 \quad i = 1, 2, \ldots, n; \quad j = 1, 2, \ldots, n \tag{7}$$

and

$$\left(\frac{\partial^2 v_j}{\partial x_i^2} + \frac{\partial^2 v_j}{\partial y_i^2}\right) = 0 \quad i = 1, 2, \ldots, n; \quad j = 1, 2, \ldots, n. \tag{8}$$

The sum of the eigenvalues (or diagonal elements) of any matrix equals its trace and thus the trace of $\nabla^2\|f\|^2$ is

$$tr(\nabla^2\|f\|^2) = \sum_i \frac{\partial^2\|f\|^2}{\partial x_i^2} + \frac{\partial^2\|f\|^2}{\partial y_i^2}$$
$$= 2\sum_j\sum_i\left[\left(\frac{\partial u_j}{\partial x_i}\right)^2 + \left(\frac{\partial u_j}{\partial y_i}\right)^2 + \left(\frac{\partial v_j}{\partial x_i}\right)^2 + \left(\frac{\partial v_j}{\partial y_i}\right)^2\right.$$
$$\left. + u_j\left(\frac{\partial^2 u_j}{\partial x_i^2} + \frac{\partial^2 u_j}{\partial y_i^2}\right) + v_j\left(\frac{\partial^2 v_j}{\partial x_i^2} + \frac{\partial^2 v_j}{\partial y_i^2}\right)\right], \tag{9}$$

which simplifies to

$$tr(\nabla^2\|f\|^2) = 2\sum_j\sum_i\left[\left(\frac{\partial u_j}{\partial x_i}\right)^2 + \left(\frac{\partial u_j}{\partial y_i}\right)^2 + \left(\frac{\partial v_j}{\partial x_i}\right)^2 + \left(\frac{\partial v_j}{\partial y_i}\right)^2\right] \tag{10}$$

for any analytical function since Eqs. 7 and 8 are always satisfied. Furthermore, because the first partial derivatives of u_j and v_j with respect to x_i and y_i for all i and j are zero at any singular point, it follows that the trace of $\nabla^2\|f\|^2$ is zero at either a degenerate or nondegenerate singular point.

To further distinguish between degenerate and nondegenerate singular points, we need to differentiate Eq. 2 with respect to x_j and y_j. This gives

$$\frac{\partial}{\partial x_j}\left(\frac{\partial\|f\|^2}{\partial x_i}\right) = \left(\frac{\partial^2\|f\|^2}{\partial x_i\partial x_j}\right) = 2\left\{\sum_k\left[\left(\frac{\partial u_k}{\partial x_j}\right)\left(\frac{\partial u_k}{\partial x_i}\right)\right.\right.$$
$$\left.\left. + u_k\left(\frac{\partial^2 u_k}{\partial x_i\partial x_j}\right) + \left(\frac{\partial v_k}{\partial x_j}\right)\left(\frac{\partial v_k}{\partial x_i}\right) + v_k\left(\frac{\partial^2 v_k}{\partial x_i\partial x_j}\right)\right]\right\}$$
$$= 2\left\{\sum_k\left[u_k\left(\frac{\partial^2 u_k}{\partial x_i\partial x_j}\right) + v_k\left(\frac{\partial^2 v_k}{\partial x_i\partial x_j}\right)\right]\right\} \tag{11}$$

since all first partial derivatives of u and v with respect to x and y are zero at a singular point. Similarly we have

$$\left(\frac{\partial^2\|f\|^2}{\partial x_i \partial y_j}\right) = 2\left\{\sum_k \left[u_k\left(\frac{\partial^2 u_k}{\partial x_i \partial y_j}\right) + v_k\left(\frac{\partial^2 v_k}{\partial x_i \partial y_i}\right)\right]\right\} \quad (12)$$

$$\left(\frac{\partial^2\|f\|^2}{\partial y_i \partial x_j}\right) = 2\left\{\sum_k \left[u_k\left(\frac{\partial^2 u_k}{\partial y_i \partial x_j}\right) + v_k\left(\frac{\partial^2 v_k}{\partial y_i \partial x_j}\right)\right]\right\} \quad (13)$$

$$\left(\frac{\partial^2\|f\|^2}{\partial y_i \partial y_j}\right) = 2\left\{\sum_k \left[u_k\left(\frac{\partial^2 u_k}{\partial y_i \partial y_j}\right) + v_k\left(\frac{\partial^2 v_k}{\partial y_i \partial y_j}\right)\right]\right\} \quad (14)$$

and Eqs. 11–14 hold for all $i, j = 1, 2, \ldots, n$. Note also that the $2n \times 2n$ real-valued matrix, $\nabla^2\|f\|^2$, is symmetric.

For any degenerate singular point, $f_k(z) = 0 + 0i$, $k = 1, 2, \ldots, n$, and Eq. 1 implies that $u_k = v_k = 0$ for all k, which in turn implies that all second partial derivatives defined by Eqs. 11–14 are zero. Thus, the matrix $\nabla^2\|f\|^2$ is the zero matrix at any turning or bifurcation point. On the other hand, at any nondegenerate singular point, $f_k(z) \neq 0 + 0i$ for at least one k. Thus at least one u_k and/or $v_k \neq 0$ and this implies that the matrix $\nabla^2\|f\|^2$ is not the null matrix. Because $\nabla^2\|f\|^2$ is a real, symmetric matrix that is not null, it has real-valued, nonzero eigenvalues. Moreover, because the trace of $\nabla^2\|f\|^2$ is zero, at least two of these eigenvalues are of the opposite sign. Hence, any nondegenerate singular point of function f corresponds to a *saddle point* of the norm of f; therefore, there is always at least one eigendirection (an eigenvector corresponding to a negative eigenvalue) at any such point of singularity that can be used to construct a path to a solution. Note that Theorem 1 applies to single- or multivariable complex-valued analytic functions!

As a simple illustration, consider first the Soave-Redlich-Kwong (SRK) equation of state and a mixture of 0.6 mol nitrogen and 0.4 mol of tetradecane at 288 K and 0.6 MPa. The critical temperatures for N_2 and $C_{14}H_{30}$ are 126.1 K and 694.0 K, respectively. The corresponding critical pressures are 33.496 and 14.192 bar, and the acentric factors are 0.045 and 0.6797. Furthermore, the compressibility roots to the equation of state are 0.048683, $0.47566 + 0.37847i$, and $0.47566 - 0.37847i$, the nondegenerate singular points, which can be computed analytically, are $0.3333 - 0.1658i$ and $0.3333 + 0.1658i$ and the Hessian matrix at either point of singularity is

$$\nabla^2\|f\|^2 = \begin{bmatrix} 0.018137 & 0.092596 \\ 0.092596 & -0.018137 \end{bmatrix}.$$

Moreover, the eigenvalues of this Hessian matrix are 0.094356 and -0.094356 and can also be computed analytically, the trace is zero and either singular point is a saddle. The eigenvectors corresponding to the two eigenvalues are **[0.1, 0.082312]** and **[0.1, −0.121487]**. A step from the singular point $0.3333 + 0.1658i$, in the direction of the eigenvector **[0.1, −0.121487]**, results in convergence to the root $0.47566 + 0.37847i$ in six iterations.

Consider the Benedict-Webb-Rubin (BWR) equation of state, which is a sixth-order transcendental function in density. Because of this, the singular points of f and eigenvalues and eigenvectors of $\|f\|^2$ can only be determined numerically. In particular, for n-pentane at 378.25 K and 2.026 MPa, one of the nondegenerate singular points is $\rho = 0.913651$. The corresponding Hessian matrix at this real-valued singular point is

$$\nabla^2\|f\|^2 = \begin{bmatrix} 343.6096 & 0 \\ 0.0 & -343.6096 \end{bmatrix}.$$

Moreover, the eigenvalues of the Hessian matrix are simply the diagonal terms, the trace is zero, and the singular point is a saddle. The eigenvectors are real and, as for any real-valued singular point, are the canonical basis **[1.0, 0.0]** and **[0.0, 1.0]**. A step from the singular point, $\rho = 0.913651$, in the direction of the eigenvector **[0.0, 1.0]** associated with the negative eigenvalue, results in convergence to the complex-valued root $0.826006 + 0.757498i$ in six iterations.

At any turning or bifurcation point, the norm takes on a global minimum, the Hessian matrix is the zero matrix and thus the singular point is degenerate. For example, for the previous mixture of 0.6 mol of nitrogen and 0.4 mol of tetradecane at 6 MPa, there is a regular (real-valued) turning point at an approximate temperature of 333.75619 K. At these conditions, the roots are (0.045744, 0.47808, 0.47808) and the singular points are (0.18954, 0.47808). Note in Figure 1 the flatness of the level curves in the neighborhood of the degenerate singular point (where a pair of roots and singular point coincide, the one on the right). Note also that the eigenvalues and eigenvectors of the Hessian matrix, $\nabla^2\|f\|^2$, at the other singular point, which is clearly nondegenerate and a saddle point, can be used to find the other root, as shown in Figure 1. If both singular points are degenerate, then the only solution is the critical point and no further computations are required. For this example, the Hessian matrix at the singular point 0.18954 is

$$\nabla^2\|f\|^2 = \begin{bmatrix} 0.02052 & 0 \\ 0 & -0.02052 \end{bmatrix},$$

the eigenvalues of this Hessian matrix are 0.02052 and -0.02052, the eigenvectors are **[1.0, 0.0]** and **[0.0, 1.0]**, respectively, and a step from the singular point 0.18954 in the negative of the eigendirection **[1.0, 0.0]** results in convergence to the root 0.045744 in four iterations.

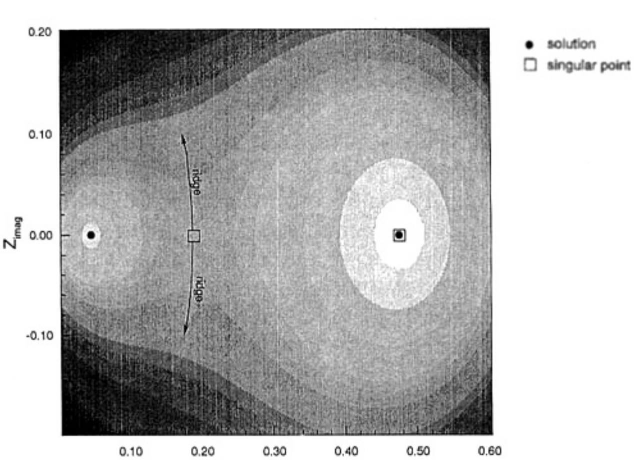

Figure 1. Level curves of $\|f\|^2$ for the SRK EOS.

Analysis of TP Flash Processes

Lucia and Taylor (1992) have used complex solutions to the SRK equation of state to solve the TP flash problem in the complex domain and have observed that all solutions to the flash problem are always real. That is, the temperature-composition surface always folds back on itself instead of bifurcating into the complex domain.

Theorem 2. For real-valued feed conditions, the isothermal isobaric flash problem admits only real-valued two-phase solutions.

Proof. Analyzing the Hessian matrix of the Rachford-Rice function at all singular points (trivial solutions) reveals why this is true. Since, by convention, the independent variables for the Rachford-Rice function are the compositions, it is more useful to perform the analysis in terms of K values and phase fraction. To do this, we write the Rachford-Rice function as

$$F(K_1, K_2, \ldots, K_{n_c}, \phi) = \sum_i \frac{z_i(K_i - 1)}{1 + (K_i - 1)\phi}. \quad (15)$$

The second partial derivative of F with respect to the phase fraction is given by

$$\frac{\partial^2 F}{\partial \phi^2} = 2 \sum_{i=1}^{n_c} \frac{z_i(K_i - 1)^3}{[1 + (K_i - 1)\phi]^3}. \quad (16)$$

At any trivial solution, $K_i = 1$ and $\partial^2 F/\partial \phi^2$ equals zero.

The second partial derivative of F with respect to K_i is given by

$$\frac{\partial^2 F}{\partial K_i^2} = -\frac{2 z_i \phi}{[1 + (K_i - 1)\phi]^2} + 2\frac{z_i(K_i - 1)\phi^2}{[1 + (K_i - 1)\phi]^3}. \quad (17)$$

Again, at any trivial solution, $K_i = 1 + 0i$ and $\partial^2 F/\partial K_i^2 = -2 z_i \phi$. Furthermore, straightforward differentiation reveals that $\partial^2 F/(\partial K_i \partial K_j) = 0$ when $i \neq j$ and that $\partial^2 F/(\partial K_i \partial \phi) = 0$ when $K_i = 1 + 0i$. Hence the Hessian matrix, $\nabla^2 F$, is a real diagonal matrix. Thus, the eigenvalues of this matrix are real, and the eigenvectors are the canonical basis that constitute the columns of the identity matrix. Since the eigenvalues and eigenvectors of the Hessian matrix are real at all singular points, the solution curve cannot bifurcate into the complex domain and must fold back on itself.

TP flash processes, in which all equilibrium phases are modeled by a single equation of state and for which the temperature and pressure specifications are in the two-phase region, admit both a nontrivial and a trivial solution. Both are global minima of $\|f\|^2$. Furthermore, the nontrivial solution is usually the desired solution, but it is not uncommon for equation-solving methods such as Newton's method to converge to the trivial solution. Theorems 1 and 2, however, provide some guidance in this regard. Because the trivial solution is also a singular point, the previous discussion of turning and bifurcation points is also relevant. In particular, Theorem 2 shows that only real solutions are possible. This does not mean the calculations have to be confined to the real domain, it simply means the solutions, trivial and nontrivial, are real! Theorem 1 and the discussion of turning and bifurcation points, on the other hand, show that if a trivial solution is calculated, then "another" singular point (or saddle point) must be located to move away from the trivial solution and toward the nontrivial solution. Note that the other singular point for $\|f\|^2$ for the SRK equation in Figure 1 (the saddle of $\|f\|^2$) lies on a ridge in the surface of the norm. Similar geometric behavior is found in TP flash problems. To see this, consider the TP flash process for a mixture of 6 kmol/h of nitrogen and 4 kmol/h of tetradecane at 300 K and 20 MPa. Figures 2 and 3 show the level curves of the

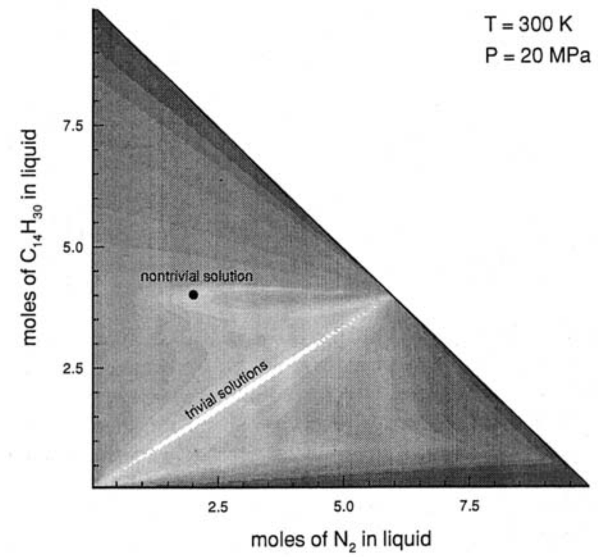

Figure 2. Level curves for $\|f\|^2$ for TP flash using a single real-valued EOS.

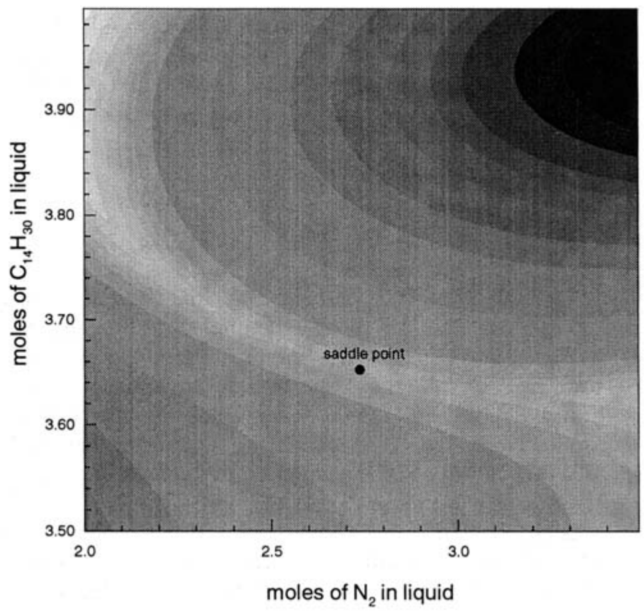

Figure 3. Enlarged level curves for $\|f\|^2$ for TP flash using a single real-valued EOS.

phase equilibrium equations projected onto the component mass-balance equations when all calculations are restricted to the real domain and the SRK equation is used. Note that there is a one-dimensional subspace of trivial solutions given by the line that runs from the origin to the hypotenuse of the triangular region. The point on the hypotenuse represents the upper limit on liquid molar flows defined by the feed molar flows. Also note that there are ridges, valleys and, most importantly, a saddle point between the subspace of trivial solutions and the nontrivial solution. Therefore, if the calculations converge to a trivial solution, a saddle point in the surface of $\|f\|^2$ must be found. Once this saddle point is located, the direction from the trivial solution to the saddle point is constructed and the saddle point is perturbed in this direction. This avoids costly eigenvalue-eigenvector calculations for high-dimensional problems. This perturbed saddle point is then used as an initial value for the flash calculations. For this example, the trivial solution calculated by Newton's method is 5.1 and 3.4 kmol/h of N_2 and $C_{14}H_{30}$, respectively. The saddle point, on the other hand, is 2.80 and 3.66 kmol/h of nitrogen and tetradecane, respectively. Perturbation of the saddle point in the direction from the trivial solution to the saddle results in convergence of Newton's method to the nontrivial solution in seven iterations. Again, here all calculations were confined to the real domain.

Figure 4 shows the level curves of $\|f\|^2$ projected onto the real-valued component mass balances for the same TP flash problem when the calculations are performed in the complex domain (the roots of the SRK equation and the iterates for the flash equations are allowed to take on complex values). The important point to note here is the absence of a subspace of trivial solutions, which clearly shows one of the primary advantages of using complex domain calculations. Note that even when the phases have equal compositions trivial solutions do not exist if the vapor and liquid compressibility roots are unequal because then K values are unequal to one. For example, for a feed mixture of 6 kmol/h of nitrogen and 4 kmol/h of tetradecane at flash conditions of 300 K and 20 MPa and initial guesses for the unknown variables of $x=(0.6, 0.4)$, $y=(0.6, 0.4)$, $L=6.25$ in kmol/h and $V=3.75$ kmol/h, real domain calculations converge immediately (in one iteration) to a trivial solution regardless of the method used to solve the model equations. On the other hand, when the calculations are performed in the complex domain from the same initial guesses the trivial solution is annihilated. This is because liquid and vapor compressibilities, which were determined to be $z_L=-0.2457-3.387i$ and $z_V=1.491$, respectively, are unequal. This, in turn, causes K values to be unequal to 1 and the two-norm of the model equations to be 7.578, which is clearly not zero. Despite this, our extended dogleg strategy, which explicitly uses Theorem 1 to calculate such things as appropriate phase compressibilities, converges to the nontrivial solution, $x=(0.3302, 0.6698)$, $y=(0.999975, 0.000025)$, $L=5.972$ kmol/h, and $V=4.028$ kmol/h, in ten iterations. However, while complex-valued calculations do not always annihilate trivial solutions, they very often do. When they do not, a saddle point can always be used to find the nontrivial solution.

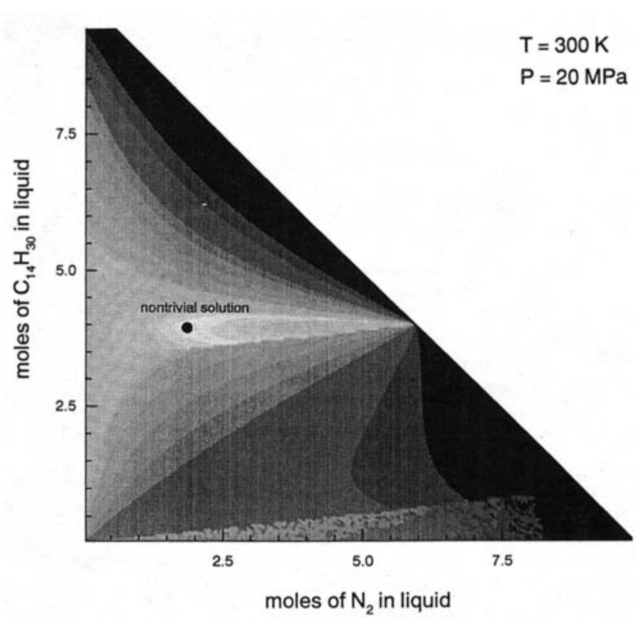

Figure 4. Level curves for $\|f\|^2$ for TP flash using a single complex-valued EOS.

Conclusions

Analysis of the Hessian matrix at singular points has led to some interesting discoveries of analytical and computational value. The fact that nondegenerate singular points of a function correspond to saddle points of the norm in the complex domain indicates that eigendirections of the Hessian matrix of the norm (or other directions) can be used to construct a path from a singular point to a solution. Similar analysis has led to the conclusion that solution curves to the TP flash problem must fold back on themselves as isola and cannot bifurcate into the complex domain.

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Notation

f = complex-valued vector function
F = Rachford-Rice function
K = K value
u = real part of f
v = imaginary part of f
x = real component of z, liquid composition
y = imaginary component of z, vapor composition
z = complex vector

Greek letters

ϕ = phase fraction
ρ = density

Subscripts

L = liquid
V = vapor

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