

Four-Component Gas/Oil Displacements in One Dimension: Part I: Global Triangular Structure

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Abstract. This paper presents an analysis of the mathematical structure of three-component and four-component gas displacements. The structure of one-dimensional flows in which components partition between two phases is governed by the geometry of a set of equilibrium tie lines. We demonstrate that for systems of four components, the governing mass conservation laws for the displacement can be represented by an eigenvalue system whose coefficient matrix has a global triangular structure, which is defined in the paper, for only specific types of phase behavior. We show that four-component systems exhibit global triangular structure if and only if (1) tie lines meet at one edge of the quaternary phase diagram or (2) if tie lines lie in planes. For such systems, shock and rarefaction surfaces coincide and are planes. We prove that systems are of category (2) if equilibrium ratios (K-values) are independent of mixture composition. In particular, for such systems shock and rarefaction curves will coincide. We also show that for systems with variable K-values, the rarefaction surfaces are almost planar in a precise sense, which is described in the paper. Therefore, systems with variable K-values may be well approximated by assuming shock and rarefaction surfaces do coincide. For these special systems the construction of solutions for one-dimensional, two-phase flow with phase behavior simplifies considerably. In Part II, we describe an application of these ideas to systems in which K-values are constant.

Key words: global triangular structure, tie line geometry, constant K-value, developable surface.

Nomenclature

- a* composition of C_1 for $P(\xi, \eta)$ in Figure 2.
- A** coefficient matrix defined in Equation (10).
- b** composition of C_2 for $P(\xi, \eta)$ in Figure 2.

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c_{ij}	volume fraction of component i in phase j .
C_i	overall volume fraction of component i .
D	defined in Equation (13).
\vec{e}_b	direction of a tie line in $C_3=0$ face.
\vec{e}_f	direction of a tie line in $C_4=0$ face.
\vec{e}_i	direction of a tie line in Γ that intersects \vec{e}_b .
F_i	overall fractional flow of component i .
g	component 2 tie line intercept at $C_1=0$ face.
G	defined in Equation (11).
h	defined in Equation (28).
H	defined in Equation (12).
h^{LR}	defined in Equation (36).
K_i	equilibrium K-value for component i .
l	parameter that traces along the nontie-line path.
l_2	component 2 tie line slope.
l_3	component 3 tie line slope.
L	defined in Equation (14).
m_2	component 2 tie line intercept at $C_1=0$ face.
m_3	component 3 tie line intercept at $C_1=0$ face.
N	defined in Equation (14).
n_c	number of components.
p	defined in Equation (28).
Q	a constant in Equation (22).
R	right-hand side of Equation (21).
s	parameter that determines the position along the tie line.
S	vapor phase saturation.
t	dimensionless time.
U	defined in Equation (27).
U	vector $(C_1, \xi, \eta)^T$.
x_i	liquid phase volume fraction of component i .
y_i	vapor phase volume fraction of component i .
z	dimensionless length.
α	see Equation (58).
β	see Equation (58).
γ	see Figure 2.
η	tie line slope in $C_3=0$ face.
κ	smooth function in Equation (25).
κ^{LR}	defined in Equation (36).
λ	eigenvalue (wave velocity).
Δ	shock wave velocity.
ξ	value of C_3 where a tie line in Γ intersects $C_1=0$ face.
τ	z/t .

1. Introduction

Interactions of equilibrium phase behavior with multiphase flow lie at the heart of displacement processes in which oil is displaced from a porous medium by a gas mixture, by a surfactant mixture, or by water containing dissolved polymer. Multicontact miscible gas/oil displacements, for

example, rely on chromatographic separations, which take place when phases with different equilibrium compositions flow at different velocities, to achieve high displacement efficiency. In any oil recovery process, hundreds of chemical components are present, but for the purposes of analysis, the phase behavior is always represented in terms of a small number of components, often only three. Recent research has indicated, however, that three-component descriptions of many processes do not reveal all the important aspects of the physical mechanisms, and hence it is desirable to increase the number of components included in the representation of the phase behavior (Zick, 1986; Monroe *et al.*, 1990; Dindoruk *et al.*, 1992, 1997; Johns *et al.*, 1992; Dindoruk *et al.*, 1993; Orr *et al.*, 1993).

Mathematically, the process of oil displacement by injection gas can be characterized by a set of nonstrictly hyperbolic mass conservation equations which, along with the initial and injection conditions, constitute a Riemann problem. The mass conservation equations have been solved repeatedly for three-component systems by investigators of alcohol flooding, surfactant flooding and gas displacement processes, and the theory of two-phase, three-component flows is largely complete. An extensive set of references to that literature is given by Johansen (1992a,b). The problem of three-phase flow with three components partitioning among the phases has been considered by LaForce and Johns (2004), who provide references to previous work for systems with three immiscible phases.

Investigations of four-component problems have been limited to gas/oil displacements. Four-component solutions were first reported by Monroe *et al.* (1990), and the properties of those solutions and many others were subsequently explored in detail by Dindoruk *et al.* (1992, 1997). Solutions were also reported by Bedrikovetsky and Chumak (1992), Entov (1997) and Voskov and Entov (2001) for displacement processes with constant K-values. Extensions to systems with more than four components were made by Johns and Orr (1996), Wang and Orr (1997, 2000), Wang (1998), Jessen (2000) and Jessen *et al.* (2001). The general Riemann problem for immiscible two phase flow with an arbitrary number of absorbing components dissolved in one of the phases was solved by Johansen and Winther (1988, 1989, 1990).

In this paper, we analyze the mathematical structure of Riemann problems for two-phase gas injection processes with three and four components. In particular, we examine the conditions under which the eigenvalue problems that describe the flow can be cast in triangular form. We also show that systems with constant K-values are triangular. Furthermore, we prove that when K-values are not constant, the rarefaction surfaces are ruled, developable surfaces (Kreyszig, 1959), which means that adjacent tie lines intersect and rarefaction surfaces are locally nearly planar. That proof reveals why it is often a reasonable approximation to assume that shock and rarefaction surfaces do coincide for systems with variable K-values.

2. Mathematical Model

For one-dimensional dispersion-free flow in which components do not change volume as they transfer between phases, the dimensionless mass conservation equations are

$$\frac{\partial C_i}{\partial t} + \frac{\partial F_i}{\partial z} = 0, \quad i = 1, \dots, n_c, \quad (1)$$

where

$$C_i = x_i(1 - S) + y_i S, \quad F_i = x_i(1 - f) + y_i f, \quad i = 1, \dots, n_c. \quad (2)$$

In Equations (1) C_i is the overall composition for component i , F_i is the overall fractional flow for component i , x_i is the liquid phase composition of component i , y_i is the vapor phase composition of component i , S is the vapor phase saturation and f is the vapor phase fractional flow function. Equations (1) are derived based on the assumptions that (1) the flow occurs in one space dimension, (2) effects of dispersion, gravity and capillary pressure can be neglected, (3) phases present at any spacial location are in thermodynamic equilibrium, and (4) equilibrium phase compositions can be calculated from a thermodynamic description of the fluid mixtures that applies throughout the displacement domain.

Equations (1) are subject to

$$\sum_{i=1}^{n_c} C_i = 1. \quad (3)$$

While we restrict the analysis in this paper to systems with no volume change upon mixing, we note that the principal results concerning tie line geometry also apply when components change volume as they transfer between phases (Dindoruk *et al.*, 1992). It would be straightforward to include gravity in the fractional flow function, but here we do not include effects of gravity.

Equations (1), along with the initial and injection conditions,

$$C_i(z, 0) = C_i^{inj} \quad z < 0, \quad i = 1, \dots, n_c, \quad (4)$$

$$C_i(z, 0) = C_i^{mi} \quad z \geq 0, \quad i = 1, \dots, n_c, \quad (5)$$

constitute a Riemann problem, whose solution consists of rarefactions, shocks and constant states. For general discussions of Riemann problems, see Lax (1957) and Smoller (1983).

In the discussion that follows, it will be convenient to specify fluid phase behavior in two ways. One is to specify the equilibrium ratios, or K-values, defined as

$$K_i = \frac{y_i}{x_i}, \quad i = 1, \dots, n_c. \quad (6)$$

The other way is to specify the geometry of tie lines and then also describe the location in composition space of the surface of phase compositions. Equilibrium compositions are then given by the intersections of tie lines with the equilibrium surface.

The analytical solution to the Riemann problem of Equations (1), (4) and (5) is constructed by solving the eigenvalue problem associated with the mass conservation laws (Helfferich, 1981). Eigenvalues give the propagation velocity of a given composition, and eigenvectors are directions of variation in composition space that satisfy the conservation equations. The solution is then constructed as a set of compatible composition variations (shocks and rarefactions) that connect the initial and injection compositions and lie on integral curves of the eigenvectors, also known as paths. To be compatible, compositions that propagate with high velocity must lie downstream of slower ones (this restriction is also known as the velocity rule).

When it is impossible to construct a solution that lies entirely on paths and satisfies the compatibility requirement, shocks are required. Any shock must satisfy an integral balance of the form

$$\Lambda = \frac{F_i^u - F_i^d}{C_i^u - C_i^d}, \quad i = 1, \dots, n_c. \quad (7)$$

When a shock connects a two-phase composition to a single-phase composition, the single-phase composition must lie on the extension of a tie line that contains the two-phase composition (Larson, 1979). When a shock connects two compositions that lie within the two-phase region, the extensions of tie lines through the compositions must intersect (Dindoruk, 1992; Johns, 1992; Dindoruk *et al.*, 1992; Orr *et al.*, 1993; Johns *et al.*, 1993).

In addition, any shocks present must satisfy an entropy condition, which requires that the shock be stable to dispersive perturbations. The entropy condition is used to determine when a shock velocity must match an eigenvalue on one side of a shock.

3. Tie Line Geometry in Four-Component Systems

In the analysis that follows, we consider flow of four components that form up to two phases in some region, Φ , of the space, Γ , of physically allowable compositions in which $C_i \geq 0$ and $C_1 + C_2 + C_3 + C_4 = 1$. Figure 1 shows a sketch of the composition space and a typical two-phase region.

We assume that tie lines do not intersect inside Γ , though extensions of tie lines can and do intersect on the boundary ($C_i = 0$ and $C_1 + C_2 + C_3 = 1$). We also assume that Φ is sufficiently regular that each tie line intersects the boundary of Φ exactly twice. Therefore the surface of Φ must be divided into two parts (hence its designation as the binodal

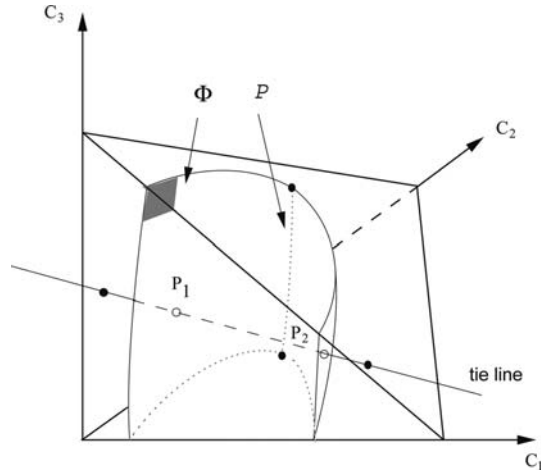


Figure 1. Composition space and two-phase region.

surface), one associated with the liquid (oil) phase and the other associated with the vapor (gas) phase. At some temperatures and pressures, the liquid and vapor portions of the binodal surface of Φ meet at a locus of critical points at which the compositions and all the properties of the two phases are identical. In Figure 1 that critical locus is labeled \mathbf{P} . When a critical locus is absent, as in the case when pressure is low, the surface of Φ may intersect any or all of the surfaces of the composition space.

3.1. GLOBAL TRIANGULAR STRUCTURE

In the analysis that follows, global triangular structure is defined as the existence of a parametric representation of tie lines for which the associated Jacobian is upper triangular for all parameter values in the two-phase region. It is convenient for analysis to write the mass conservation equations in terms of the geometric properties of tie lines, which control solution structure and behavior. To do so, we represent the equation of a general tie line again in terms of tie line slopes and intercepts

$$C_2 = l_2(\xi, \eta)C_1 + m_2(\xi, \eta), \quad C_3 = l_3(\xi, \eta)C_1 + m_3(\xi, \eta). \quad (8)$$

Substitution of Equations (8) into Equations (1) yields the following

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial z} = 0, \quad (9)$$

where $\mathbf{U} = (C_1, \xi, \eta)^T$, and

$$\mathbf{A}(\mathbf{u}) = \begin{bmatrix} \frac{\partial F_1}{\partial C_1} & \frac{\partial F_1}{\partial \xi} & \frac{\partial F_1}{\partial \eta} \\ 0 & \frac{G}{D} & \frac{(C_1 - F_1)L}{D} \\ 0 & \frac{(C_1 - F_1)N}{D} & \frac{H}{D} \end{bmatrix}. \quad (10)$$

The entries in $\mathbf{A}(\mathbf{u})$ are given by

$$G = \left(C_1 \frac{\partial l_3}{\partial \eta} + \frac{\partial m_3}{\partial \eta} \right) \left(F_1 \frac{\partial l_2}{\partial \xi} + \frac{\partial m_2}{\partial \xi} \right) - \left(C_1 \frac{\partial l_2}{\partial \eta} + \frac{\partial m_2}{\partial \eta} \right) \left(F_1 \frac{\partial l_3}{\partial \xi} + \frac{\partial m_3}{\partial \xi} \right), \quad (11)$$

$$H = \left(C_1 \frac{\partial l_2}{\partial \xi} + \frac{\partial m_2}{\partial \xi} \right) \left(F_1 \frac{\partial l_3}{\partial \eta} + \frac{\partial m_3}{\partial \eta} \right) - \left(C_1 \frac{\partial l_3}{\partial \xi} + \frac{\partial m_3}{\partial \xi} \right) \left(F_1 \frac{\partial l_2}{\partial \eta} + \frac{\partial m_2}{\partial \eta} \right), \quad (12)$$

$$D = \left(C_1 \frac{\partial l_2}{\partial \xi} + \frac{\partial m_2}{\partial \xi} \right) \left(C_1 \frac{\partial l_3}{\partial \eta} + \frac{\partial m_3}{\partial \eta} \right) - \left(C_1 \frac{\partial l_3}{\partial \xi} + \frac{\partial m_3}{\partial \xi} \right) \left(C_1 \frac{\partial l_2}{\partial \eta} + \frac{\partial m_2}{\partial \eta} \right), \quad (13)$$

$$L = \frac{\partial l_3}{\partial \eta} \frac{\partial m_2}{\partial \eta} - \frac{\partial l_2}{\partial \eta} \frac{\partial m_3}{\partial \eta}, \quad N = \frac{\partial l_2}{\partial \xi} \frac{\partial m_3}{\partial \xi} - \frac{\partial l_3}{\partial \xi} \frac{\partial m_2}{\partial \xi}. \quad (14)$$

We assume that the mapping $(C_1, \xi, \eta) \rightarrow (C_1, C_2, C_3)$ is 1-1, and therefore, that $D \neq 0$.

It is obvious that Equations (9) have global triangular structure if and only if either

$$L = 0, \quad (15)$$

or

$$N = 0. \quad (16)$$

We now examine tie line geometry for which either of the conditions for triangular structure (Equations (15) or (16)) holds true. The geometry of the parametrization is illustrated in Figure 2. We choose η to be the slope of a tie line in the $C_3 = 0$ face. For simplicity of description only, we assume that $\eta \geq 0$. Let $\gamma(\eta)$ be the intercept of the tie line with the C_2 axis. Let $C_2 = g(C_3, \eta)$ be any smooth function such that its graph in the $C_1 = 0$ face passes through the point $(0, \gamma(\eta), 0)$. We choose the second parameter ξ to be the value of C_3 where a tie line in the interior of Γ intersects the $C_1 = 0$ face. A point on the g curve then determines a single tie line in the interior that intersects the $C_1 = 0$ surface at the point $(0, g(\xi, \eta), \xi)$.

A general tie line \mathbf{PQ} (shown in Figure 2) is given by

$$C_1 = -sa, \quad C_2 = g + s(g - b), \quad C_3 = \xi + s\xi, \quad (17)$$

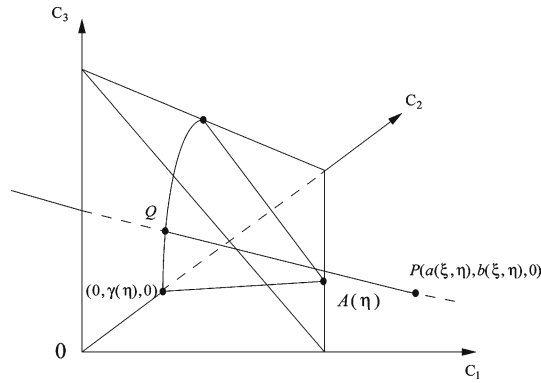


Figure 2. Representation of tie lines.

which leads to

$$l_2 = \frac{b(\xi, \eta) - g(\xi, \eta)}{a(\xi, \eta)}, \quad m_2 = g(\xi, \eta), \quad (18)$$

$$l_3 = -\frac{\xi}{a(\xi, \eta)}, \quad m_3 = \xi. \quad (19)$$

Two tie line geometries are of interest. The geometries of tie lines that result in triangular structure are illustrated in Figures 3 and 4. Tie line geometry for (i) is shown in Figure 3. While this tie line geometry produces triangular structure, it is not a reasonable representation of the behavior of gas/oil systems, and hence we focus our attention here on the situation (ii) illustrated in Figure 4, where tie lines lie in planes. Detailed analysis of the geometry of tie lines leads to the following observation.

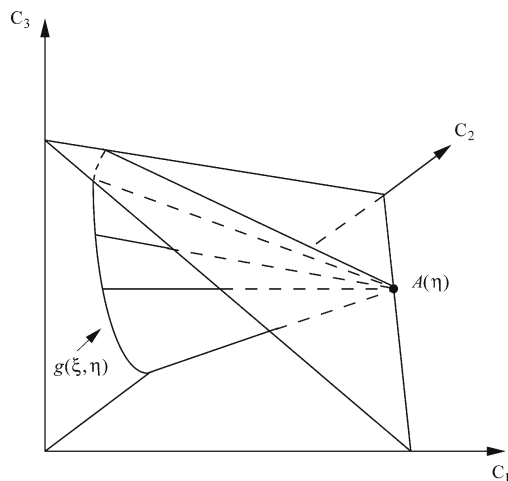


Figure 3. Tie-line geometry for global triangular systems.

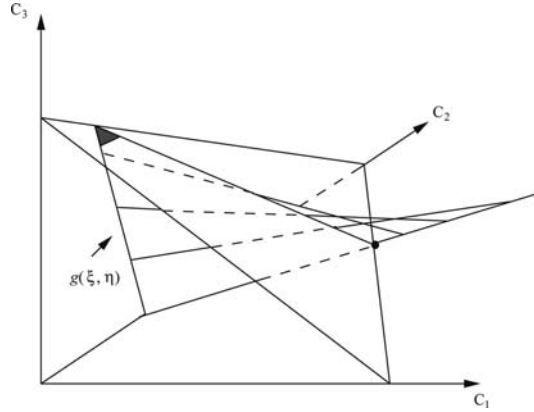


Figure 4. Tie-line geometry for global triangular systems.

A system has global triangular structure if and only if either (i) all tie line extensions intersect the C_1/C_2 edge of the quaternary diagram, or (ii) all tie line extensions lie in planes spanned by two intersecting tie lines that lie in the $C_3=0$ and $C_4=0$ faces of the quaternary diagram.

To prove the above observation, we assume first that the model has global triangular structure (Equation (16) is satisfied). Equation (16) is satisfied if and only if

$$\frac{\partial a}{\partial \xi} \left(\xi \frac{\partial g}{\partial \xi} + b - g \right) = a \frac{\partial b}{\partial \xi}. \quad (20)$$

If $\partial a/\partial \xi = 0$, then $\partial b/\partial \xi$ must also be zero. That can happen only if all tie lines corresponding to a given η pass through a single point, which must lie on the C_1/C_2 axis, because tie lines that lie in both the $C_3=0$ and $C_4=0$ faces must pass through it. Hence, that point must be $A(\eta)$ in Figure 3, and part (i) of our observation follows from triangularity.

If $\partial a/\partial \xi \neq 0$, (except possibly at isolated points), Equation (20) can be written for fixed η (and for $\xi \neq 0$) as

$$\frac{dg}{d\xi} - \frac{g(\xi)}{\xi} = \frac{a(db/d\xi) - b(da/d\xi)}{\xi(da/d\xi)}. \quad (21)$$

Let the right side of Equation (21) be $\xi R(\xi)$. It follows that

$$g(\xi) = \xi \left[Q + \int R(\xi) d\xi \right], \quad (22)$$

where Q is a constant. Differentiation of Equation (22) gives an expression for $dg/d\xi$, which can be differentiated again to obtain an expression for

$d^2g/d\xi^2$. Substitution for $R(\xi)$ and $dR/d\xi$ in that expression gives

$$\frac{d^2g}{d\xi^2} = \frac{a}{\xi} \frac{d}{d\xi} \left(\frac{db}{da} \right). \quad (23)$$

According to Equation (23), if $d^2g/d\xi^2 = 0$, then db/da is a constant, which can only be true if a and b lie on a straight line. That line must be the tie line in the $C_3=0$ face with slope η , as Figure 4 shows.

Next, we show that if part (i) or part (ii) of our observation is satisfied, then the system has global triangular structure. If part (i) of our observation is true, then $\partial a/\partial\xi = \partial b/\partial\xi = 0$, and Equation (20) is trivially satisfied. Hence, part (i) of the observation is shown to be true.

If part (ii) is true, then

$$b(\xi, \eta) = \eta a(\xi, \eta) + \gamma(\eta) \quad (24)$$

and

$$g(\xi, \eta) = \kappa(\eta)\xi + \gamma(\eta), \quad (25)$$

where $\kappa(\eta)$ is some smooth function. Differentiation of Equations (24) and (25) followed by substitution into the left side of Equation (20) gives $\eta a(da/d\xi)$, which is also the right side of Equation (20). Hence, the condition for global triangular structure is satisfied, and part (ii) of the observation is demonstrated.

3.2. WAVE ANALYSIS FOR GLOBAL TRIANGULAR SYSTEMS

In this section, we derive the basic wave properties for the planar tie lines of part (ii) of the observation. A detailed analysis for the tie line situation for part (i) is given by Johansen (1992a, b) and Johansen *et al.* (1994).

The matrix, $\mathbf{A}(\mathbf{u})$, now becomes

$$\mathbf{A}(\mathbf{u}) = \begin{bmatrix} \frac{\partial F_1}{\partial C_1} & \frac{\partial F_1}{\partial \xi} & \frac{\partial F_1}{\partial \eta} \\ 0 & \frac{F_1+p}{C_1+p} & U \\ 0 & 0 & \frac{F_1+h}{C_1+h} \end{bmatrix}, \quad (26)$$

where

$$U = \frac{\xi(C_1 - F_1)}{Da^2} \frac{\partial a}{\partial \eta} \frac{\partial g}{\partial \eta}, \quad (27)$$

$$p = \frac{a^2}{\xi(\partial a/\partial \xi) - a}, \quad h = \frac{a(\xi(d\kappa/d\eta) + (d\gamma/d\eta))}{\xi(d\kappa/d\eta) - a}. \quad (28)$$

We now consider the rarefaction waves associated with the eigenvalues of $\mathbf{A}(\mathbf{u})$

$$\lambda_1 = \frac{\partial F_1}{\partial C_1}, \quad \lambda_2 = \frac{F_1+p}{C_1+p}, \quad \lambda_3 = \frac{F_1+h}{C_1+h}. \quad (29)$$

Rarefaction waves corresponding to λ_1 take place at constant values of ξ and η , and hence they represent variations along fixed tie lines. These waves correspond, therefore, to rarefaction waves of the scalar mass conservation equation

$$\frac{\partial C_1}{\partial t} + \frac{\partial F_1(C_1, \xi_0, \eta_0)}{\partial z} = 0 \quad (30)$$

for constant ξ_0 and η_0 . Equation (30) is an analog of the familiar Buckley–Leverett equation (Buckley and Leverett, 1941).

The rarefaction waves for λ_2 are determined by

$$(\lambda_1 - \lambda_2) \frac{dC_1}{d\tau} + \frac{\partial F_1}{\partial \xi} \frac{d\xi}{d\tau} + \frac{\partial F_1}{\partial \eta} \frac{d\eta}{d\tau} = 0, \quad (31)$$

$$(\lambda_3 - \lambda_2) \frac{d\eta}{d\tau} = 0, \quad U \frac{d\eta}{d\tau} = 0, \quad (32)$$

where $\tau = z/t$. It follows that the λ_2 waves take place at constant values of η . For $\eta = \eta_0$, these waves are determined by

$$(\lambda_1 - \lambda_2) \frac{dC_1(\xi)}{d\xi} + \frac{dF_1(C_1, \xi, \eta_0)}{d\xi} = 0. \quad (33)$$

Next we consider shock waves for a planar structure of tie lines (part (ii) of the observation). The Rankine–Hugoniot shock balances are

$$\Lambda = \frac{F_1^L - F_1^R}{C_1^L - C_1^R}, \quad (34)$$

$$\Lambda = \frac{l_2^L F_1^L + m_2^L - l_2^R F_1^R - m_2^R}{l_2^L C_1^L + m_2^L - l_2^R C_1^R - m_2^R}, \quad \Lambda = \frac{l_3^L F_1^L + m_3^L - l_3^R F_1^R - m_3^R}{l_3^L C_1^L + m_3^L - l_3^R C_1^R - m_3^R}. \quad (35)$$

It is clear that Equations (34) and (35) can be satisfied with $\xi^L = \xi^R$ and $\eta^L = \eta^R$. These are tie-line shocks that correspond to the scalar mass conservation equation, Equation (30). Rearrangement of Equation (34) shows that when a shock connects a composition point in the single-phase region with a composition point in the two-phase region, the single-phase composition point must lie on the extension of a tie line, as several investigators have shown (Larson, 1979; Helfferich, 1981; Dumore *et al.*, 1984).

When $\xi^L \neq \xi^R$, we define

$$\kappa^{LR} = \frac{m_2^L - m_2^R}{l_2^L - l_2^R}, \quad h^{LR} = \frac{m_3^L - m_3^R}{l_3^L - l_3^R}. \quad (36)$$

Therefore,

$$\Lambda = \frac{F_1^L + \kappa^{LR}}{C_1^L + \kappa^{LR}} = \frac{F_1^R + \kappa^{LR}}{C_1^R + \kappa^{LR}} = \frac{F_1^L + h^{LR}}{C_1^L + h^{LR}} = \frac{F_1^R + h^{LR}}{C_1^R + h^{LR}}. \quad (37)$$

It is now easy to show that $h^{LR} = \kappa^{LR}$ if $\xi^L \neq \xi^R$ and $\eta^L = \eta^R$, which is a sufficient condition for Equations (34) and (35) to be satisfied. Thus, shocks satisfying Equation (37) are contained in the tie-line surfaces. That result is consistent with the observation that a shock that connects any two compositions inside the two-phase region (which therefore lie on two different tie lines) can only occur if the extensions of the two tie lines intersect. As Figure 4 shows, all the tie lines that lie in the plane at constant η intersect. The statement that tie lines connected by a shock must intersect is also true for systems with any number of components (Johns, 1992; Johns *et al.*, 1993), whether or not components change volume as they change phase (Dindoruk, 1992; Dindoruk *et al.*, 1992).

We summarize these results in the following observation:

Rarefaction and shock waves corresponding to λ_1 take place along fixed tie lines, whether or not the system has triangular structure. The rarefaction and shock waves corresponding to λ_2 are contained in the tie-line planes at constant values of η .

A similar result holds when the global triangular structure results from tie lines that extend through an edge of the quaternary diagram (Johansen, 1992a, b). Thus, we have shown that when a system is globally triangular, the shock and rarefaction surfaces coincide.

The behavior of the second surface is determined by waves associated with the λ_3 eigenvalue,

$$(\lambda_1 - \lambda_3) \frac{dC_1}{d\tau} + \frac{\partial F_1}{\partial \xi} \frac{d\xi}{d\tau} + \frac{\partial F_1}{\partial \eta} \frac{d\eta}{d\tau} = 0, \quad (38)$$

$$(\lambda_2 - \lambda_3) \frac{d\xi}{d\tau} + U \frac{d\eta}{d\tau} = 0. \quad (39)$$

When a λ_3 shock exists, it is defined by

$$h^{LR} = \kappa^{LR}, \quad \xi^L \neq \xi^R, \quad \eta^L = \eta^R. \quad (40)$$

For such waves, both η and ξ will change across the shock (Johansen, 1992a, b), and again, tie lines connected by the shock must intersect. Wave analysis of similar systems can be found in Entov (1997) and Voskov and Entov (2001).

3.3. FOUR-COMPONENT SYSTEMS WITH CONSTANT K-VALUES

We now turn to four-component systems with constant K-values. *These are systems that have global triangular structure.* To prove this, we need only show that tie lines for constant K-value systems lie in planes like that shown in Figure 4. To do so, we consider three vectors: \vec{e}_b , the direction of

a tie line in the $C_3=0$ face, \vec{e}_f , the direction of a tie line in the $C_4=0$ face, and \vec{e}_i , the direction of a tie line in the interior of Γ that also intersects the first tie line. Those vectors are

$$\vec{e}_b = (K_1 - 1)c_{11}^b \vec{e}_b + (K_2 - 1)c_{21}^b \vec{e}_2, \quad (41)$$

$$\vec{e}_f = (K_1 - 1)c_{11}^f \vec{e}_1 + (K_2 - 1)c_{21}^f \vec{e}_2 + (K_3 - 1)c_{31}^f \vec{e}_3, \quad (42)$$

$$\vec{e}_i = (K_1 - 1)c_{11}^i \vec{e}_1 + (K_2 - 1)c_{21}^i \vec{e}_2 + (K_3 - 1)c_{31}^i \vec{e}_3, \quad (43)$$

where c_{ij} is the volume fraction of component i in phase j .

The tie line can be chosen by selecting c_{11}^b . The remaining compositions are determined by selecting an intersection point on the tie line in the $C_3=0$ face and solving the equations of the three tie lines simultaneously. A lengthy but straightforward calculation shows that $\vec{e}_i \cdot (\vec{e}_b \times \vec{e}_f) = 0$, i.e., the three vectors line in the same plane. Hence, the solution composition route lies entirely in planes in constant K -values. It shows that for systems with constant K -values, shock and rarefaction surfaces coincide, and they are all planes. As a result the solution to a Riemann problem with global triangular structure is determined by three key tie lines, one that extends through the injection fluid composition, one that extends through the initial fluid composition, and one known as the *crossover tie line* (Monroe *et al.*, 1990) that is determined easily as the intersection of the planes of tie lines associated with the first two tie lines. In addition, for four-component constant K -value systems, the nontie-line paths connecting two key tie lines can be obtained in a closed-form integration. Therefore, complete analytical solutions can be constructed for four-component systems with constant K -values (see Part II).

3.4. GENERAL TIE LINE GEOMETRY

We have shown here that for systems with constant K -values, even if two key tie lines are connected by a rarefaction, the extensions of these two tie lines still intersect. Therefore shock and rarefaction surfaces are all planes (or hyperplanes for systems with more than four components). For constant K -value systems, therefore, the ruled surface (a surface generated by the continuous motion of a straight line in space) generated by a nontie-line path takes the simplest form of a plane. Thus, for constant K -value systems, the key tie lines found by using the global property of intersecting tie lines are rigorously accurate. Therefore solutions for constant K -value systems serve as the starting point for the development of methods to determine key tie lines for general systems with realistic phase behavior characterized by an equation of state.

For systems with composition-dependent K -values, however, the nontie-line rarefaction surfaces are no longer planes. Hence, shock and rarefaction

surfaces are different. In general, in order to find the nontie-line paths along which rarefactions occur, one must integrate the appropriate eigenvectors numerically. Examination of the structure of those integrals indicates that the geometry of the rarefaction surfaces depends on the phase behavior of the system. We show, however, that a local geometric property of the rarefaction surface is, in fact, independent of the phase behavior. In addition, the geometry of the rarefaction surface is strikingly simple. The analysis that follows shows that for four-component systems, the rarefaction surfaces are developable surfaces, which means that locally, two adjacent tie lines along the nontie-line path must intersect, even though the nontie-line path is not self-sharpening.

Every point on a “ruled surface” can be defined by the following equation

$$\vec{Z} = \vec{C} + t\vec{e}_t, \quad (44)$$

where \vec{Z} is the vector that defines the ruled surface, \vec{e}_t is the vector of the straight line (a tie line in this case) that lies in the ruled surface and passes through the composition point (denote point \mathbf{Z}) of the vector \vec{C} , and t is a parameter that sets the position along the tie line. A ruled surface defined by Equation (44) is developable if (Kreyszig, 1959)

$$\frac{d\vec{C}}{d\eta} \cdot \left(\vec{e}_t \times \frac{d\vec{e}_t}{d\eta} \right) = 0, \quad (45)$$

or

$$\vec{e}_{nt} \cdot \left(\vec{e}_t \times \frac{d\vec{e}_t}{d\eta} \right) = 0, \quad (46)$$

where \vec{e}_{nt} is the nontie-line eigenvector at point \mathbf{Z} , and η is the arc length of the nontie-line path. Notice that the nontie-line eigenvector is the tangent vector of the nontie-line path.

Mass conservation along the tie line that passes through \mathbf{Z} can be written as

$$\vec{F} = \vec{X} + fl_t\vec{e}_t \quad (47)$$

and

$$\vec{C} = \vec{X} + Sl_t\vec{e}_t, \quad (48)$$

where

$$l_t = \sqrt{\sum_{i=1}^3 (y_i - x_i)^2} \quad (49)$$

and

$$\vec{X} = (x_1, x_2, x_3)^T, \quad (50)$$

where x_i and y_i are the liquid and vapor phase compositions of the tie line. Therefore for point \mathbf{Z} along the nontie-line path

$$\vec{F}(\eta) - \vec{C}(\eta) = (f(\eta) - S(\eta))l_t(\eta)\vec{e}_t(\eta) = g(\eta)\vec{e}_t(\eta), \quad (51)$$

where $g(\eta)$ is a function of the arc length η only.

Differentiation of Equation (51) with respect to η leads to

$$\frac{d\vec{F}}{d\eta} - \frac{d\vec{C}}{d\eta} = \frac{dg}{d\eta}\vec{e}_t + g\frac{d\vec{e}_t}{d\eta}. \quad (52)$$

It must also be true that

$$\frac{d\vec{F}}{d\eta} = \frac{\partial F_i}{\partial C_j} \frac{\partial C_j}{\partial \eta} = \bar{A} \cdot \vec{e}_{nt}, \quad (53)$$

and the nontie-line path equation is

$$\bar{A} \cdot \vec{e}_{nt} = \lambda_{nt} \vec{e}_{nt}, \quad (54)$$

where matrix \bar{A} is defined as

$$A_{ij} = \frac{\partial F_i}{\partial C_j}, \quad i = 1, \dots, n_c - 1, \quad j = 1, \dots, n_c - 1. \quad (55)$$

and λ_{nt} is the nontie-line eigenvalue. In Equation (53), summation convention is assumed for index j .

Hence, Equation (52) becomes

$$(\lambda_{nt} - 1)\vec{e}_{nt} = \frac{dg}{d\eta}\vec{e}_t + g\frac{d\vec{e}_t}{d\eta}, \quad (56)$$

or

$$\vec{e}_{nt} = \frac{(dg/d\eta)}{\lambda_{nt} - 1}\vec{e}_t + \frac{g}{\lambda_{nt} - 1}\frac{d\vec{e}_t}{d\eta} = \alpha\vec{e}_t + \beta\frac{d\vec{e}_t}{d\eta}, \quad (57)$$

where

$$\alpha = \frac{(dg/d\eta)}{\lambda_{nt} - 1}, \quad \beta = \frac{g}{\lambda_{nt} - 1}. \quad (58)$$

Because of the following two identities:

$$\vec{e}_t \cdot \left(\vec{e}_t \times \frac{d\vec{e}_t}{d\eta} \right) = 0 \quad (59)$$

and

$$\frac{d\vec{e}_t}{d\eta} \cdot \left(\vec{e}_t \times \frac{d\vec{e}_t}{d\eta} \right) = 0 \quad (60)$$

it follows from Equation (57) that

$$\vec{e}_{nt} \cdot \left(\vec{e}_t \times \frac{d\vec{e}_t}{d\eta} \right) = 0. \quad (61)$$

Therefore the rarefaction ruled surface is in fact a developable surface. Geometrically, developable surfaces are special kinds of ruled surfaces. In general, they are not planes, and therefore shock and rarefaction surfaces are not the same. Only if K-values are constant will rarefaction surfaces become planes, which are the simplest form of developable surfaces. It can be proved, however, that a sufficiently small area of a developable surface can be mapped isometrically into a plane (Kreyszig, 1959). Thus, locally, at least, rarefaction surfaces are nearly planar, even when K-values are variable.

Direct calculation of developable surfaces generated by the nontie-line paths for realistic gas/oil K-values indicates that they are numerically not far from planes. Dindoruk (1992), Johns (1992) and Wang and Orr (2000) showed that, in fact, the nontie-line rarefaction surfaces are so close to planes that two key tie lines connected by a rarefaction almost intersect (they strictly intersect each other if they are connected by a shock). Consequently, the notion of intersecting key tie lines is a very good approximation to the tie line geometry and can be used to find good estimates of all key tie lines, a tactic that has been exploited by Jessen *et al.* (2001).

4. Conclusions

In this paper we present a comprehensive analysis of the tie line geometry associated with the Riemann problem of four-component gas/oil displacements in one dimension. The analysis reveals important geometric structures that form the basis for the analytical solutions obtained in Part II of this paper series. The following conclusions can be drawn from the analysis:

1. Four-component systems exhibit global triangular structure if and only if (1) tie lines meet at one edge of the quaternary phase diagram or (2) if tie lines lie in planes spanned by pairs of tie lines in opposite faces of the composition space.
2. Systems are of category (2), and therefore have triangular structure, if K-values are constant.
3. When a system contains global triangular structure, the wave analysis indicates that the shock and rarefaction surfaces coincide.

4. For systems with composition-dependent K -values, the rarefaction surfaces are shown to be developable surfaces that are nearly planar. This leads to the general conclusion that systems with variable K -values may be well approximated by assuming shock and rarefaction surfaces do coincide.

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