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## SI Metric Conversion Factors

g/U.S. gal	× 2.641	720	E -01	= kg/m <sup>3</sup>
in.	× 2.54*		E +00	= cm
in. <sup>3</sup>	× 1.638	706	E +01	= cm <sup>3</sup>
mile	× 1.609	344*	E +00	= km
psi	× 6.894	757	E -03	= MPa

\*Conversion factor is exact.

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# Theory of Multicomponent, Multiphase Displacement in Porous Media

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## Abstract

The basis of a general theory of multicomponent, multiphase displacement in porous media is presented. The theory is applicable to an arbitrary number of phases, an arbitrary number of components partitioning between the phases, and variable initial and injection conditions. Only the effects of propagation are considered; phase equilibria and dependence of fractional flows on phase compositions and saturations are required as input, but any type of equilibrium and flow behavior can be accommodated. The principal simplifying assumptions are the restriction to one dimension, local phase equilibria, volume additivity on partitioning, idealized fluid dynamic behavior, and absence of temperature and pressure effects. The theory is an extension of that of multicomponent chromatography and has taken from it the concept of "coherence" and, for practical application, the tools of composition routes and distance/time diagrams. The application of the theory to a surfactant flood is illustrated in a companion paper.<sup>1</sup>

## Introduction

A key problem in modern methods of enhanced oil recovery is that of multicomponent, multiphase displacement in porous media. This term means the induced flow of any number of simultaneous, not fully miscible fluid phases consisting of any number of components. The components may partition between the phases; moreover, the physical properties of the phases (densities, viscosities, interfacial tensions, etc.) depend on composition and, therefore, on partitioning of the components.

Multicomponent, multiphase displacement may be viewed as a generalization and combination of two different and independent approaches. The first of

these is the highly developed theory of multicomponent chromatography,<sup>2</sup> which allows for any number of components affecting one another's distribution behavior but admits only one mobile and one stationary phase. This theory has to be extended to more than one mobile phase. The second is the fluid dynamic theory of immiscible displacement in porous media, allowing for more than one mobile phase but not for partitioning of components. This theory was developed in the 1940's for two mobile phases<sup>3</sup> and so far has not been stated in general form for more than two phases. It has to be extended to include partitioning of the components between the phases and its effects on phase properties. A summary of the state of the art, including recent work on systems with up to three components and two phases, has been given by Pope.<sup>4</sup>

This paper describes the extension of the theory to multicomponent, multiphase displacement with partitioning and for arbitrary initial and boundary conditions. The theory concerns itself only with transport behavior. Phase equilibrium and flow properties of the phases (relative permeabilities) as a function of composition are considered as given. Application of the theory, therefore, requires as input either empirical correlations or experimental data on phase equilibria and properties or theories predicting these. Moreover, the theory concentrates exclusively on multicomponent, multiphase effects and does not attempt to account for the complex fluid dynamic situation in real, three-dimensional, and nonuniform reservoirs.

## Theoretical Basis

### Scope

The scope of the theory is to accommodate an arbitrary number of fluid phases, arbitrary partitioning of components between the phases (including the solid phase), arbitrary dependence of phase

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equilibria and properties on composition, and arbitrary initial and injection conditions.

#### Premises and Limitations

To reduce the problem to a manageable form and bring out clearly the effects of multicomponent, multiphase partitioning, a number of simplifications and idealizations are introduced, most of which are common practice in basic theories of fluid dynamics and chromatography.

1. The problem is presented in one-dimensional form.

2. The porous medium is uniform and isotropic with respect to all relevant properties.

3. The porous medium is considered as quasihomogeneous (i.e., effects of pore structure such as excluded volume, capillary imbibition, etc. are neglected, empirical permeabilities are taken at face value, and fractional flows are unique functions of composition).

4. All fluids are incompressible.

5. The effect of pressure on equilibrium and relative permeabilities is negligible.

6. The system is isothermal.

7. Partial molar volumes of components are constant (volume additivity of components in all phases, including the adsorbed phase if any; no change in total volume upon transfer of components from one phase to another).

8. The phases are in local equilibrium everywhere.

9. Effects of fluid dynamic dispersion and of dispersion through molecular diffusion are neglected.

In other respects, the treatment is kept as general as possible. In particular, no restrictive assumptions are made regarding phase equilibria, relative permeabilities, and viscosities and their dependence on composition (other than that the respective functions be univaled and differentiable).

#### Units and Definitions

We are considering a system with  $n$  components and  $m$  phases,  $n$  and  $m$  being arbitrary numbers. The count of phases includes the adsorbed phase, if one is present.

**Concentrations** are expressed conveniently as volume fractions  $c_{ij}$  of component  $i$  in phase  $j$ . Saturations  $S_j$  of phases  $j$  are defined, as usual, as volume fractions of total pore volume (here taken to include any volume occupied by an adsorbed phase). The following relations then hold.

$$\sum_{i=1}^n c_{ij} = 1, \quad j=1, \dots, m. \quad (1)$$

$$\sum_{j=1}^m S_j = 1. \quad (2)$$

If an adsorbed phase is present, its "saturation"  $S_m$  is the volume occupied by adsorbed components per unit total pore volume. With this definition, in a uniform reservoir, the porosity and cross-sectional pore area remain constant even if the volume occupancy of the adsorbed phase is not negligible.

Volumetric flow rates  $q_j$ , velocities  $v_j$ , and

fractional flows  $f_j$  of phases  $j$ , the mean interstitial velocity  $v$ , and total volumetric flow  $q$  are defined in the usual manner, so that

$$v_j = v f_j / S_j, \quad j=1, \dots, m, \quad (3)$$

$$f_j = q_j / q, \quad j=1, \dots, m, \quad (4)$$

and

$$\sum_{j=1}^m f_j = 1. \quad (5)$$

Independent variables are distance  $z$  and time  $t$ .

For convenience, the "overall concentration"  $C_i$  and "overall fractional flow"  $F_i$  are introduced, defined by

$$C_i = \sum_{j=1}^m S_j c_{ij}, \quad i=1, \dots, n. \quad (6)$$

and

$$F_i = \sum_{j=1}^m f_j c_{ij}, \quad i=1, \dots, n. \quad (7)$$

In view of Eqs. 1, 2, 4, 6, and 7,

$$\sum_{i=1}^n C_i = 1, \quad (8)$$

+ 0.6 - C

and

$$\sum_{i=1}^n F_i = 1. \quad (9)$$

(For any adsorbed phase  $m$ ,  $f_m = 0$ , so this phase does not contribute to the sums in Eqs. 5 and 7.)

#### Concepts

Since not all concepts of the theory are in standard use, brief descriptions are provided here for reference. (For more details, see Ref. 5.)

**Composition.** The complete set of concentrations of all components in all phases and of all phase saturations constitutes a composition. (Granted the premise of local phase equilibrium, a composition is fully characterized by the complete set of overall concentrations of all components).

**Profiles and Histories.** A graph showing a dependent variable as a function of distance at fixed time is called a profile. A graph showing a dependent variable as a function of time at fixed location is called a history.

**Waves.** A wave is a composition variation, usually propagated in the direction of flow. (Under certain conditions a wave may have zero propagation velocity and, thus, remain in place.)

**Sharpening Behavior of Waves.** At any moment in time, a wave may be "sharp" or "diffuse"—i.e., the composition variation it represents may extend over a short or long distance, respectively.

With respect to their behavior on propagation, waves can be grouped into three different categories. A "self-sharpening wave," if initially diffuse, sharpens as it travels and eventually becomes a shock (discontinuity). A "nonsharpening" wave spreads as

it travels, and an "indifferent" wave neither sharpens nor spreads. (These explanations refer to the behavior under the premises accepted here, under which sharpening or spreading is caused exclusively by the dependence of the intrinsic composition velocity on composition. They must be qualified when fluid dynamic dispersion or finite mass transfer rates are taken into account—e.g., see Lake and Helfferich.<sup>6</sup>) A wave also can be self-sharpening in one part and nonsharpening in another.

**Velocities.** It is important to distinguish between "particle velocities" and "wave velocities." The former describe rates of travel of distinguishable particles or volume elements; the latter are rates of advance of given values of physical variables.

The *phase velocity* of a fluid phase (a particle velocity) is the velocity of a volume element of that phase. The *concentration velocity* of a component and the *composition velocity* (both wave velocities) are the velocities at which a given concentration or composition advance. (The composition velocity can be defined only for coherent waves, because only in these do compositions advance unchanged.)

**Composition Space.** The composition space is a coordinate system with the overall concentrations  $C_i$  of all components as the coordinates. Thus, a composition corresponds to a point in the composition space; a wave corresponds to a curve between two points which represent the compositions on its upstream and downstream sides.

**Composition Paths.** The composition space will be seen to contain curves in discrete directions, representing composition variations which meet the coherence condition (see Coherence). These curves are called composition paths, or paths for short. The grid of mutually intersecting paths is determined uniquely by the equations for phase equilibria and fractional flows (at least under the premises listed at the outset) and is independent of the initial and injection conditions.

**Composition Routes.** In contrast to a composition path, a composition route, or route for short, is a curve in the composition space corresponding to the sequence of compositions in a system with specified initial and boundary conditions. A distinction may be made between history routes (for fixed location) and profile routes (at fixed time). By convention, routes are symbolized by arrows pointing in the direction of flow. This paper uses history routes, which thus appear as sequences of arrows pointing from the composition last injected to the composition initially present. In a system which is coherent everywhere in space and time, the route follows a sequence of paths, switching from one to another at their intersections. In general, however, routes temporarily may contain noncoherent segments that do not follow any paths.

**Coherence.** The key concept of the theory is that of "coherence," originally developed for chromatographic phenomena.<sup>2</sup> Coherence is a shorthand expression of what could be called, in the

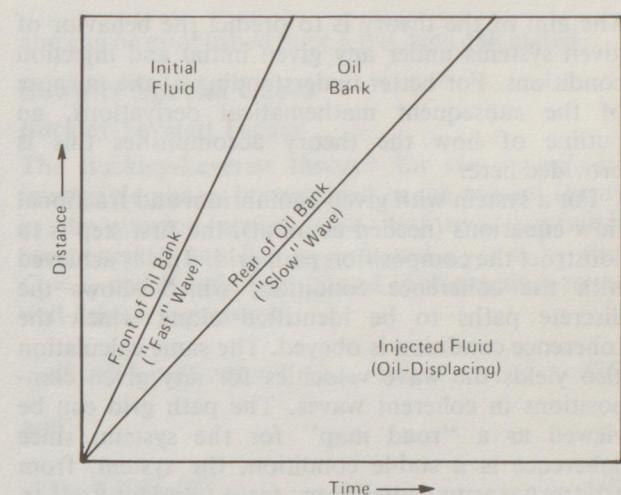
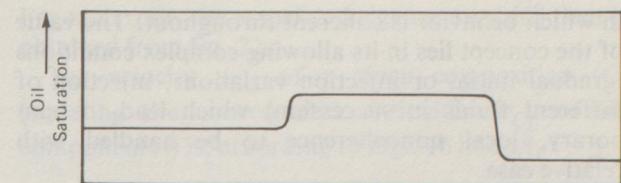


Fig. 1—Schematic oil-saturation/distance/time diagram for an oil-displacing process.

present context, propagational stability. An arbitrary composition variation—e.g., existing initially at some distance from the injection point or generated at that point by injection of a fluid different from that present initially—in general is propagationally unstable—i.e., it cannot be propagated with integrity as one single wave. Rather, it separates into several propagationally stable ("coherent") waves which travel at different speeds and between which new zones of different, uniform compositions arise.

The generation of several waves of different velocities by a single injection or initial variation may appear unfamiliar but is the normal behavior in multicomponent dynamics and is well known to the reservoir engineer in at least one manifestation: the formation of an oil bank by injection of an oil-displacing fluid. (See Fig. 1, which shows the schematic distance/time diagram and an oil saturation history of such an operation.)

A wave in a multicomponent system in general is a composite of waves of all the dependent variables. For the multicomponent wave to be propagated with integrity—to be "coherent"—the waves of all the dependent variables must stay together—i.e., advance at the same speed. Accordingly, *coherence requires all dependent variables at any given point in space and time to have the same wave velocity*. This is the "coherence condition."

The proof of development toward coherence from arbitrary starting conditions can be given with the method of characteristics as outlined in Appendix A.

The coherence concept contributes little in cases with simple initial and injection conditions (e.g., uniform initial and constant injected compositions)



and  $C$  and  $\bar{C}$  are the total concentrations in the mobile and stationary phase, respectively.) This analogy between multicomponent chromatography and multiphase immiscible displacement will be discussed more fully in a future publication.

The same equations and rules as for immiscible components ( $c_{ij}=0$  for all  $i \neq j$ ) also apply for composition-space domains in which the number of phases equals the number of components and, according to the phase rule, the phase compositions remain constant. This is true although each phase then may consist of more than one component. A simple example is the three-phase region in a three-component system with partial miscibility.

### Three-Component Systems

For three-component systems, the characteristic equation (Eq. 22) reduces to the quadratic equation in  $\lambda$ :

$$(F'_{11} - \lambda)(F'_{22} - \lambda) - F'_{12}F'_{21} = 0, \quad \dots \dots \dots \quad (28)$$

with the roots (eigenvalues)

$$\lambda = \frac{1}{2} \{ F'_{11} + F'_{22} \pm [ (F'_{11} - F'_{22})^2 + 4F'_{12}F'_{21} ]^{1/2} \} \quad \dots \dots \dots \quad (29)$$

and

$$dC_2/dC_1 = -\frac{1}{2F'_{12}} [ F'_{11} - F'_{22} \pm [ (F'_{11} - F'_{22})^2 + 4F'_{12}F'_{21} ]^{1/2} ] \quad \dots \dots \dots \quad (30)$$

giving the directions of the eigenvector  $[dC_1, dC_2]$ .

### Composition Paths and Path Grids

For any given composition  $[C]$ , the eigenvectors  $[dC]$  obtained with the differential coherence condition indicate the directions of the composition paths in the composition space. Only composition variations along these discrete directions are compatible with coherence.

In an  $n$ -component system with one constraint (Eq. 8), as considered here, the characteristic equation for a given composition  $[C]$  has  $n-1$  eigenvalues  $\lambda$  each associated with an eigenvector  $[dC]$ . Accordingly, the composition is at an intersection of  $n-1$  different paths (singular and degenerate cases excepted; discussion to follow). Thus, the composition can exist in  $n-1$  different coherent waves and in each of these will have a different velocity.

### Path Grid Construction

A starting point is selected, preferably near (but not on) one of the borders of the composition space. The eigenvalue problem is solved for this starting-point composition. The first eigenvector (associated with the smallest eigenvalue) is selected, and a path that follows the direction of the first eigenvector through the entire composition space is calculated by integration from the chosen starting point. The procedure then is repeated with the second eigen-

vector, the third eigenvector, and so on, always from the same starting point. After all  $n-1$  paths originating from the starting point have been calculated in this manner, the entire procedure is repeated with various other starting points until a sufficiently dense path grid has been generated.

In many cases, the step-by-step integration to obtain the path grid can be obviated. If the general topology of the grid is known, it is usually sufficient to establish the locations of a few key points and then to interpolate the rest of the grid. Examples will be given later.

### Grid Topology

The topology of the path grid reflects the general nature of the equilibrium and fractional flow equations. Once the grid topology of a class of systems is understood, approximate grids can be constructed without much calculation. Of the almost countless possibilities, two examples are given here.

**Three-Phase Immiscible System With Constant Phase Velocity Ratios.** The very simple grid of a system with three entirely immiscible phases and constant phase velocity ratios is shown in Fig. 2. Such grids are the same as for chromatographic systems with constant separation factors and have been discussed at length in that context for any number of components.<sup>2</sup> The salient features include the following. (For proofs, see Ref. 2.)

1. Each composition is at the intersection of a "slow" and a "fast" path (corresponding to the smaller and the larger eigenvalue  $\lambda$ , respectively).
2. Each "slow" path crosses all "fast" paths. Each "fast" path crosses all "slow" paths. No two "slow" or "fast" paths cross one another.
3. All "slow" paths connect Side 2-3 with one segment of Side 1-3. All "fast" paths connect Side 1-2 with another segment of Side 1-3 (apexes being numbered so that  $v_1 < v_2 < v_3$ ).
4. A "watershed point" divides Side 2-3 into the two segments of origin of "slow" and "fast" paths.
5. All paths are straight and regularly spaced.

All that is needed to construct the complete grid is the exact location of the watershed point. That location is given by<sup>2</sup>

$$S_1 = (1 - \beta_{12})/(1 - \beta_{13}), \quad S_2 = 0. \quad \dots \dots \dots \quad (31)$$

**Three-Component System With Two-Phase Region and S-Shaped Fractional Flow Curves.** Such systems, one of which is shown in Fig. 3, often are used as simplified models for surfactant flooding (with pseudocomponents brine, oil, and surfactant) and  $\text{CO}_2$  flooding (heavy oil, light oil, and  $\text{CO}_2$ ). The application to surfactant flooding is discussed in more detail in Ref. 1.

Because of the presumed S-shape of the fractional flow curves, the two-phase region is divided into two domains: in one, the aqueous phase is faster than the oleic phase; in the other, the opposite is true.  $[v_j = v_f/S_j < v(1-f_j)/(1-S_j) = v_k]$  if  $f_j < S_j$ —i.e., where the fractional curve  $f_j(S_j)$  is below the diagonal (dashed line in Fig. 3b); and  $v_j > v_k$  if

$f_j > S_j$ —i.e., where the curve is above the diagonal.] The curve separating the two domains is called "equivelocity curve"—the locus of compositions at which both phases move with equal velocity. Also, the minority phase usually, but not necessarily, remains immobile ("trapped") if present at less than some finite saturation. [Curve  $f_j(S_j)$  then has finite horizontal segments with  $f_j = 0$  and  $f_j = 1$ .]

For a system with these properties, the salient features of the path grid include the following.

1. The single-phase region contains no paths, any direction within that region being coherent.
2. All tie lines are paths.
3. The equivelocity curve is a path.
4. The envelope of the two-phase region is a path.
5. From any point on the envelope, the tie line is the only path leading into the interior of the two-phase region (except at the plait point).
6. Each tie line has two singular points (at which two paths are tangential), one on each side of the equivelocity curve.
7. Each tie line is a "fast" path between the two singular points and is a "slow" path between the envelope and the singular points.

The proofs are outlined in Appendix B. Fig. 3a shows a grid with the respective topological properties.\*

One additional property is of practical importance. If the slant of the tie lines increases steadily and monotonically as the plait point is approached (as is usually the case) the velocity eigenvalues  $\lambda$  for the nontie-line paths are smaller than unity on the side of the equivelocity curve where the tie lines are spaced more narrowly and are greater than unity on the other side. At the envelope of the two-phase region and at the equivelocity curve, these  $\lambda$  values for the nontie-line paths are unity. (See also Ref. 1.)

For construction of a reasonable approximation of the path grid, only the equivelocity points and points of singularity on a few tie lines need to be calculated. The equivelocity point on a tie line is found readily as the point where the fractional flow curve  $f_j(S_j)$  for that tie line intersects the diagonal  $f_j = S_j$ . An approximate equivelocity curve then can be drawn through these points, starting from the plait point. The locations of the two singular points on a tie line can be calculated from the condition that the two eigenvalues are equal at these points. According to Eq. 29, this calls for

$$(F'_{11} - F'_{22})^2 + 4F'_{12}F'_{21} = 0. \quad \dots \dots \dots \quad (32)$$

Knowing the equivelocity curve and the locations of the points at which the nontie-line paths are tangential to the tie lines, one can draw the grid with fair accuracy.

### Construction of Composition Routes

Given the path grid, the construction of composition routes is usually a simple matter of tracing a curve, or curves, from the point(s) corresponding to the injected fluid(s) to that or those corresponding to the

\*This type of topology was discovered by G.J. Hirasaki in 1977 by numerical computation.

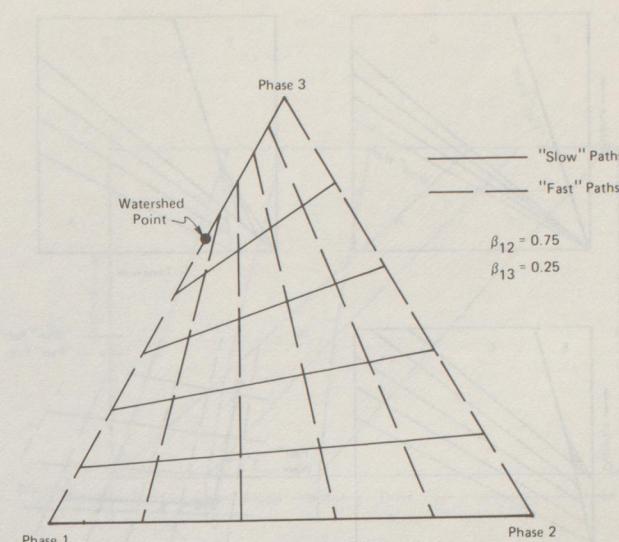


Fig. 2—Path grid for system with three immiscible phases and constant phase velocity ratios.

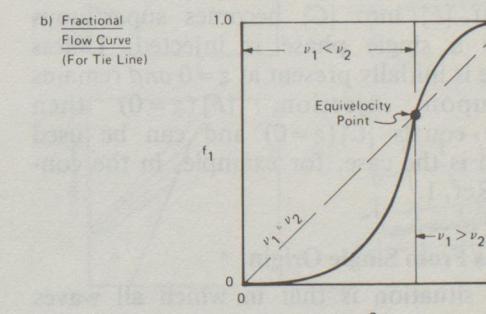
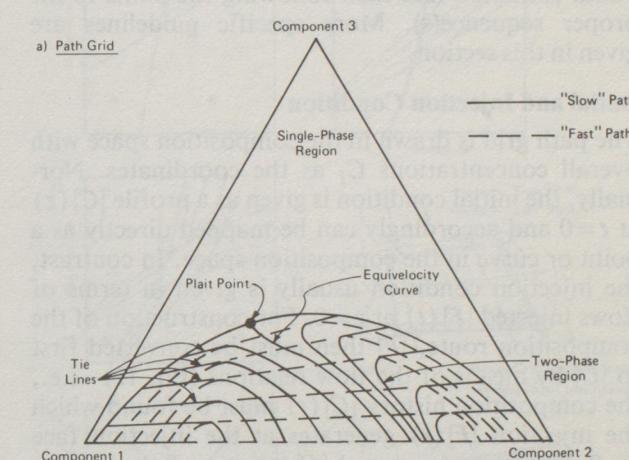


Fig. 3—Path grid topology for typical three-component system with two-phase region and S-shaped fractional flow curves.

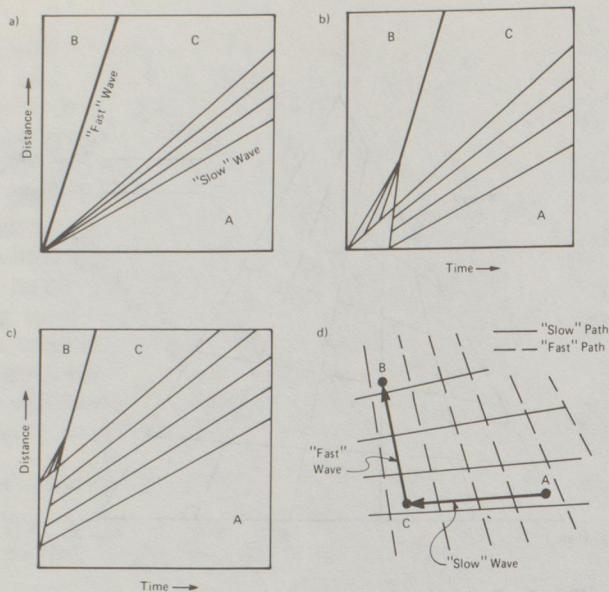


Fig. 4 – Distance/time diagrams (a,b,c) and coherent route (d) for wave patterns from a single origin (three-component system).

initial condition and then following the paths in the proper sequence(s). More specific guidelines are given in this section.

#### Initial and Injection Condition

The path grid is drawn in the composition space with overall concentrations  $C_i$  as the coordinates. Normally, the initial condition is given as a profile  $\{C\}(z)$  at  $t=0$  and accordingly can be mapped directly as a point or curve in the composition space. In contrast, the injection condition usually is given in terms of flows injected  $\{F\}(t)$  at  $z=0$ . For construction of the composition route,  $\{F\}$  then must be converted first to  $\{C\}$  by means of the flow relations (Eq. 12)—i.e., the composition history  $\{C\}(t)$  must be found which the injection  $\{F\}(t)$  generates at the injection face  $z=0$ . The point (or curve)  $\{C\}(t)$  at  $z=0$  then serves as the starting point(s) for route construction.

In a number of cases of practical importance, this translation of  $\{F\}$  into  $\{C\}$  becomes superfluous because only a single phase is injected. Unless another phase is initially present at  $z=0$  and remains immobile upon injection,  $\{F\}(z=0)$  then automatically equals  $\{C\}(z=0)$  and can be used directly. Such is the case, for example, in the constructions in Ref. 1.

#### Wave Patterns From Single Origin

The simplest situation is that in which all waves originate from a single noncoherent variation. For example, such a variation may exist in the initial profile or be generated by injection. Various cases are shown in Fig. 4.

Let the composition upstream of this original variation be A (usually the injected fluid) and the composition downstream be B (usually the initial or a previously injected fluid). The original variation AB,

unless it happens to coincide with a path, is noncoherent and splits up into  $n-1$  coherent waves (two waves in a three-component system, as used for the diagrams). Of these waves, the slower one will have traveled the shorter distance at any given time and, therefore, is upstream of the faster one. Accordingly, the rules for construction of the route from A (upstream) to B (downstream) after attainment of coherence are that *the route runs exclusively along paths and the route follows the paths in the sequence of increasing wave velocities*. In the three-component system, the route follows the "slow" path from A and then switches to the "fast" path which leads to B. (See Fig. 4d.)

It makes no difference for the eventual, coherent route whether the original variation is sharp or diffuse and where in the distance/time plane it is located. However, while a sharp original variation is resolved immediately into a fully coherent pattern (Fig. 4a), a diffuse original variation requires a finite time and distance for such resolution (Figs. 4b and 4c and Ref. 2.).

These rules call for some qualifications and amplifications. Specifically, the first rule does not prevent the route from transversing regions in which *any* composition variation is coherent and which, therefore, contain no discrete paths (e.g., single-phase regions). In the second rule, "wave velocity" refers to the step velocity of a self-sharpening wave and the composition velocities of a nonsharpening wave. At an intersection, the route thus may switch only from a "slower" to a "faster" path. Along any one path, the composition velocity may increase or decrease in the direction of the route (direction of flow), producing either a self-sharpening or a nonsharpening wave. The diagrams in Fig. 4 presume the "slow" wave is nonsharpening ( $v_{[C]}$  increasing along path from A to C) and the "fast" wave is self-sharpening ( $v_{[C]}$  decreasing along path from C to B).

An additional complication is that the two endpoints of a coherent shock wave do not necessarily fall onto the same composition path if that path is curved. With respect to shocks, the route then may deviate slightly from a course exclusively along paths. A more exact route construction then must replace, for each shock wave, the composition path [obtained from the differential coherence condition (Eq. 18)] by the locus of points that obey the integral coherence condition (Eq. 19).

#### Interference of Wave Patterns

In many cases of practical importance, the distance/time plane contains more than one point (or region) of noncoherence. A typical example is the preflood-flood-drive sequence often employed in enhanced oil recovery and illustrated schematically in Fig. 5 (for a three-pseudocomponent system). Each injection of a new fluid generates its own pattern of coherent waves according to the rules already established. However, at some distances from the injection face, faster waves from later injections catch up with slower waves from earlier injections; the previously separate wave patterns of different origins now begin to "interfere."

Such a collision between two waves of different origins and with routes along different paths creates a temporary state of noncoherence. This noncoherent wave, in turn, is resolved into coherent ones according to the rules already stated. (One might say the noncoherent variation does not know or care whether it arose from a collision of waves somewhere in the interior of the distance/time plane or exists in the initial profile or injection history; wherever its location, it develops toward the stable condition of coherence.)

Schematic distance/time and route diagrams of the typical types of interference of shocks or diffuse waves are shown in Fig. 6. The first three cases refer to interference of waves of different "families" (with routes along different paths); the last two refer to waves of the same family. Two shocks of the same family merge (Fig. 6d); this is so because they would not be shocks unless the composition velocity decreased along the route, necessarily making the downstream shock the slower one. A shock and nonsharpening wave of the same family, necessarily with "backtracking" route, also merge (Fig. 6e); the shock weakens, and the backtracking portion of the route gradually shortens and disappears. (See also Ref. 2.)

#### Phase Region Transitions

Additional rules are needed for construction of routes which cross from composition regions into others with different number of phases. Only the rules for transition from single-phase to two-phase regions and vice versa, important for the constructions in Ref. 1, are stated here. The rules are phrased for wave patterns from a single origin and apply to systems with S-shaped fractional flow curves and any number of components. Since, by convention, routes are viewed in the direction of flow, a region "entered" is downstream of the region from which it is entered.

**Entry Into Two-Phase Region.** A two-phase region can be entered from a single-phase region in only two ways (see Fig. 7).

- If the starting point of the route is on an extension of a tie line, the two-phase region may be entered only on that tie-line extension and tie line. The wave corresponding to the entering route segment is a "slow" shock.

- If the starting point of the route is outside the region of tie-line extensions, the two-phase region may be entered only through the plait point. The corresponding wave is an indifferent step of unit normalized velocity ( $\lambda = 1$ ).

**Exit From Two-Phase Region.** A route may exit a two-phase region into a single-phase region in only these ways (see Fig. 8).

- If the endpoint of the route is on a tie-line extension and the route crosses the equivelocity hypersurface (curve in three-component system), the route may exit only along that tie line and extension. The corresponding wave is a "fast" shock.

- If the endpoint is outside the region of tie-line extensions or if the route does not cross the

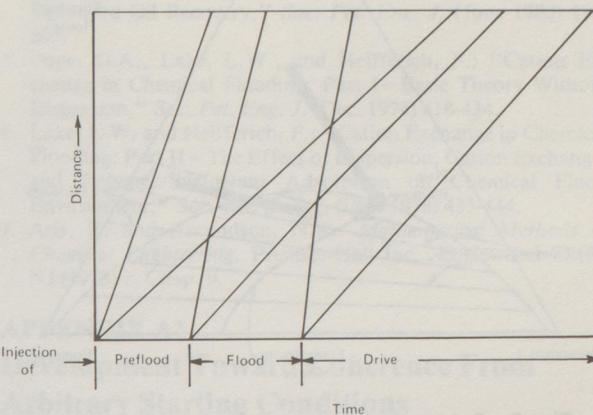


Fig. 5 – Schematic distance/time diagram for a typical preflood-flood-drive sequence.

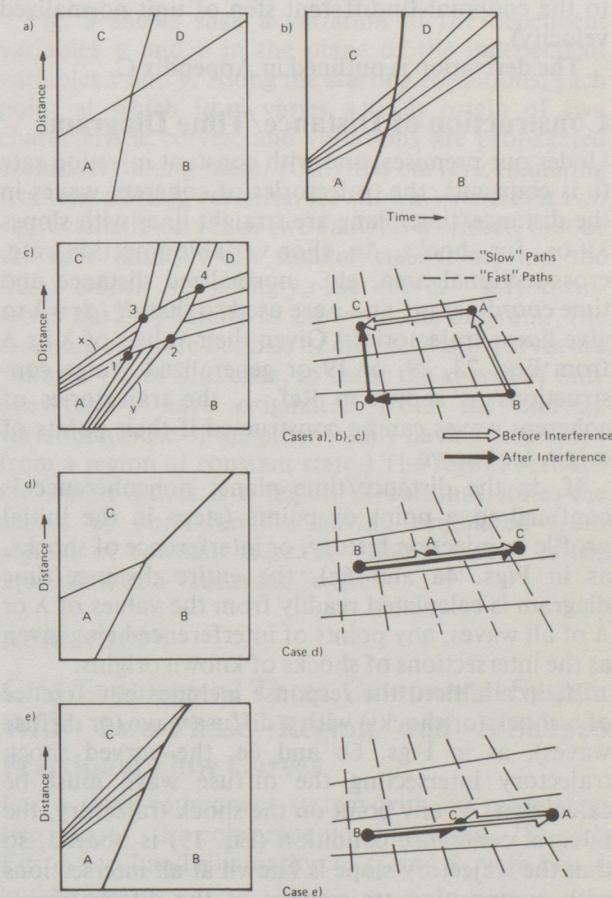


Fig. 6 – Types of interference of coherent waves.

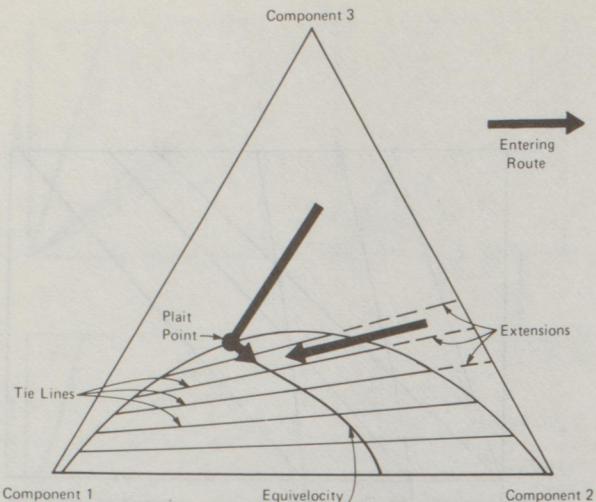


Fig. 7 – Coherent routes entering two-phase region.

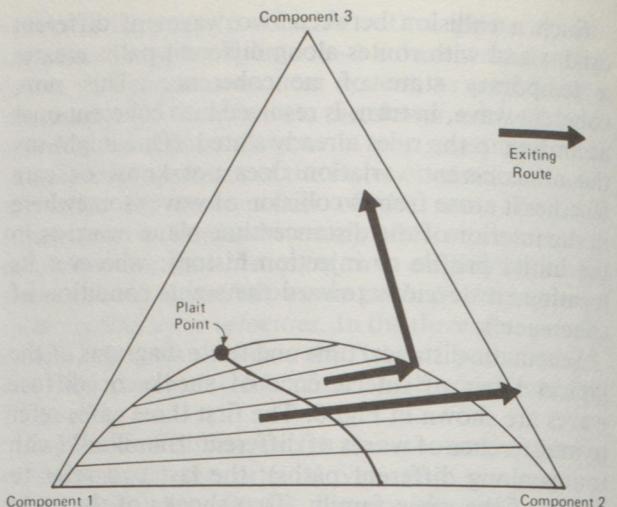


Fig. 8 – Coherent routes exiting two-phase region.

equivalency hypersurface, the route first follows a tie line to the envelope ("slow" shock) and the proceeds to the endpoint (indifferent step of unit normalized velocity).

The derivation is outlined in Appendix C.

### Construction of Distance/Time Diagrams

Under our premises, and with constant injection rate ( $v$  is constant), the trajectories of coherent waves in the distance/time plane are straight lines with slopes  $\lambda v$  or, for shocks,  $\Lambda v$ . (For variable injection rate, cross-sectional area, etc., normalized distance and time coordinates  $\xi$  and  $\tau$  are used so that  $d\xi/d\tau = \lambda$  to give linear trajectories.) Given their values of  $\lambda$  or  $\Lambda$  from Eqs. 23, 29, or 19 or generalized Welge constructions as shown in Ref. 1, the trajectories of coherent waves can be constructed if their points of origin are known.

If, in the distance/time plane, noncoherence is confined to a point or points (steps in the initial profile or injection history, or interference of shocks, as in Figs. 4a and 6a), the entire distance/time diagram is calculated readily from the values of  $\lambda$  or  $\Lambda$  of all waves, any points of interference being given as the intersections of shocks of known origins.

If, in addition, the response includes interference of a shock (or shocks) with a diffuse wave (or diffuse waves), as in Figs. 6b and 6e, the curved shock trajectory intersecting the diffuse wave must be calculated. At any point on the shock trajectory, the integral coherence condition (Eq. 19) is obeyed, so that the trajectory slope is known at all intersections with composition trajectories of the diffuse wave. The curved shock trajectory, thus, can be calculated by integration. Such calculations have been described previously.<sup>2,5</sup>

If the distance/time plane contains finite regions of noncoherence (from gradual variations in the initial profile or injection history or from interference of diffuse waves, as in Figs. 4b, 4c, or 6c), their calculation requires fairly lengthy integration

over space and time—for example, by the method of characteristics.<sup>7</sup>

It is usually possible to avoid the integration to calculate curved shock trajectories of finite regions of noncoherence by the following approximation procedure, illustrated here for the most complicated case of interference of two diffuse waves (see Fig. 6c). The slopes of the trajectories at Corner Points 1, 2, 3, and 4 of the region are known, and so is the position of Point 1 as the intersection of straight trajectories of known origins. Straight lines with average slopes of the 12 and 13 trajectories are drawn through Point 1, and their intersections with Trajectories X and Y (straight and of known origins) give approximate locations of Points 2 and 3. Straight lines with average slopes of the 24 and 34 trajectories are now drawn through Points 2 and 3, and their intersection gives an approximate location of Point 4. The new trajectories (after interference) emanating from Points 2, 3, and 4 are once again straight, and their slopes are known, so they can be drawn once their points of origin have been established. In effect, the procedure has calculated "around" the region of noncoherence.

The construction of the distance/time diagram completes the quantitative calculation of the response.

Constructions for systems with more than three components are based on the same principles but may entail slight complications which are not discussed here.

### Overview

A general theory for multicomponent, multiphase displacement in porous media with mass transfer between phases and for arbitrary initial and injection conditions has been presented. The key concept is that of "coherence," a state of propagational stability which the system strives to attain. The coherence condition is used to construct a "composition path grid" to which the composition

variations of the system tend to adapt themselves. With the grid as a road map, the "composition route" describing the sequences of compositions which will occur under given initial and injection conditions can be found. The construction of a distance/time diagram completes the quantitative description.

The concepts and tools have been used extensively in earlier work on multicomponent chromatography.<sup>2</sup> The necessary extension of chromatographic theory from one to an arbitrary number of fluid phases is achieved by the use of overall "blind man's" variables  $C_i$  and  $F_i$ , which are the concentrations and flows which would be seen by an observer who can analyze for components but not distinguish between phases. In this way, the difficulty of dealing with multiple phases is shifted from calculus to algebra: the differential equations retain their simplicity, and the complication is merely in the dependence of overall flows on composition.

The principal value of the theory is in that it affords almost immediate qualitative predictions, requiring very little calculation, about how a system is affected by changes in properties or conditions. An example is given in Ref. 1.

### Nomenclature

$c_{ij}$  = concentration (volume fraction) of component  $i$  in phase  $j$

$C_i$  = overall concentration of  $i$  (Eq. 6)

$f_j$  = fractional flow of phase  $j$

$F_i$  = overall fractional flow of component  $i$  (Eq. 7)

$m$  = number of phases

$n$  = number of components

$q$  = total volumetric flow

$q_j$  = volumetric flow of phase  $j$

$S_j$  = saturation of phase  $j$

$t$  = time

$v$  = mean velocity

$v_j$  = velocity of phase  $j$

$v_x$  = velocity of given value of variable  $x$

$z$  = distance from injection face

$\beta_{jk}$  = phase velocity ratio of phases  $j$  and  $k$

$\Delta$  = (operator) difference across shock or step

$\lambda$  = eigenvalue (Eq. 18)

$\Lambda$  = common coefficient in integral coherence condition (Eq. 19)

### Vector Notation

$[C] = [C_1, C_2, \dots, C_{n-1}]$  etc.

### Indices

$i$  = components

$j$  = phases

$k$  = additional components or phases

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### APPENDIX A\*

#### Development Toward Coherence From Arbitrary Starting Conditions

In the language of the method of characteristics, the coherence principle can be stated as follows. *An arbitrary variation in the starting condition, if embedded between sufficiently large regions of constant state, sorts itself out into simple waves between which new regions of constant state arise.*

Fig. 9 shows such a variation of the dependent variables  $u$  and  $v$  in the plane of the independent variables  $x$  and  $y$ . Along the starting conditions, each point at which  $\{u, v\}$  varies acts as origin of two characteristic curves, and variations are propagated exclusively along these. (Only the curves originating from the starting variation are shown.) Wherever two characteristic curves of two families intersect, that of the first family (with smaller eigenvalue) has the lesser slope. Accordingly, the curves "sort themselves out" by family as shown in the diagram. The resulting separate bundles of characteristic curves are "simple waves" because, in each, the curves of only one family have originated from the starting variation (those of the other family having originated from a region of constant state.) The region between the simple waves is a region of constant state, the curves of both families having originated from regions of constant state. A "simple wave" is the equivalent of a "coherent" wave.

### APPENDIX B

#### Grid Topology of Three-Component System With Two-Phase Region and S-Shaped Fractional Flow Curves

For a three-component system with no more than two phases, the coherence condition (Eq. 18) with Eqs. 6 and 7 and elimination of  $f_2$  and  $S_2$  with Eqs. 1 and 5 gives

$$\frac{f_1 (dc_{i1} - dc_{i2}) + dc_{i2} + (c_{i1} - c_{i2})df_1}{S_1 (dc_{i1} - dc_{i2}) + dc_{i2} + (c_{i1} - c_{i2})dS_1} = \lambda, \\ i=1,2. \dots \quad (33)$$

For the single-phase region,  $f_1 = S_1$  and

\*Only outlines of the derivations can be given here.

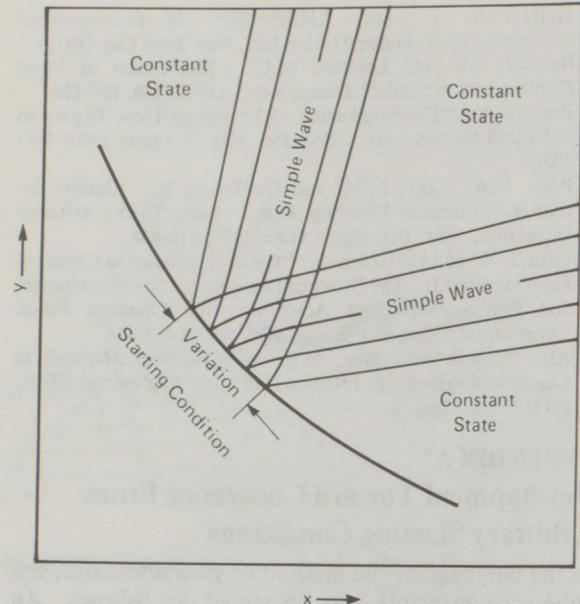


Fig. 9—"Sorting out" of families of characteristic curves from arbitrary starting variation between regions of constant state.

$df_1 = dS_1 = 0$ , so that Eq. 33 is obeyed automatically for all  $\{c\}$  and  $\{dc\}$ . Thus, any direction in the composition space meets the coherence condition.

In the two-phase region, Eq. 33 is obeyed in these cases: (1) along tie lines, along which all  $dc_{ij} = 0$ , (2) along the equivelocity curve, along which  $f_1/S_1 = 1$  and  $df_1 = dS_1$ , and (3) along the envelope of the two-phase region, for which  $f_1 = S_1$  and  $df_1 = dS_1$ .

The existence of two singular points (at which paths are tangential) on each tie line, one on each side of the equivelocity curve, is proved as follows. For the tie line, by virtue of the presumed S-shape of the fractional flow curve,  $\lambda = dF_i/dC_i < 1$  at both ends and  $\lambda > 1$  in the vicinity of the equivelocity curve (see Fig. 3b). For the paths intersecting the tie line,  $\lambda = 1$  at both ends of the tie line (envelope of the two-phase region) and at the equivelocity curve. Accordingly, if the flows and, thus,  $\lambda$  are continuous functions of composition, the tie line must have, on each side of the equivelocity curve one point at which  $\lambda$  has the same value for the tie-line path and the nontie-line path. Equality of the eigenvalues entails equality of the eigenvectors so that the nontie-line path is tangential to the tie line.

The simplest grid topology consistent with these results is shown in Fig. 3a.

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## APPENDIX C

### Route Entry Into and Exit From Two-Phase Regions

It is shown first that the route of a shock between a single-phase composition  $\{C^I\}$  and a two-phase composition  $\{C^{II}\}$  must coincide with a tie line and its extension. For the single-phase composition,  $C_i = F_i$ , so that the integral coherence condition (Eq. 19) for the shock becomes

$$F_i^{II} - C_i^I = \Lambda(C_i^{II} - C_i^I), \quad i=1, \dots, n-1. \quad (34)$$

Replacement of  $C_i^{II}$  and  $F_i^{II}$  with Eqs. 6 and 7 gives, after arrangement,

$$C_i^I = \sum_{j=1}^2 [c_{ij}(f_j - \Lambda S_j)]^{II}/(1 - \Lambda), \quad i=1, \dots, n-1. \quad (35)$$

Accordingly,  $\{C^I\}$  is a linear combination of the compositions of the two phases of  $\{C^{II}\}$  and, therefore, must lie on an extension of the tie line of  $\{C^{II}\}$  into the single-phase region.\*

For systems with the presumed S-shape of the fractional flow curves, a generalized Welge construction (in an  $F_i$  vs.  $C_i$  diagram<sup>1</sup>) shows that a route entering the two-phase region along a tie line and extension must correspond to a "slow" shock ( $\Lambda < 1$ ) and that a route exiting the two-phase region along a tie line and extension corresponds to a "fast" shock ( $\Lambda > 1$ ) if it crosses the equivelocity curve and to a "slow" shock if it does not. In wave patterns with single origin, no single-phase variation (necessarily with  $\lambda = 1$ ) can be upstream of a "slow" shock or downstream of a "fast" shock.

These constraints provide rules for all cases, except for entry from points not on tie-line extensions. In such cases, Eq. 34 can be obeyed only if  $F_i^{II} = C_i^I$ . This corresponds to an indifferent step ( $\lambda = 1$  for entire route) between  $\{C^I\}$  and any point on the equivelocity curve. Since  $\lambda$  must remain equal to one along the entire route, the latter should be drawn formally through the plait point and along the equivelocity curve. Since any path crossing the equivelocity curve is "fast," the step with  $\lambda = 1$  can be upstream of a two-phase composition variation but not downstream of such a variation.

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\*A proof along these lines and for three-component systems was given first by R.G. Larson (1976).

## Formulation of a General Multiphase, Multicomponent Chemical Flood Model

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### Abstract

A general multiphase, multicomponent chemical flood model has been formulated. The set of mass conservation laws for each component in an isothermal system is closed by assuming local thermodynamic (phase) equilibrium, Darcy's law for multiphase flow through porous media, and Fick's law of diffusion. For the special case of binary, two-phase flow of nonmixing incompressible fluids, the equations reduce to those of Buckley and Leverett. The Buckley-Leverett equations also may be obtained for significant fractions of both components in the phases if the two phases are sufficiently incompressible. To illustrate the usefulness of the approach, a simple chemical flood model for a ternary, two-phase system is obtained which can be applied to surfactant flooding, polymer flooding, caustic flooding, etc.

### Introduction

Field tests of various forms of surfactant flooding currently are under way or planned at a number of locations throughout the country.<sup>1</sup> The chemical systems used have become quite complicated, often containing up to six components (water, oil, surfactant, alcohol, salt, and polymer). The interactions of these components with each other and with the reservoir rock and fluids are complex and have been the subject of many laboratory investigations.<sup>2-22</sup> To aid in organizing and understanding laboratory work, as well as providing a means of extrapolating laboratory results to field situations, a mathematical description of the process is needed. Although it seems certain that mathematical simulations of such processes are being performed, models aimed specifically at the process have been reported only recently in the literature.<sup>23-31</sup> It is likely that many

such simulations are being performed on variants of immiscible, miscible, and compositional models that do not account for all the facets of a micellar/polymer process.

To help put the many factors of such a process in proper perspective, a generalized model has been formulated incorporating an arbitrary number of components and an arbitrary number of phases. The development assumes isothermal conditions and local phase equilibrium. Darcy's law<sup>32,33</sup> is assumed to apply to the flow of separate phases, and Fick's law<sup>34</sup> of diffusion is applied to components within a phase. The general development also provides for mass transfer of all components between phases, the adsorption of components by the porous medium, compressibility, gravity segregation effects, and pressure differences between phases. With the proper simplifying assumptions, the general model is shown to degenerate into more familiar special cases. Numerical solutions of special cases of interest are presented elsewhere.<sup>35</sup>

### General Multiphase Chemical Flood Equations

Here we consider an  $n_c$ -component,  $n_p$ -phase system. We assume the system is isothermal, although temperature variations can be included in a straightforward manner. For isothermal flow we need to consider only the  $n_c$  local mass conservation laws (continuity equations) for the (assumed chemically nonreacting) components. These are

$$\frac{\partial \bar{\rho}_i}{\partial t} + \nabla \cdot (\vec{g}_i) = 0, \quad i = 1 \dots n_c, \dots \quad (1)$$

where  $\bar{\rho}_i$  is the mass density of the  $i$ th species and  $\vec{g}_i$  is the corresponding momentum density. These conservation equations are valid for all possible motions involving molecules of the  $n_c$  components (i.e., they are true microscopically). However, for the