

Chapter 8 1-D, Multiphase - Multicomponent Displacement

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Definitions

i	component index
j	phase index
m	number of phases
n	number of components
S_j	saturation of phase j
f_j	fractional flow of phase j

c_{ij} concentration of component i in phase j

C_i overall concentration of component i

F_i overall fractional flow of component i

$C = \{C_1, C_2, \dots, C_n\}^t$ composition

$\left(\frac{dx}{dt}\right)_{dC_i=0} = v_{C_i}$ concentration velocity of component i

$\left(\frac{dx}{dt}\right)_{dC=0} = v_C$ composition velocity

$v = u/\phi$ mean interstitial velocity

Assumptions:

1. One dimensional
2. No capillary pressure or dispersion, i.e. first order partial derivatives
3. Properties depend only on composition, i.e., are independent of pressure.
4. Homogeneous system, i.e., properties do not depend explicitly on position.
5. Ideal volume of mixing, i.e. no volume change on mixing
6. Phase composition are locally at equilibrium.

Overall Concentration and Fractional Flow

$$C_i = \sum_{j=1}^m S_j c_{ij}$$

$$F_i = \sum_{j=1}^m f_j c_{ij}, \quad m = N_p$$

$$\sum_{i=1}^n c_{ij} = 1, \quad n = N_c$$

$$\sum_{j=1}^m S_j = 1$$

$$\sum_{j=1}^m f_j = 1$$

\Rightarrow

$$\sum_{i=1}^n C_i = 1$$

$$\sum_{i=1}^n F_i = 1$$

Differential Conservation Equations

$$\frac{\partial C_i}{\partial t} + v \frac{\partial F_i}{\partial x} = 0, \quad i = 1, 2, \dots, n-1$$

Concepts

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.)

$$\mathbf{C} = \{C_1, C_2, \dots, C_n\}^t$$

Profiles and history. A graph showing a dependent variable as a function of distance at a 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, or a part of a wave may be “sharp” or it may be “diffuse”.

With respect to their behavior on propagation, waves can be grouped into three categories. A “self-sharpening wave”, if initially diffuse, sharpens as it travels and eventually becomes a shock (discontinuity). A “spreading wave” spreads or becomes more diffuse as it propagates. An “indifferent wave” neither sharpens nor spreads on propagation. A wave can also be sharpening in one part and spreading in another. (These definitions apply in the absence of dispersion or capillary pressure.)

Velocities. It is important to distinguish between “particle velocity” and “wave velocity”. The former describes the rate of travel of matter; the latter, the rate of advance of physical variables.

The phase velocity of a fluid phase (an average particle velocity) is the average 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 advances. (The composition velocity can be defined only for coherent waves, because only in these waves do composition advance unchanged.)

Composition Space. The composition space is a coordinate system with the overall concentrations, C_i , of all components as coordinates. A composition

thus corresponds to a point in the composition space. A wave corresponds to a curve between two points which represents 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 below). These curves are called composition paths or paths for short. The grid of mutually intersecting paths is uniquely determined from the partial differential equations and equilibrium phase properties. The paths are independent of initial and boundary conditions.

Composition Routes. The 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 can 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, i.e. from B.C. to I.C. In a system that is coherent everywhere in space and time, the route follows a sequence of paths, switching from one to another at their intersections. In general, routes may at least temporally contain noncoherent segments that do not follow any paths.

Coherence. Coherence is a short-hand expression for what in the present context could be called the condition for propagational stability of a composition wave. A wave in a multicomponent system is in general a composite of waves of all the overall concentrations. For the multicomponent wave to be “coherent” upon propagation, the waves of all the concentrations must stay together, i.e., they must have the same velocity. The “coherence condition” is the condition that all concentration waves at any given point in space and time have the same wave velocity. We will see that this condition is satisfied for only a finite number of directions in the composition space. These directions are the directions of the composition paths.

Concentration Velocities in Multicomponent Systems

The concentration velocity is defined as the velocity at which a given value of concentration propagates through the system.

$$v_{C_i} \equiv \left(\frac{dx}{dt} \right)_{dC_i=0}$$

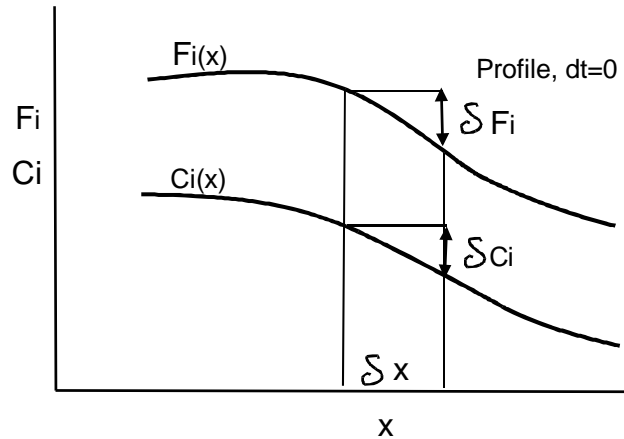
The concentration velocity can be determined from the expression for the total differential and the conservation equation for component i .

$$dC_i = \frac{\partial C_i}{\partial t} dt + \frac{\partial C_i}{\partial x} dx, \quad i = 1, 2, \dots, n-1$$

$$\begin{aligned} \left(\frac{dx}{dt}\right)_{dC_i=0} &= -\frac{\partial C_i / \partial t}{\partial C_i / \partial x} \\ &= v \frac{\partial F_i / \partial x}{\partial C_i / \partial x} \\ &= v \left(\frac{dF_i}{dC_i}\right)_{dt=0} \end{aligned}$$

Define:

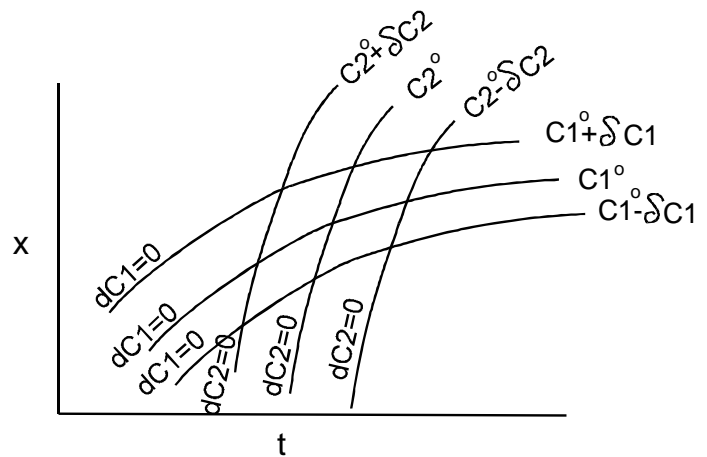
$$\begin{aligned} \delta F_i &\equiv (dF_i)_{dt=0} \\ \delta C_i &\equiv (dC_i)_{dt=0} \end{aligned}$$



These quantities represent changes in F_i and C_i along a profile, i.e., $dt=0$. The concentration velocity can now be expressed in terms of these changes.

$$v_{C_i} = v \frac{\delta F_i}{\delta C_i}$$

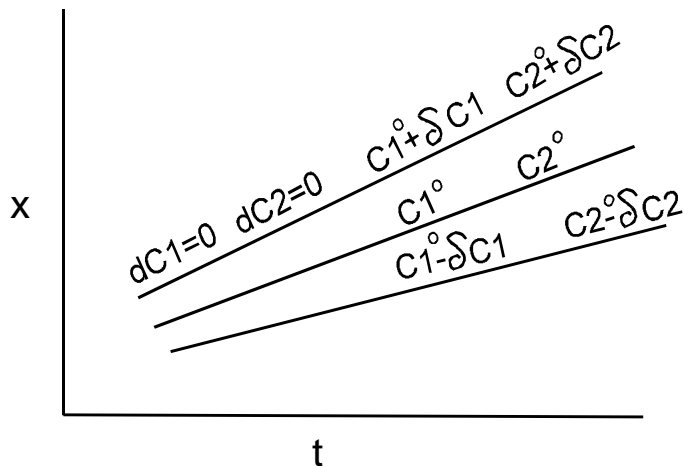
In general, not all of the v_{C_i} are equal to each other. In such a case, the trajectories of $dC_i=0$ will be crossing each other in a distance-time diagram. If the trajectories are crossing each other, then the composition (set of all concentrations) does not remain constant along the trajectories. e.g., We see that along a trajectory of C_1 constant, $C_1=C_1^0$, the value of C_2 changes from $C_2^0+\delta C_2$, to C_2^0 , to $C_2^0-\delta C_2$. If C_2 is changing along the trajectory of constant C_1 and the concentration velocity is a function of both C_1 and C_2 , then the trajectory may not be straight because the slope (equal to the concentration velocity) may be changing.



On the other hand, suppose that the concentration velocities are equal to each other, i.e., $v_{C_1} = v_{C_2} = \dots = v_{C_{n-1}}$. This implies that

$$\left(\frac{dx}{dt}\right)_{dC_1=0} = \left(\frac{dx}{dt}\right)_{dC_2=0} = \dots = \left(\frac{dx}{dt}\right)_{dC_{n-1}=0}$$

The trajectories all have the same direction, thus they coincide and all



concentrations remain constant on the trajectory. Thus the composition remains constant along the trajectory.

This condition that the concentrations velocities are equal is called the **coherence condition**: $v_{C1} = v_{C2} = \dots = v_{Cn} = v_C$. This is not a general condition, but it is satisfied over much of the distance-time domain in problems in which the initial and boundary conditions make only discrete changes or make continuous changes only a finite interval. We will first study the properties of waves that satisfy the coherence conditions. Then we will show when waves are coherent and when they are non-coherent.

$$dC_i = \frac{\partial C_i}{\partial t} dt + \frac{\partial C_i}{\partial x} dx, \quad i = 1, 2, \dots, n-1$$

$$0 = -v \frac{\partial F_i}{\partial x} + \frac{\partial C_i}{\partial x} \left(\frac{dx}{dt} \right)_{dC_i=0}$$

$$0 = -v \sum_k \frac{\partial F_i}{\partial C_k} \frac{\partial C_k}{\partial x} + v_{C_i} \sum_k \delta_{ik} \frac{\partial C_k}{\partial x}$$

$$0 = \sum_k \left(-v \frac{\partial F_i}{\partial C_k} + \delta_{ik} v_{C_i} \right) \frac{\partial C_k}{\partial x}$$

$$\frac{\partial C_k}{\partial x} = \lim_{\delta x \rightarrow 0} \frac{\delta C_k}{\delta x}$$

Since equation is homogeneous, factor out δx .

$$0 = \sum_k \left(-v \frac{\partial F_i}{\partial C_k} + \delta_{ik} v_{C_i} \right) \delta C_k$$

Divide by $-v$ and use $v_{C_i} = v_C$.

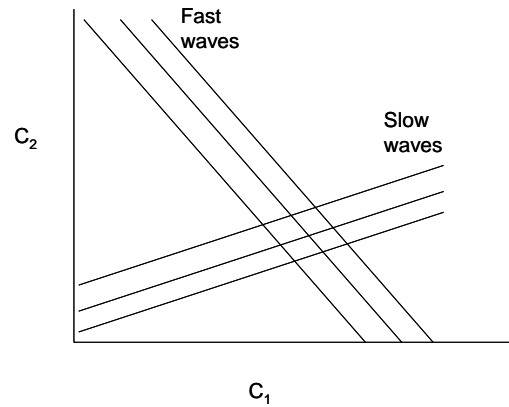
$$\sum_k \left(\frac{\partial F_i}{\partial C_k} - \delta_{ik} \frac{v_C}{v} \right) \delta C_k = 0, \quad i = 1, 2, \dots, n-1$$

$$(\mathbf{M} - \lambda \mathbf{I}) \delta \mathbf{C} = \mathbf{0}$$

$$\lambda = v_C / v$$

The solution to this system of equations is an eigenvalue problem with eigenvalues, λ and the eigenvectors, $\delta \mathbf{C}$. A solution to the eigenvalue problem satisfies the condition that $v_{C1} = v_{C2} = \dots = v_C$, i.e., the coherence condition.

There are as many solutions, $\delta\mathbf{C}$ as there are distinct eigenvalues. The set of solutions can be identified by the relative values of the eigenvalues, i.e., the relative values of v_C . Set 1 corresponds to the smallest (slowest) value of v_C and set $n-1$ corresponds to the largest (fastest) value of v_C . $\delta\mathbf{C}$ is a direction vector in the composition space. Thus the solutions, $\delta\mathbf{C}$ define as many directions as the number of distinct eigenvalues.



Examine the properties of the composition variation, $\{\delta C_k\} = (\delta C_1, \delta C_2, \dots, \delta C_{n-1})$, along the profile (i.e., along a wave) that satisfies the coherence condition, i.e., $v_{C1} = v_{C2} = \dots = v_C$.

1. Along a trajectory of $dC_i = 0$, all of the other concentrations are also constant, i.e., the composition remains constant along a trajectory.

$$\left(\frac{dx}{dt}\right)_{dC_1=0} = \left(\frac{dx}{dt}\right)_{dC_2=0} = \dots = v_C$$

Thus the trajectory of $dC_i = 0$, $i = 1, 2, \dots, n-1$ all coincide.

2. The trajectory is a straight line. We have assumed that F_i is a function of only the composition, i.e., independent of x and t . Thus the Jacobian matrix, $[\partial F_i / \partial C_k]$ is a function of only composition. Thus the eigenvalues is a function only of composition. Since along a trajectory, the composition is constant, the eigenvalues, the velocity v_C , and the slope of the trajectory, $(dx/dt)_{dC=0}$ must all be constant.