"Transport Phenomena" R. B. Bird, 1960.

CHAPTER 20

Concentration Distributions in Turbulent Flow

In the preceding chapters we have derived the equations for diffusion in a fluid or solid, and we have shown how one can obtain expressions for the concentration distribution, provided the flow is not turbulent. Here we turn our attention to turbulent mass transport, a subject about which not a great deal can be said at the present time.

The discussion here is quite similar to that in Chapter 12. In fact, the treatment is kept quite short in view of the fact that much of the material is taken over by analogy. We restrict ourselves in this chapter to isothermal binary systems with approximately constant mass density ρ and diffusivity $\mathscr{D}_{AB}$. Therefore, the partial-differential equation describing the diffusion in a flowing fluid (Eq. 18.1–17) is of exactly the same form as that for heat transport in an incompressible fluid (Eq. 10.1–25) except for the inclusion of a chemical reaction term.

§20.1 CONCENTRATION FLUCTUATIONS AND THE TIME-SMOOTHED CONCENTRATION

The comments made in §12.1 regarding the physical picture can be taken over by analogy. We shall work here in terms of the molar concentration c_A. In a turbulent stream c_A will be a rapidly oscillating function of the time.

It is then convenient to replace c_A by the sum of a time-smoothed value $\bar{c}_A$ and a turbulent concentration fluctuation c_A':

$$c_A = \bar{c}_A + c_A' \qquad (20.1\text{–}1)$$

analogously to Eq. 12.1–1 for temperature. By virtue of the definition of c_A', we see that $\overline{c_A'} = 0$. However, quantities such as $\overline{v_x'c_A'}$, $\overline{v_y'c_A'}$, and $\overline{v_z'c_A'}$ are not zero because the local fluctuations in concentration and velocity are not independent of one another.

The time-smoothed concentration profiles $\bar{c}_A(x, y, z, t)$ are those measured, for example, by the withdrawal of samples from the stream. In tube flow with mass transfer at the tube wall, one expects that the time-smoothed concentration $\bar{c}_A$ will vary only slightly in the turbulent core, where the eddy transport is predominant. In the slowly moving stream near the wall, on the other hand, the concentration $\bar{c}_A$ will be expected to change rapidly from the turbulent core value to the wall value in a short distance. The steep concentration gradient is then associated with the slow molecular diffusion process in the laminar sublayer, as opposed to the rapid eddy transport in the fully developed turbulent core.

§20.2 TIME-SMOOTHING THE EQUATION OF CONTINUITY OF A

We begin with the equation of continuity of substance A, which we presume to be disappearing by an nth-order chemical reaction.[1] (See Eq. 18.1–17.)

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial}{\partial x} v_x c_A + \frac{\partial}{\partial y} v_y c_A + \frac{\partial}{\partial z} v_z c_A\right) + \mathscr{D}_{AB}\left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2}\right) - k_n''' c_A^{\ n} \qquad (20.2\text{–}1)$$

Here k_n''' is the reaction-rate constant for the nth-order homogeneous reaction; it is presumed that k_n''' is independent of position. In subsequent equations we shall consider $n = 1$ and $n = 2$ just to emphasize the difference between a first-order and a sample higher-order reaction.

When c_A and v_i are replaced by $\bar{c}_A + c_A'$ and $\bar{v}_i + v_i'$, we obtain after time averaging

$$\frac{\partial \bar{c}_A}{\partial t} = -\left(\frac{\partial}{\partial x} \bar{v}_x \bar{c}_A + \frac{\partial}{\partial y} \bar{v}_y \bar{c}_A + \frac{\partial}{\partial z} \bar{v}_z \bar{c}_A\right) - \underline{\left(\frac{\partial}{\partial x} \overline{v_x' c_A'} + \frac{\partial}{\partial y} \overline{v_y' c_A'} + \frac{\partial}{\partial z} \overline{v_z' c_A'}\right)} + \mathscr{D}_{AB}\left(\frac{\partial^2 \bar{c}_A}{\partial x^2} + \frac{\partial^2 \bar{c}_A}{\partial y^2} + \frac{\partial^2 \bar{c}_A}{\partial z^2}\right) - \begin{cases} k_1''' \bar{c}_A & \text{or} \\ k_2'''(\bar{c}_A^{\ 2} + \underline{\overline{c_A'^2}}) \end{cases} \qquad (20.2\text{–}2)$$

[1] S. Corrsin, *Physics of Fluids*, **1**, 42–47 (1958).

Comparison of this equation with Eq. 20.2–1 indicates that the time-smoothed equation differs only in the appearance of some extra terms (dashed underline). The terms containing $\overline{v_i' c_A'}$ describe the turbulent mass transport, and we designate the ith component of this flux by $\bar{j}_i^{(t)}$. We have now met the third of the turbulent fluxes, and we may summarize them thus:

turbulent momentum flux (tensor) $$\bar{\tau}_{ij}^{(t)} = \rho\overline{v_i' v_j'} \tag{20.2–3}$$

turbulent energy flux (vector) $$\bar{q}_i^{(t)} = \rho\hat{C}_p\overline{v_i' T'} \tag{20.2–4}$$

turbulent mass flux(vector) $$\bar{j}_i^{(t)} = \overline{v_i' c_A'} \tag{20.2–5}$$

All of these are defined as fluxes with respect to the mass average velocity.

It is interesting to note that there is an essential difference between the behavior of chemical reactions of different orders. The first-order reaction is described by a linear differential equation, and the chemical reaction term has the same form in the time-smoothed equation as in the original equation. The second-order reaction is described by a nonlinear equation, and time-smoothing generates the extra term $-k_2'''\overline{c_A'^2}$. That is, for a first-order decomposition, the mean conversion rate is independent of the concentration fluctuations, whereas an explicit dependence on the concentration fluctuations is predicted for higher-order reactions.

By way of summary, we now list all three of the time-smoothed equations of change for turbulent flow of an isothermal, binary fluid mixture with constant ρ, $\mathscr{D}_{AB}$, and μ:

time-smoothed equation of continuity $$(\nabla \cdot \bar{v}) = 0 \tag{20.2–6}$$

time-smoothed equation of motion $$\rho\frac{D\bar{v}}{Dt} = -\nabla\bar{p} - [\nabla \cdot \bar{\tau}^{(l)}] - \underline{[\nabla \cdot \bar{\tau}^{(t)}]} + \rho g \tag{20.2–7}$$

time-smoothed equation of continuity of A $$\frac{D\bar{c}_A}{Dt} = -(\nabla \cdot \bar{J}_A^{(l)}) - \underline{(\nabla \cdot \bar{J}_A^{(t)})} - \begin{Bmatrix} k_1'''\bar{c}_A \quad \text{or} \\ k_2'''(\bar{c}_A^{\,2} + \underline{\overline{c_A'^2}}) \end{Bmatrix} \tag{20.2–8}$$

Here $\bar{J}^{(l)} = -\mathscr{D}_{AB}\nabla\bar{c}_A$, and the D/Dt operator is understood to be written with the time-smoothed velocity $\bar{v}$ in it.

§20.3 SEMIEMPIRICAL EXPRESSIONS FOR THE TURBULENT MASS FLUX

The turbulent mass flux $\bar{J}^{(t)}$ appearing in Eq. 20.2–8 has to be related to $\bar{c}_A$ or its gradient if Eq. 20.2–8 is to be solved. Just as for the turbulent momentum and energy fluxes, there are several semiempirical expressions available. Since they are all analogous to the expressions given in §12.3, we do little more than list them here:

The Eddy Diffusivity[1]

By analogy with Fick's law of diffusion, we write

$$\bar{J}_{Ay}^{(t)} = -\mathscr{D}_{AB}^{(t)}\frac{d\bar{c}_A}{dy} \tag{20.3–1}$$

in which $\mathscr{D}_{AB}^{(t)}$ is the "turbulent diffusivity" or "eddy diffusivity." Because of the analogy between heat and mass transfer, it is often assumed that $\mathscr{D}_{AB}^{(t)}/\alpha^{(t)} = 1$, in which $\alpha^{(t)}$ is the eddy thermal diffusivity. One also assumes that $\nu^{(t)}/\mathscr{D}_{AB}^{(t)}$ is between 0.5 and 1. (See §12.3.)

The Mixing Length Expressions of Prandtl and Taylor

By analogy with Eq. 12.3–2, we write

$$\bar{J}_{Ay}^{(t)} = -l^2\left|\frac{d\bar{v}_x}{dy}\right|\frac{d\bar{c}_A}{dy} \tag{20.3–2}$$

Here l is the mixing length, which is usually set equal to $\kappa_1 y$ for flow in conduits, where y is the distance from the wall.

Expression Based on the von Kármán Similarity Hypothesis

By analogy with Eq. 12.3–3, we write

$$\bar{J}_{Ay}^{(t)} = -\kappa_2^{\,2}\left|\frac{(d\bar{v}_x/dy)^3}{(d^2\bar{v}_x/dy^2)^2}\right|\frac{d\bar{c}_A}{dy} \tag{20.3–3}$$

in which κ_2 is the same constant appearing in Eqs. 5.3–3 and 12.3–3.

Deissler's Empirical Formula for the Region Near the Wall

By analogy with Eq. 12.3–4, Deissler proposed

$$\bar{J}_{Ay}^{(t)} = -n^2\bar{v}_x y\left[1 - \exp\left(\frac{-n^2\bar{v}_x y}{\nu}\right)\right]\frac{d\bar{c}_A}{dy} \tag{20.3–4}$$

The n here is the same as in Eqs. 5.3–4 and 12.3–4.

[1] For a summary of experimental eddy diffusivity measurements, see T. K. Sherwood and R. L. Pigford, *Absorption and Extraction*, McGraw-Hill, New York (1952), Chapter II, and J. B. Opfell and B. H. Sage, *Turbulence in Thermal and Material Transport*, chapter in *Advances in Chemical Engineering*, Vol. I, pp. 242–290 (1956).