Intensity of Segregation Revisited

H. L. Toor
Chemical Engineering Dept., Carnegie Mellon University, Pittsburgh, PA 15213

Danckwerts' (1958) measure of micromixing is discussed, and a related measure is introduced.

Variance with Nondiffusive Mixing

Mix a volume f of a fluid containing a nondiffusing tracer at unit concentration with a volume $1-f$ of the pure fluid. Then, f is the mean-tracer concentration after mixing. Clumps of tracer fluid with concentration unity are now interspersed through the pure fluid. (Ignore the irrelevant diffusion of the fluid medium.) As mixing progresses, f remains constant as the size of the clumps of tracer fluid diminish and the number increases.

Now, consider a system like a turbulent jet of tracer fluid mixing with pure fluid. f now decreases in both the radial and axial directions as the mixing progresses, and this is due both to turbulent dispersion and molecular diffusion. f is now the local time average tracer concentration, and without molecular diffusion f measures the time-average volume fraction of tracer fluid at a point.

When tracer fluid is present at a particular position, the concentration fluctuation is 1-f and its square is $(1-f)^2$. When pure fluid is present the fluctuation is $-f$ and the square is f^2.

The variance of the fluctuations is the volume weighted average of the squared fluctuations so

$$\sigma_o^2 = (f(1-f)^2 + (1-f)f^2)/(f+1-f) \tag{1}$$

which gives

$$\sigma_o^2 = f(1-f) \tag{2}$$

σ_o^2 is the variance in the absence of molecular diffusion so it applies at the instant of mixing. Equal volume mixing gives a variance of 0.25, the maximum possible value.

The above derivation is in the pre-BSL (Bird et al., 1960) style of Danckwerts (1957), but Eq. 2 can also be derived in a contemporary fashion (more mathematical, less physical, more cumbersome) from the convective diffusion equation by showing that σ_o^2 satisfies the standard variance evolution equation (Spalding, 1971) when the diffusivity is set equal to zero. And Eq. 2 was actually obtained earlier in a quite different context by Shenoy and Toor (1989).

Intensity of Segregation

Danckwerts (1958) used Eq. 2 in his original definition of the intensity of segregation,

$$I_S = \sigma^2/f(1-f) \tag{3}$$

where σ^2 is the variance, and he obviously knew the meaning of Eq. 2 when he stated that I_S is "...unity when segregation is complete...". Lee and Brodkey (1964) used Eq. 3 to interpret their mixing data and Brodkey (1975) clarified it further by stating that if there were no diffusion, and only the eddies were present, the value of the intensity of segregation would still be unity.

In an idealized one-dimensional reactor where f is constant after the initial instantaneous macromixing, both the variance and a more limited definition of the intensity, I'_S (Brodkey, 1967)

$$I'_S = \sigma^2/\sigma^2_i \tag{4}$$

are suitable micromixing measures (where i refers to the initial value). Otherwise, as noted by Lee and Brodkey (1964), Eq. 3 is appropriate since tracer fluid must mix intimately with pure fluid (micromix) for I_S to decrease, while dispersing tracer without any intimacy at all (macromix) can still decrease or even increase the variance and I'_S. At the mouth of the earlier jet, for example, the variance is initially zero, and as the jet mixes with the surroundings the variance rises to a maximum (less than 0.25 at the position where f has fallen to 0.5) and then decreases, eventually approaching zero with f. Meanwhile, I_S decreases monotonically reflecting the smoothing of the choppy concentration field by molecular diffusion.

Relationship of I_S to FUDL

The following development gives another view of I_S. Consider the same system as before, where now diffusion out of the tracer fluid has reduced the average tracer concentration within the tracer fluid to f_1 and raised the average in the originally pure fluid to f_2. Since tracer is conserved

$$f_1 f + f_2(1-f) = f \tag{5}$$

The *minimum* value of the variance is now given by

$$\sigma^2 = f(f_1 - f)^2 + (1-f)(f_2 - f)^2 \tag{6}$$

Equations 3, 5 and 6 give

$$I_S > ((f_1 - f)/(1-f))^2 \tag{7}$$

For the particular value of f, the term on the right of Eq. 7 is the square of the amount of tracer still to leave the tracer fluid divided by the total amount which could leave—the square of the fractional unaccomplished diffusive loss FUDL. Hence

$$\text{FUDL} < I_S^{1/2} \tag{8}$$

Acknowledgment

The author would like to thank Robert Brodkey for his help.

Literature Cited

Bird, R. B., E. W. Stewart, and E. N. Lightfoot, *Transport Phenomena*, Wiley, New York (1960).
Brodkey, R. S., *The Phenomena of Fluid Motions*, Addison-Wesley, p. 332 (1967); Dover, New York (1995).
Brodkey, R. S., *Turbulence in Mixing Operations*, R. S. Brodkey, ed., Academic Press, New York, p. 59 (1975).
Danckwerts, P. V., "Measurement of Molecular Homogeneity in a Mixture," *Chem. Eng. Sci.*, **7**, 116 (1957).
Danckwerts, P. V., "The Effect of Incomplete Mixing on Homogeneous Reactions," *Chem. Eng. Sci.*, **8**, 93 (1958).
Lee, J., and R. S. Brodkey, "Turbulent Motion and Mixing in a Pipe," *AIChE J.*, **10**, 187 (1964).
Shenoy, V. V., and H. L. Toor, "Turbulent Micromixing Parameters From Reactive Mixing Measurements," *AIChE J.*, **35**, 1692 (1989).
Spalding, D. B., "Concentration Fluctuations in a Round Turbulent Free Jet," *Chem. Eng. Sci.*, **26**, 95 (1971).

Manuscript received Mar. 25, 1996, and revision received July 1, 1996.