Diffusion across interface. Extra material for *Introduction to Chemical Engineering Computing,* 2nd ed., Bruce A. Finlayson, Wiley (2012).

If two immiscible fluids are flowing at the same velocity, and one contains a chemical and the other doesn't, then the diffusion across the interface is governed by

$$u\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial x^2}, \frac{\partial c}{\partial x}(\pm\infty, z) = 0$$

$$c(x,0) = 1 \text{ for } x > 0 \text{ and } 0 \text{ for } x \le 0$$

This is the same equation governing diffusion in a slab, with $t = z/u$. The solution for $x > 0$ is

$$c = 0.5\,erfc(\eta), \quad \eta \equiv \frac{x}{\sqrt{4\frac{Dz}{u}}}$$

The solution for $x < 0$ is

$$c = 1 - 0.5\,erfc(\eta), \quad \eta \equiv \frac{-x}{\sqrt{4\frac{Dz}{u}}}$$

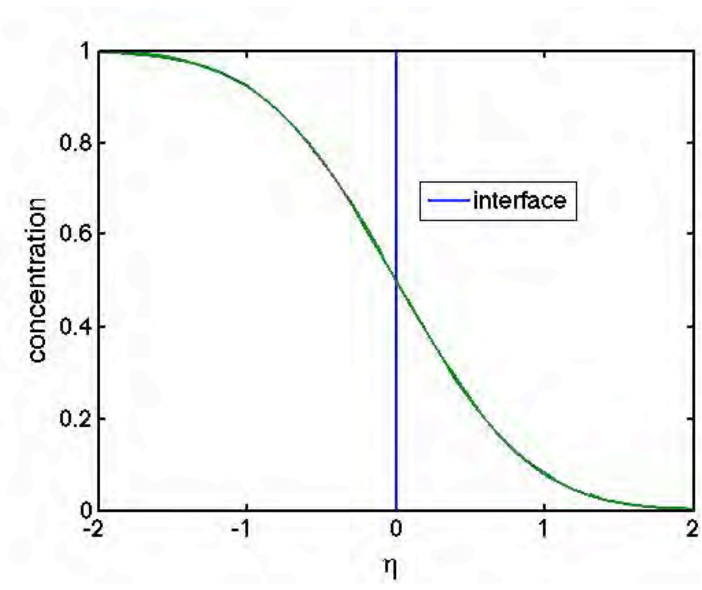

Figure 1. Diffusion across interface

The thickness of the diffusion layer is taken as the distance over which the concentration falls from 0.5 to 0.01 (2% criterion). This happens when the complementary error function is 0.01/0.5 = 0.02, or at an argument of η=1.645.

$$\delta = \sqrt{10.8\frac{Dz}{u}}$$

This solution obviously cannot be used once the diffusion thickness reaches one of the walls. This is the thickness that the fluid diffuses from one fluid to another in a distance z downstream. An approximate solution to this problem for $x > 0$ is (Finlayson, 1972, p. 45)

$$c = 0.5(1-\eta^2),\ \eta = \frac{x}{\delta},\ \delta = \sqrt{12\frac{Dz}{u}}$$

Either of these functions can be used to estimate the diffusion thickness above and below the dividing streamline under the stated assumptions. Other numerical experience has shown that these assumptions are quite good in realistic cases. In the case of albumin and creatinine (Problems 10.27 and 11.28), in a length of 2 cm with a velocity of 2 mm/sec, the creatinine diffusion length (D = 9.2 10^{-10} m^2/s) was 315 μm, but the albumin diffusion length (D = 6.7 10^{-11} m^2/s) was 85 μm. The microfluidic device thus could provide one stream that had creatinine but very little albumin in it provided it was obtained at a distance δ_{albumin} away from the interface.

Variance

An approximation to the variance can be derived analytically (see below).

$$\sigma^2 = \begin{cases} 0.25\left(1-1.476\sqrt{2z'/Pe}\right), z'/Pe \le 0.05 \\ 0.220\exp(-10z'/Pe), z'/Pe > 0.05 \end{cases},\ z'/Pe = \frac{z}{x_s}\frac{D}{ux_s}$$

In this formula, the characteristic distance is the total width of the T-sensor and the velocity is the inlet average velocity. It is plotted below on the composite graphs. For comparison, a finite difference solution was used. For a flat velocity profile, the approximate solution and finite difference solution for 20 and 40 points superimpose in Figure 2. When the velocity profile is quadratic (for fully developed flow between two flat plates, but not derived here) the variance is slightly smaller.

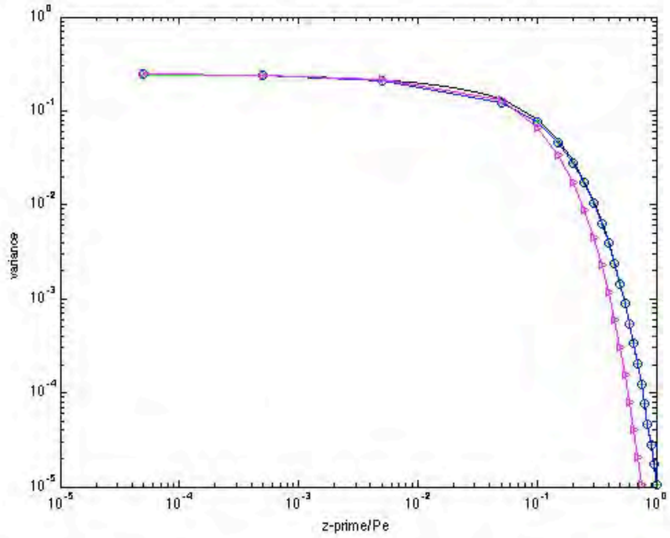

Figure 2. Variance for T-sensor
o – finite difference results and approximate solution, flat velocity profile; triangle – finite difference results with quadratic velocity profile

Approximate Solution

An approximate solution for diffusion in the T-sensor is developed using the Method of Weighted Residuals, as described by Finlayson [pp. 45-46, (1972) and pp. 179-180, 190 (1980]. Finlayson, pp. 45-46, 1972) Notice that in Figure 1 the concentration at the midpoint remains at c = 0.5. On the right of the mid-point, the concentration is initially zero, then a diffusion zone moves from the midpoint to the edge, and then the concentration increases. Thus, we pose the following problem to represent this case. Only the case of uniform velocity is done.

The diffusion equation is solved on x = 0 to h (from the midpoint to the edge; thus h is the half-thickness).

$$u_{avg}\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial x^2}$$

With boundary conditions of $c = 0.5$ at $x = 0$ and zero flux at $x = h$, and initial conditions of $c = 0$, the problem is fully specified. It is made non-dimensional using the variables

$$\frac{\partial c}{\partial z''} = \frac{\partial^2 c}{\partial x'^2}, z'' = \frac{zD}{u_{avg}h^2}, x' = \frac{x}{h}$$

$$c(0,z'') = 0.5, c(x',0) = 0, \partial c / \partial x'(1,z'') = 0$$

For the first part of the time, the concentration is zero almost everywhere with a concentration increase at $x = 0$ to $c = 0.5$. Then a thin diffusion layer grows out towards the far wall. During this time, the approximations solution is taken as

$$c = \begin{cases} 0.5 * (1 - a\eta)^2, \eta < 1/a \\ 0, \eta \geq 1/a \end{cases}, \quad \eta = \frac{x'}{\sqrt{4z''}}$$

This function is substituted into the differential equation to form the residual. In the Galerkin method the residual is made orthogonal to the trial function, which in this case is the derivative of the function with respect to the unknown parameter, a. This is the same procedure that is used in the Galerkin finite element method, except that the trial function and weighting function are not finite elements here. Solving for a gives a^2 = 2/5. This solution holds until the diffusion front meets the wall, which is $z'' \leq 0.1$. Calculating the variance gives

$$\sigma^2 = 0.25\left(1 - 1.476\sqrt{z''}\right), z'' \leq 0.1$$

At $z'' = 0.1$ the variance is 0.133. After this time another form of the solution is used.

$$c = 0.5 + d(z'')(x'^2 - 2x')$$

The initial condition is $d(0.1) = 0.5$ to make the start of this solution agree with the end of the previous one. Substituting this formula into the differential equation forms the residual. In the Galerkin method this time the weighting function is

$$(x'^2 - 2x')$$

and the solution for d is

$$d(z'') = 0.642\exp(-2.5z'')$$

The variance is

$$\sigma^2 = 0.220\exp(-5z''), z'' > 0.1$$

In these formulas the distance is the half-thickness and the velocity is the velocity out. In the figures shown above the total thickness is used and the velocity is the average velocity in, which is half as big. Thus, the formula for z'' is multiplied by 2^2 and divided by 2, giving the variance as shown above.

References

Finlayson, B. A., *The Method of Weighted Residuals and Variational Principles,* Academic Press (1972).

Finlayson, B. A., *Nonlinear Analysis in Chemical Engineering*, McGraw-Hill (1980).