Diffusion Methodology

3.185

Fall, 2003

This will describe the 3.185 methodology for deriving the equations which give solutions to diffusion problems. The methodology carries over to the other areas of 3.185, heat transfer and fluid dynamics, which is why so much time is being spent on it in the beginning of the course.

This handout also presents the error function, which may be new to some students taking this course.

The Methodology

We begin with a statement about conservation of species over a "differential volume" of constant concentration, of the form:

$$\text{accumulation} = \text{in} - \text{out} + \text{generation}$$

The in and out represent the diffusive flux over an area on each side of the volume, generation is the production (or destruction) of the species by chemical reactions in the solid throughout the volume, and accumulation is the time derivative over the volume. This leads to a difference equation of the form:

$$V\frac{\partial C}{\partial t} = (J_\xi \cdot A)|_\xi - (J_\xi \cdot A)|_{\xi+\Delta\xi} + V \cdot G$$

where ξ is the direction in which concentration varies. If the concentration varies only in the x-direction, then this is a planar sheet of thickness Δx, so the area does not vary with x and the volume is the area times Δx. We can divide by the volume and let Δx shrink to zero to give the differential equation:

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x} + G$$

In cylindrical coordinates with concentration varying only in the r-direction, the "differential volume" is a thin cylindrical sheet whose area at a given radius is $2\pi rL$ and volume is $2\pi rL\Delta r$, giving the difference equation

$$2\pi rL\Delta r\frac{\partial C}{\partial t} = -\Delta(J_r \cdot 2\pi rL) + 2\pi rL\Delta r \cdot G$$

We divide by $2\pi L\Delta r$ and shrink Δr to zero to give the differential equation

$$r\frac{\partial C}{\partial t} = -\frac{\partial(rJ_r)}{\partial r} + rG$$

In spherical coordinates if concentration varies only with radius, then the differential volume is a thin spherical shell, and we have:

$$4\pi r^2\Delta r\frac{\partial C}{\partial t} = -\Delta(J_r \cdot 4\pi r^2) + 4\pi r^2\Delta rG$$

This reduces to the differential equation

$$r^2 \frac{\partial C}{\partial t} = -\frac{\partial (r^2 J_r)}{\partial r} + r^2 G$$

In many situations we can neglect species generation and set G to zero. In some processes which take sufficiently long to establish steady-state, we solve for the time-independent solution by setting $\frac{\partial C}{\partial t}$ to zero.

With the conservation equation in hand, we turn to the constitutive equation, which describes the material behavior. For diffusion in most isotropic materials, this is given by Fick's first law:

$$J = -D \frac{\partial C}{\partial \xi}$$

where ξ can be x in cartesian coordinates or r in cylindrical or spherical coordinates. Substituting this into the above differential equations gives a differential equation for concentration as a function of distance and time which may be solved to give a general solution.

Because the diffusion equation is second-order in x (or r) and first-order in time, it requires two boundary conditions in x and an initial condition in time. For this course, we will only deal with uniform or periodic (sine or square wave) initial conditions. Boundary conditions can take the form:

$$C = C_s$$

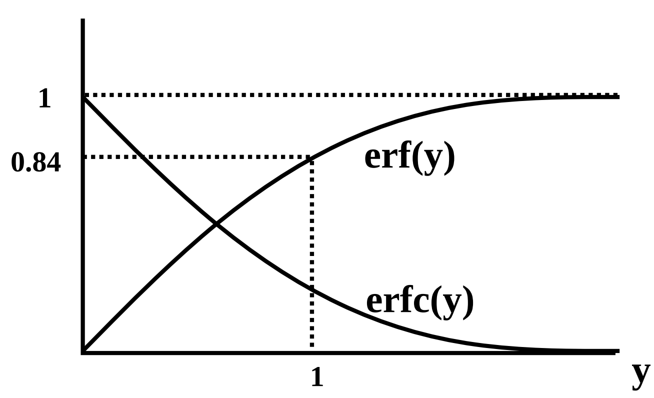
$$J = \text{constant}$$

$$J = h_D(C - C_0) \text{ or} J = k'(C - C_{\text{eq}})$$

These are used to obtain values for the constants in the general solution.

We now know the concentration profile (as a function of time for transient problems), which solves many problems in itself, and can be used with Fick's first law to evaluate the flux at surfaces which solves many other problems.

The Error Function



The error function $\text{erf}(y)$ is defined by

$$\text{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-\beta^2} d\beta$$

To differentiate it, we use the fundamental theorem of calculus:

$$\frac{d}{dy}\mathrm{erf}(y) = \frac{2}{\sqrt{\pi}}\exp(-y^2)$$

The error function is important to diffusion because one solution to the 1-D transient diffusion equation is given by

$$\frac{C - C_s}{C_\infty - C_s} = \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

where C_s is the surface concentration and C_∞ is the initial concentration and the concentration at infinity. This solution applies where we have diffusion from an infinite source of solute and a constant concentration boundary condition $x = 0 \Rightarrow C = C_s$ and the solute is diffusing into a semi-infinite medium.

The complementary error function erfc(y) is just 1–erf(y). The diffusion equation solution using erfc takes the form

$$\frac{C - C_\infty}{C_s - C_\infty} = \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

This version is used because it visually looks like the concentration profile seen in many problems.

What follows is a table of the error function and associated functions, including ierfc(x), the integral complementary error function, which is defined as

$$\mathrm{ierfc}(x) = \int_x^\infty \mathrm{erfc}(y)dy$$

x	$\frac{2}{\sqrt{\pi}}e^{-x^2}$	erf(x)	erfc(x)	2ierfc(x)	e^{x^2}erfc(x)
0	1.1284	0	1	1.1284	1
0.05	1.1254	0.056372	0.943628	1.0312	0.9460
0.1	1.1172	0.112463	0.887537	0.9396	0.8965
0.15	1.1033	0.167996	0.832004	0.8537	0.8509
0.2	1.0841	0.222703	0.777297	0.7732	0.8090
0.25	1.0600	0.276326	0.723674	0.6982	0.7703
0.3	1.0313	0.328627	0.671373	0.6284	0.7436
0.35	0.9983	0.379382	0.620618	0.5639	0.7015
0.4	0.9615	0.428392	0.571608	0.5043	0.6708
0.45	0.9215	0.475482	0.524518	0.4495	0.6423
0.5	0.8788	0.520500	0.479500	0.3993	0.6157
0.55	0.8338	0.563323	0.436677	0.3535	0.5909
0.6	0.7872	0.603856	0.396144	0.3119	0.5678
0.65	0.7395	0.642029	0.357971	0.2742	0.5462
0.7	0.6913	0.677801	0.322199	0.2402	0.5259
0.75	0.6429	0.711156	0.288844	0.2097	0.5069
0.8	0.5950	0.742101	0.257899	0.1823	0.4891
0.85	0.5479	0.770668	0.229332	0.1580	0.4723
0.9	0.5020	0.796908	0.203092	0.1364	0.4565
0.95	0.4576	0.820891	0.179109	0.1173	0.4416
1.0	0.4151	0.842701	0.157299	0.1005	0.4276
1.1	0.3365	0.880205	0.119795	0.0729	0.4017
1.2	0.2673	0.910314	0.089686	0.0521	0.3785
1.3	0.2082	0.934008	0.065992	0.0366	0.3576
1.4	0.1589	0.952285	0.047715	0.0253	0.3387
1.5	0.1189	0.966105	0.033895	0.0172	0.3216
1.6	0.0872	0.976348	0.023652	0.0115	0.3060
1.7	0.0627	0.983790	0.016210	0.0076	0.2917
1.8	0.0442	0.989091	0.010909	0.0049	0.2786
1.9	0.0305	0.992790	0.007210	0.0031	0.2665
2.0	0.0207	0.995322	0.004678	0.0020	0.2554
2.1	0.0137	0.997021	0.002979	0.0012	0.2451
2.2	0.0089	0.998137	0.001863	0.0007	0.2356
2.3	0.0057	0.998857	0.001143	0.0004	0.2267
2.4	0.0036	0.999311	0.000689	0.0002	0.2185
2.5	0.0022	0.999593	0.000407	0.0001	0.2108
2.6	0.0013	0.999764	0.000236	0.0001	0.2036
2.8	0.0004	0.999925	0.000075		0.1905
3.0	0.0001	0.999978	0.000022		0.1790