Appendix C

The Error Function

The error function is frequently encountered in solutions to the diffusion equations for infinite and semi-infinite media. It is defined by

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-u^2)\,du$$

with u a dimensionless, dummy variable. The function has the properties

$$\mathrm{erf}(0) = 0$$

$$\mathrm{erf}(\infty) = 1$$

$$\mathrm{erf}(z) = -\mathrm{erf}(-z)$$

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

For small z

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)n!}$$

and for $z > 1$

$$\mathrm{erf}(z) \approx 1 - \frac{\exp(-z^2)}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n [1 \cdot 3 \cdot 5 \cdot \ldots (2n-1)]}{2^n z^{2n+1}}$$

The error function is available on spreadsheets. Its tabulated values (and those of its derivatives and integrals) are available in [1], and Table C1 lists some numerical values.

The complementary error function defined by

$$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$$

also appears in a number of solutions to the diffusion equations.

TABLE C1 The Error Function

z	erf (z)
0	0
0.05	0.056 372
0.1	0.112 463
0.15	0.167 996
0.2	0.222 703
0.25	0.276 326
0.3	0.328 627
0.35	0.379 382
0.4	0.428 392
0.45	0.475 482
0.5	0.520 500
0.55	0.563 323
0.6	0.603 856
0.65	0.642 029
0.7	0.677 801
0.75	0.711 156
0.8	0.742 101
0.85	0.770 668
0.9	0.796 908
0.95	0.820 891
1.0	0.842 701
1.1	0.880 205
1.2	0.910 314
1.3	0.934 008
1.4	0.952 285
1.5	0.966 105
1.6	0.976 348
1.7	0.983 790

TABLE C1 The Error Function—cont'd

z	erf (z)
1.8	0.989 091
1.9	0.992 790
2.0	0.995 322
2.2	0.998 137
2.4	0.999 311
2.6	0.999 764
2.8	0.999 925
3.0	0.999 978

Solutions to the Fick Equations which take error function forms

$$C(x,t) = F\left[\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right]$$

correspond to parabolic penetration kinetics. If a location of fixed composition, $C(x,t) = C_1$, such as a phase boundary, moves with time, it follows from the above solution that

$$\operatorname{erf}\left(\frac{X}{2\sqrt{Dt}}\right) = \text{Constant}$$

with $x = X$ where $C = C_1$. Therefore

$$X = \text{Constant } 2\sqrt{Dt}$$

If the error function has the value 0.84, the well-known approximation

$$X^2 \approx 4Dt$$

is arrived at.

REFERENCE

[1] H.S. Carslaw, J.C. Jaeger, Conduction of Heat in Solids, Clarendon Press, Oxford, 1959.