Graphing to Explore Equations
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One technique for helping students understand the role of variables and parameters in an equation is to explore graphical representations. Several computer programs are commercially available for this purpose including Matlab (http://www.mathworks.com/), Mathmatica (http://www.wolfram.com/), Genplot (http://www.genplot.com/), or Excel (http://serc.carleton.edu/introgeo/models/mathematical/UsingXL.html). We illustrate this point with two examples.

Example 1:

The rate of diffusion of atoms or ions through a rock is described by a diffusion coefficient, D, a parameter that increases exponentially with increasing temperature, T. The diffusion coefficient is expressed as an Ahrrenius equation of the form

$$D = D_o \exp\left(-\frac{Q}{RT}\right) \tag{1a}$$

where the pre-exponential factor, D_o, is material-dependent parameter, Q is the activation energy, and R is the gas constant. It may not be obvious from this equation that D increases with increasing temperature. Therefore, I ask students to use their calculators to help me make a plot of D versus $1/T$ on the blackboard using $Q = 150$ kJ/mol and $D_o = 1$ m^2/s with R = 8.314 kJ/mol/K. After plotting D versus T on the blackboard, I handout a hard copy of Figure 1. From this graph, it is clear that D indeed increases with increasing T. In addition, I find it valuable to discuss the behavior of D in the limits that T goes to zero and T goes to infinity. Figure 1 illustrates that D goes to zero as T goes to 0 and that D goes to infinity at T goes to infinity. [Aside: It may be helpful to ask students to compare values of D/D_o for the case in which $Q/RT = 1$ with the case in which $Q/RT = 2$, noting that the first case corresponds to a lower temperature than the second case. With this approache, I find it useful to rewrite Equation (1a) as

$$D = D_o \frac{1}{\exp\left(\frac{Q}{RT}\right)} \tag{1b}$$

so that the students are comparing 1/e (low temperature) with 1/e^2 (high temperature).]

Because the dependence of D on T is exponential in form, it is instructive for the students if you rewrite Eq. (1) as

$$\ln D = = \ln D_o - \frac{Q}{R}\frac{1}{T} \tag{2a}$$

which is a linear equation of the usual form

$$y = b + mx \tag{2b}$$

I again ask the students to use their calculators to help me plot the diffusion data on a semi-log graph to emphasize the linear relationship between $\ln(D)$ and $1/T$, as illustrated in Figure 2. To complete this part of the exercise, I point out that if they were given a set of diffusion data such as shown in Figure 3, they can determine the activation energy from the slope, since the slope m = -Q/R such that Q = -m/R. Likewise, they can determine D_o from the intercept, since b = $\ln(D_o)$ such that D_o = exp(b).

Example 2:

Next, I extend this example to examine an important problem in diffusion kinetics, namely the case in which diffusion occurs not only through the interiors of grains but also along boundaries or interfaces between neighboring grains. The activation energy for diffusion along grain boundaries, Q_{gb}, is almost always smaller than the activation energy for diffusion through the grain interiors (which I call the grain matrix), Q_{gm}. Typically, $Q_{gb} \approx 2/3\ Q_{gm}$. Based on Equation (1a), the magnitude of Q directly affects the rate of change of D.

The question then arises, which diffusion path is most important at low temperatures? At high temperatures? A convenient way to explore the effect of Q on D is in graphical form. As demonstrated above in Figures 1 and 2, two types of plots are useful for discussing this problem, a plot of D versus T and a plot of $\ln(D)$ verus $1/T$.

In the plot of D versus T in Figure 4, grain boundary diffusion (the process with the smaller activation energy) dominates at low temperatures, while grain matrix diffusion is faster at high temperatures. This point is amplified in the plot of $\ln(D)$ verus $1/T$ in Figure 5. Again, we see that the rate of diffusion along grain boundaries is faster than the rate of diffusion through grain interiors at low temperatures. This situation is reversed at high temperatures. As before, the activation energies for grain matrix and grain boundary diffusion can calculated from the slopes of the two lines.
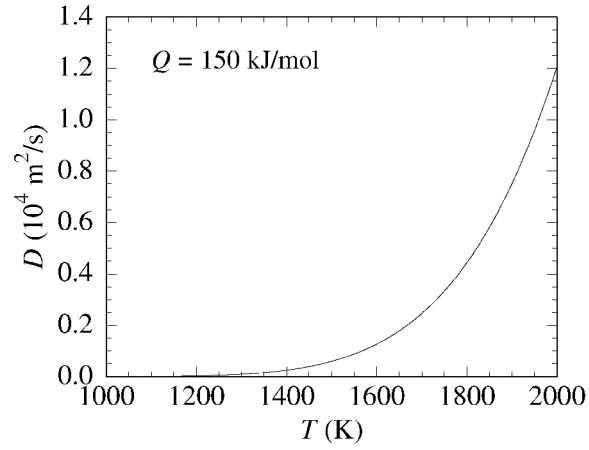
Figure 1: Plot of D versus T for an a ctivation energy $Q = 150$ kJ/mol with $D_o = 3 \times 10^{-3}$ m^2/s.

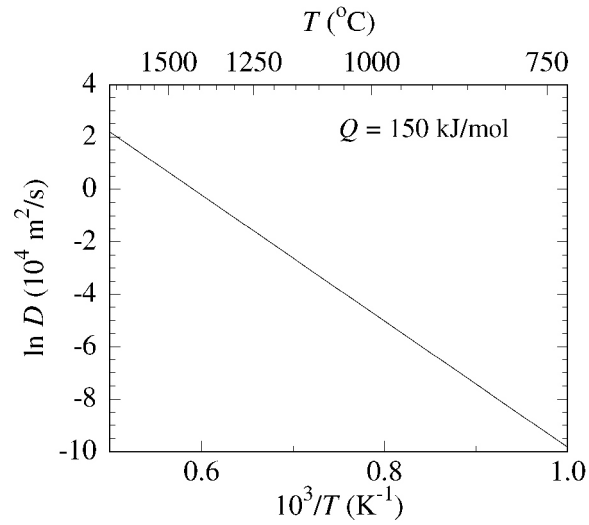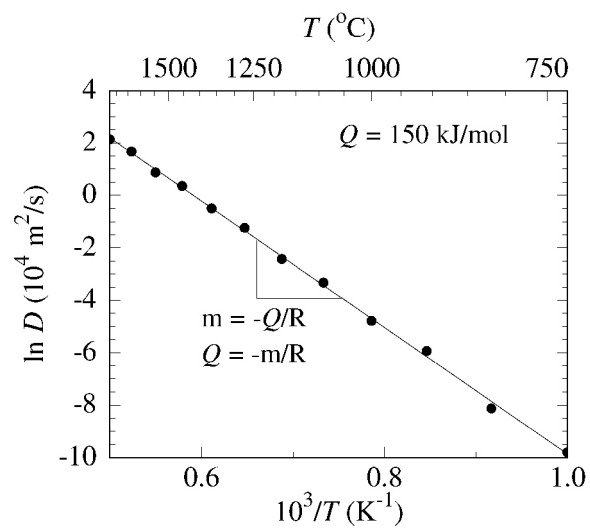Figure 2: Plot of ln(D) versus $1/T$ for an activation energy $Q = 150$ kJ/mol with $D_o = 3 \times 10^{-3}$ m^2/s.

Figure 3: Plot of experimentally determined diffusion data as ln(D) versus $1/T$. Note that the activation energy, Q, can be directly calculated from the slope, m, of this plot.
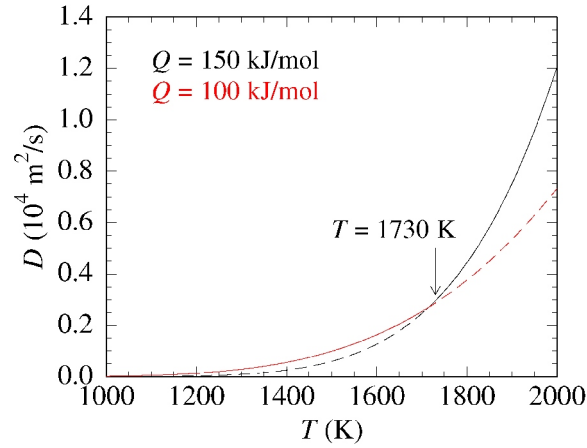
Figure 4: Plot of D versus T for an activation energy for diffusion through the grain interior/matrix of Q_{gm} = 150 kJ/mol with D_o = 1m^2/s (black curve) and an activation energy for diffusion along the grain boundaries of Q_{gb} = 100 kJ/mol with D_o = 3×10^{-2} m^2/s (red curve). The solid line identifies the faster mechanism, and the dashed line denotes the slower mechanism. With increasing temperature, a transition occurs grain boundary dominated diffusion to grain matrix dominated diffusion.
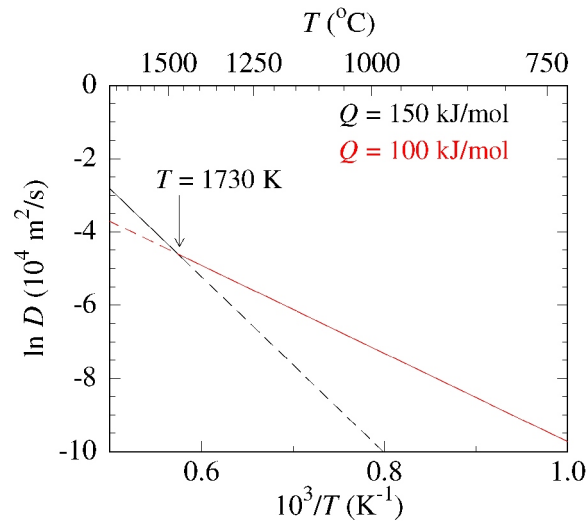

Figure 5: Plot of ln(D) versus 1/T for an activation energy for diffusion through the grain interior/matrix of Q_{gm} = 150 kJ/mol with D_o = 1m^2/s (black) and an activation energy for diffusion along the grain boundaries of Q_{gb} = 100 kJ/mol with D_o = 3×10^{-2} m^2/s (red). With increasing temperature (i.e., moving from right to left) a transition occurs from diffusion dominated by transport along grain boundaries to diffusion dominated by transport through the grain interiors (matrix). Solid lines indicate the dominate diffusion path.