9.1: Response Surfaces

One of the most effective ways to think about an optimization is to visualize how a system's response changes when we increase or decrease the levels of one or more of its factors. We call a plot of the system's response as a function of the factor levels a response surface. The simplest response surface has one factor and is drawn in two dimensions by placing the responses on the *y*-axis and the factor's levels on the *x*-axis. The calibration curve in Figure $9.1.1$ is an example of a one-factor response surface. We also can define the response surface mathematically. The response surface in Figure $9.1.1$, for example, is

$$A = 0.008 + 0.0896 C_A$$

where A is the absorbance and C_A is the analyte's concentration in ppm.

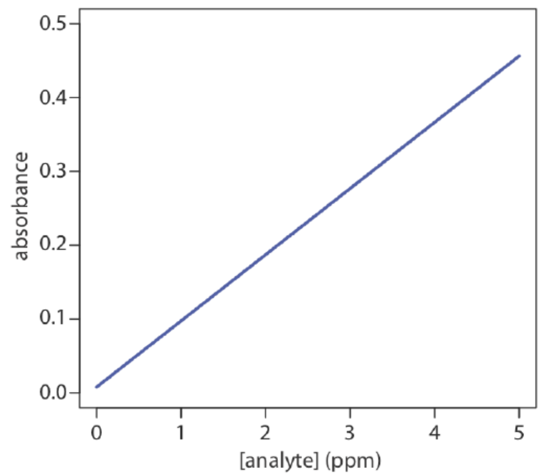

Figure 9.1.1. A calibration curve is an example of a one-factor response surface. The responses (absorbance) are plotted on the *y*-axis and the factor levels (concentration of analyte) are plotted on the *x*-axis.

For a two-factor system, such as the quantitative analysis for vanadium described earlier, the response surface is a flat or curved plane in three dimensions. As shown in Figure $9.1.2$, we place the response on the *z*-axis and the factor levels on the *x*-axis and the *y*-axis. Figure $9.1.2a$ shows a pseudo-three dimensional wireframe plot for a system that obeys the equation

$$R = 3.0 - 0.30A + 0.020AB$$

where R is the response, and A and B are the factors. We also can represent a two-factor response surface using the two-dimensional level plot in Figure $9.1.2b$, which uses a color gradient to show the response on a two-dimensional grid, or using the two-dimensional contour plot in Figure $9.1.2c$, which uses contour lines to display the response surface.

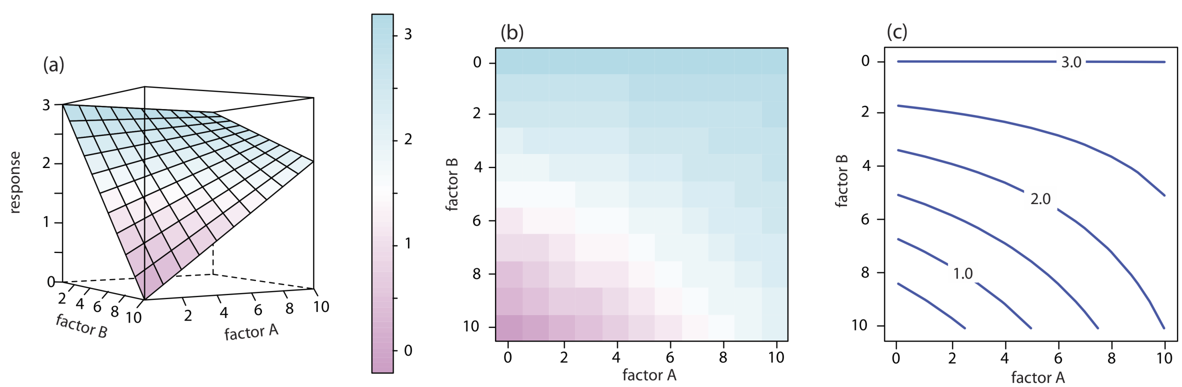

Figure 9.1.2. Three examples of a two-factor response surface displayed as (a) a pseudo-three-dimensional wireframe plot, (b) a two-dimensional level plot, and (c) a two-dimensional contour plot. We call the display in (a) a pseudo-three dimensional response surface because we show the presence of three dimensions on the page's flat, two-dimensional surface.

The response surfaces in Figure $9.1.2$ cover a limited range of factor levels ($0 \le A \le 10$, $0 \le B \le 10$), but we can extend each to more positive or to more negative values because there are no constraints on the factors. Most response surfaces of interest to an analytical chemist have natural constraints imposed by the factors, or have practical limits set by the analyst. The response surface in Figure $9.1.1$, for example, has a natural constraint on its factor because the analyte's concentration cannot be less than zero; that is, $C_A \geq 0$.

If we have an equation for the response surface, then it is relatively easy to find the optimum response. Unfortunately, we rarely know any useful details about the response surface. Instead, we must determine the response surface's shape and locate its optimum response by running appropriate experiments. The focus of this chapter is on useful experimental methods for characterizing a response surface. These experimental methods are divided into two broad categories: searching methods, in which an algorithm guides a systematic search for the optimum response, and modeling methods, in which we use a theoretical model or an empirical model of the response surface to predict the optimum response.