DOWNLOAD PDF PRACTICAL EXPERIMENTAL DESIGNS AND OPTIMIZATION METHODS FOR CHEMISTS

Chapter 1 : experimental design and process optimization | Download eBook PDF/EPUB

This book introduces statistically designed experiments to chemists who conduct experiments for the purpose of making inferences from data. It emphasizes statistical considerations for preliminary planning of experiments, standard statistical designs that may be used for experiments, and the underlying logic for using these designs.

To optimize the method we need to find the best combination of factor levels. Usually we seek a maximum response, as is the case for the quantitative analysis of vanadium as VO 2 SO4 3. Note We will return to this analytical method for vanadium in Example The calibration curve in Figure We also can define the response surface mathematically. The response surface in Figure The response absorbance is plotted on the y-axis and the factor levels concentration of analyte is 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 We can also represent a two-factor response surface using the two-dimensional level plot in Figure Note We also can overlay a level plot and a contour plot. The response surfaces in Figure Most response surfaces of interest to an analytical chemist have natural constraints imposed by the factors or have practical limits set by the analyst. 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. The focus of this section is on useful experimental designs for characterizing response surfaces. These experimental designs are divided into two broad categories: Suppose you wish to climb to the highest point of this ridge. Because the shortest path to the summit is not obvious, you might adopt the following simple ruleâ€”look around you and take a step in the direction that has the greatest change in elevation. The route you follow is the result of a systematic search using a searching algorithm. Of course there are as many possible routes as there are starting points, three examples of which are shown in Figure Note that some routes do not reach the highest pointâ€”what we call the global optimum. Instead, many routes reach a local optimum from which further movement is impossible. Note Searching algorithms have namesâ€”the one described here is the method of steepest ascent. The path on the far right reaches the highest point, or the global optimum. The other two paths reach local optima. You can read about the geology of the park as www. We can use a systematic searching algorithm to locate the optimum response for an analytical method. We begin by selecting an initial set of factor levels and measure the response. Next, we apply the rules of our searching algorithm to determine a new set of factor levels, continuing this process until we reach an optimum response. Effectiveness and Efficiency A searching algorithm is characterized by its effectiveness and its efficiency. A searching algorithm may fail to find the global optimum for several reasons, including a poorly designed algorithm, uncertainty in measuring the response, and the presence of local optima. An algorithm must be that responds to a change in the direction of steepest ascent is effective. All measurements contain uncertainty, or noise, that affects our ability to characterize the underlying signal. When the noise is greater than the local change in the signal, then a searching algorithm is likely to end before it reaches the global optimum. Because the variation in local height exceeds the slope, our searching algorithm stops the first time we step up onto a less weathered surface. The yellow rod at the bottom of the figure, which marks a trail, is about 18 in high. Finally, a response surface may contain several local optima, only one of which is the global optimum. If we begin the search near a local optimum, our searching algorithm may not be capable of reaching the global optimum. The ridge in Figure Only those searches beginning at the far right reach the highest point on the ridge. Ideally, a searching algorithm should reach the global optimum regardless of where it starts. A searching algorithm always reaches an optimum. Our problem, of course, is that we do not know if it is the global optimum. If we arrive at the same optimum response after starting from very different locations on the response surface, then we are more confident that is it the global optimum. Efficiency is the second desirable characteristic for a searching algorithm. An efficient algorithm moves from the initial set of factor levels to the optimum response in as few steps as possible. We can increase the rate at which we approach the

optimum by taking larger steps. If the step size is too large, however, the difference between the experimental optimum and the true optimum may be unacceptably large. One solution is to adjust the step size during the search, using larger steps at the beginning and smaller steps as we approach the global optimum. One-Factor-at-a-Time Optimization A simple algorithm for optimizing the quantitative method for vanadium described earlier is to select initial concentrations for H2O2 and H2SO4 and measure the absorbance. We can stop this process, which we call a one-factor-at-a-time optimization, after one cycle or repeat it until the absorbance reaches a maximum value or it exceeds an acceptable threshold value. A one-factor-at-a-time optimization is consistent with a notion that to determine the influence of one factor we must hold constant all other factors. This is an effective, although not necessarily an efficient experimental design when the factors are independent.

Chapter 2 : Optimizing the Experimental Procedure - Chemistry LibreTexts

Practical experimental designs and optimization methods for chemists, Charles K. Bayne and Ira B. Rubin, VCH Publishers, Inc., Deerfield Beach, FL, U.S.A.

Chapter 3 : QbD - Product & Process Optimization using Design of Experiments - CfPIE

Search the history of over billion web pages on the Internet.