# Find Optimum Operating Conditions Fast

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Process optimization is essential for gaining and maintaining a competitive edge. The simplex method may provide the optimal strategy for discovering the true optimum.

In today's world of intense financial competition, chemical processes must be optimized quickly if they are to become successful. These successful processes must continue to be operated optimally if they are to retain their competitive edge. In this article, we discuss statistically-based optimization strategies that can be used to achieve these two goals of achieving and maintaining optimized processes.

To illustrate a typical situation, let's consider the yield of a hypothetical unit operation. Figure 1 shows elliptical contours of constant yield as a function of two factors, temperature and pressure. These contours suggest a rising, mountainous response surface that has an optimal yield near a temperature of 370°F and a pressure of 30 psi. We do not know this behavior when we start investigating the system — this mountain must be discovered by experimentation. But, how?

## Flawed approaches

Unfortunately, several popular optimization methods usually do not work very well.

*The consultant approach.* Here, a company simply hires a consultant to recommend the conditions of temperature and pressure that will give the best yield. Let's say the consultant suggests a temperature of 332°F and a pressure of 42 psi. When an experiment is carried out at these conditions, the yield is better than currently achieved. Some organizations will accept these conditions as the optimum and, thus, will specify them as the set points for the future operation of the process.

It is evident in this example that the consultant has made a good suggestion. But, as Figure 1 shows, the optimum lies elsewhere. This discrepancy between the conditions suggested by the consultant and the conditions of the true optimum might be critically important — if a rival runs its process at the actual optimum, it will have the competitive edge.

The consultant approach can give a good set of starting conditions, but additional experimental work must be done to find the true optimum.

*The shotgun approach.* Figure 2 shows the familiar shotgun approach to optimization. There are many things wrong with this approach — it is inefficient, for one. But, let's just focus on the well-known "lamp post effect" that often occurs, and which is seen here in the cluster of experiments that are found on the response surface ridge near a temperature of 334°F and a pressure of 56 psi.

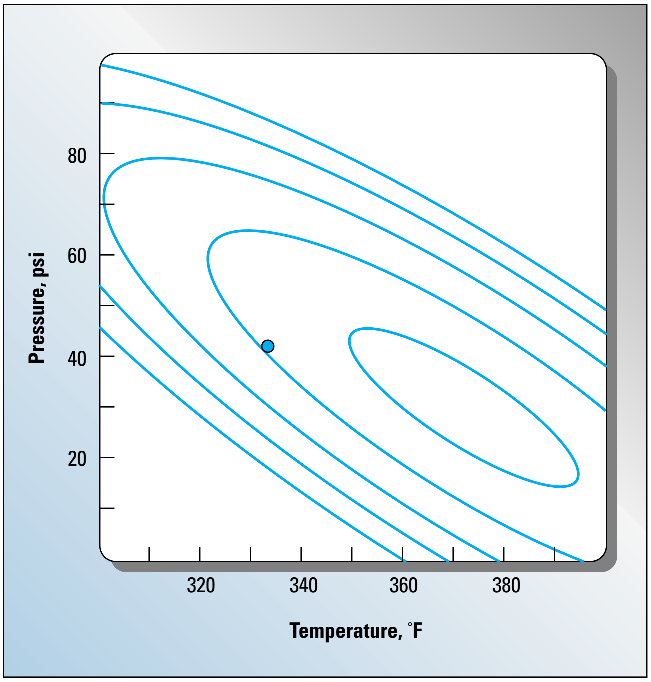



Figure 1. Yield variation with temperature and pressure.

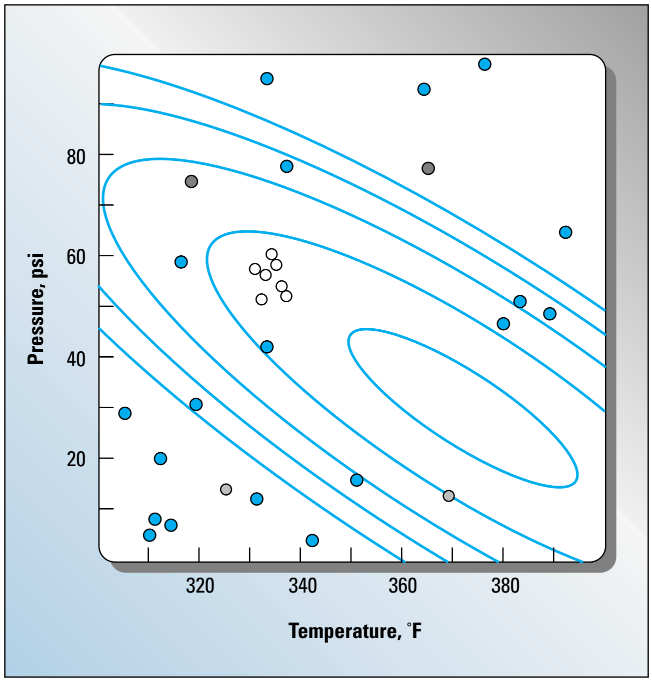



Figure 2. The shotgun approach to optimization

Experiments frequently are carried out under conditions where the "light is brighter," that is, there is a tendency to continue to experiment in tight regions that give good results rather than risk conditions farther away that might give a bad response. This leads to experimentation becoming too conservative too fast, and aggressiveness being lost. It is not a competitive strategy.

*The "good science" approach.* Many of us have been taught that one aspect of "good science" is that if you want to find the effect of a factor, then all other factors must be held constant while this one factor is varied. What we are not told is that the effect we see is conditional on the values specified for the factors that are held constant. A different effect might be observed if one or more of the other factors were held constant at another value.

As an optimization strategy, changing only one factor at a time can be misleading. In Figure 3, a researcher has held the pressure constant at a value of 50 psi while varying the temperature to find that an optimal yield occurs at 342°F. When the temperature now is held constant at this "optimal" value and the pressure is varied, the optimal pressure is found to be the original 50 psi.

Some researchers might take great pride in the fact that the "optimal" pressure turns out to be the value they initially chose. Unfortunately for their egos, the reason this pressure appears to be optimal is that varying the temperature alone took the operating conditions of the system onto a ridge, and varying the pressure alone will not move the operating conditions off that ridge. In short, the single-factor-at-a-time optimization strategy (doing "good science") might improve a system, but it can be stranded by diagonal ridges and often fails to find the true optimum.

For the system shown in Figure 3, it clearly is necessary to change more than one factor at a time to move toward the optimum. This is where statistical experimental design comes in.

## The design-of-experiments approach

The full factorial design is the basis of most classical statistical experimental designs. Figure 4 shows a two-level two-factor full factorial design (a $2^2$ design).

In statistics, the word "factorial" means "related to the factors," and the word "level" means "value." Thus, a two-level design is a two-value design in which each factor is set to either a low or a high value. In a "full" factorial design, the factors are set to all possible combinations of these low and high values; thus, a two-level two-factor full factorial design contains the $2^2 = 4$ design points shown in Figure 4.

Factorial designs are valuable, because they can be used to detect "factor interaction," that is, where the effect of one factor on the response (the slope) depends upon the level of another factor. In the

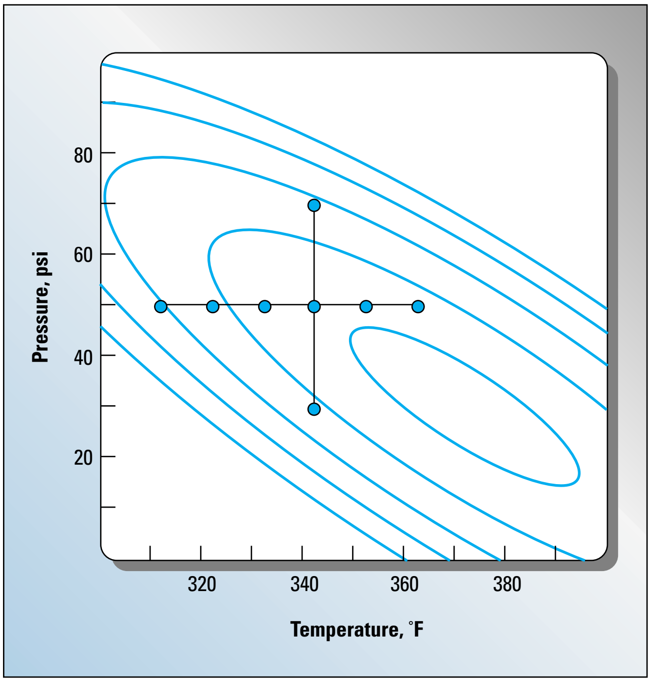



Figure 3. The "good science" approach.

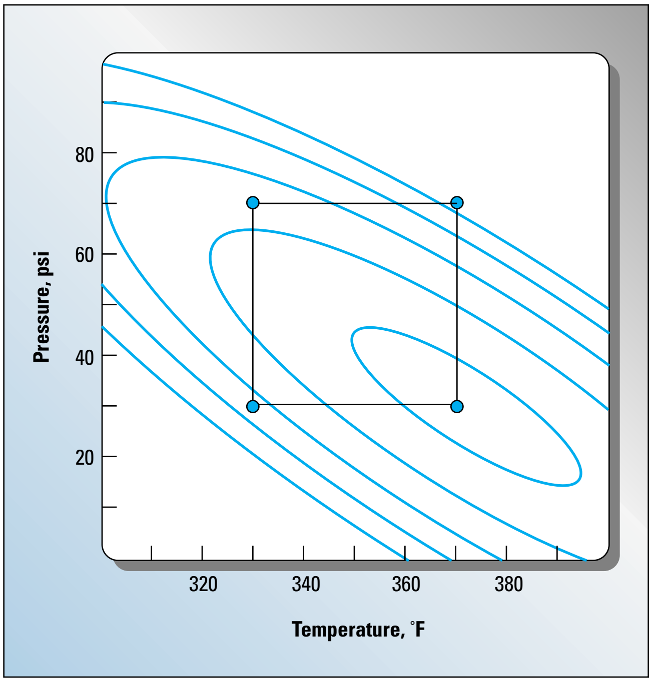



Figure 4. Two-level, two-factor full factorial design.

example shown in Figure 4, the effect of temperature clearly depends upon the value of pressure — at low pressures, increasing the temperature causes the yield to rise; at high pressures, temperature has the opposite effect. In this figure, temperature and pressure are said to interact.

Factorial designs often are augmented with star designs to give composite designs. Figure 5 illustrates a "central composite design," because the centers of the factorial and star designs coincide. These "response surface designs" give a more complete view of the local response surface, a view sufficiently complex to draw the elliptical contours of constant response shown in the figure.

When fitting a more limited model, factorial designs frequently are "fractionalized" — only a fraction of the possible experiments is carried out. Figure 6 shows the four experiments of a $2^{3-1}$ fractional factorial design being used to estimate the main effects of each of the three factors (no curvature or interaction terms can be calculated from this limited set of data).

## The traditional statistical approach

Statistics often have been used to help find optimal operating conditions for processes. The traditional statistical approach to optimization *(1)* seeks to answer, in order, three questions:

**1.** Does an experimentally measured response depend upon certain factors?

**2.** What equation does the dependence best fit?

**3.** What are the optimal levels of the important factors?

It is easy to get lost with this approach. As Driver has pointed out *(1)*, "The questions are so related that it is possible for the experimenter not to know which one he wishes to answer and, in particular, many people try to answer question 2, when in fact they need the answer to the narrower question 3."

*The first question.* To answer this question, fractional factorial designs (including Plackett-Burman designs, also known as Hadamard or Taguchi designs *(2)*) often are used to "screen" (or sieve) the factors — to choose the factors that have the greatest effect and ignore (but hold constant) those less useful factors that have only a small effect. Screening is efficient and effective, but is not without difficulty.

For example, as shown in Figure 7, two-level screening designs can miss an important factor if the levels straddle an optimum and give essentially identical responses. Figure 7 also depicts the situation where a factor might not have much of an effect over the region it is investigated, but exhibits an important effect elsewhere. In both cases, the screening design will fail to show that this is an important factor.

A separate, subtle problem with screening occurs when decisions are made with stated levels of statistical confidence. Ideally, it is desirable to know if a factor is *unimportant* at a certain level of confidence (with a "Type II" error of being wrong to omit the factor

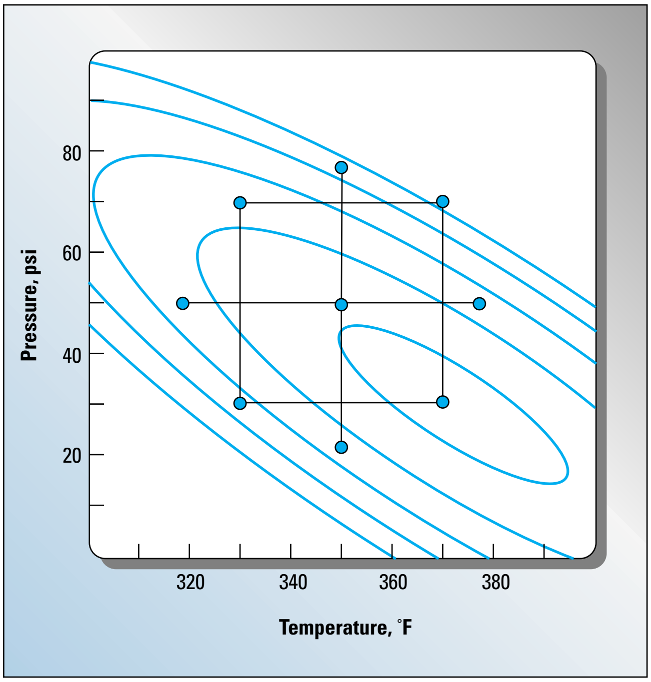



Figure 5. Central composite design.

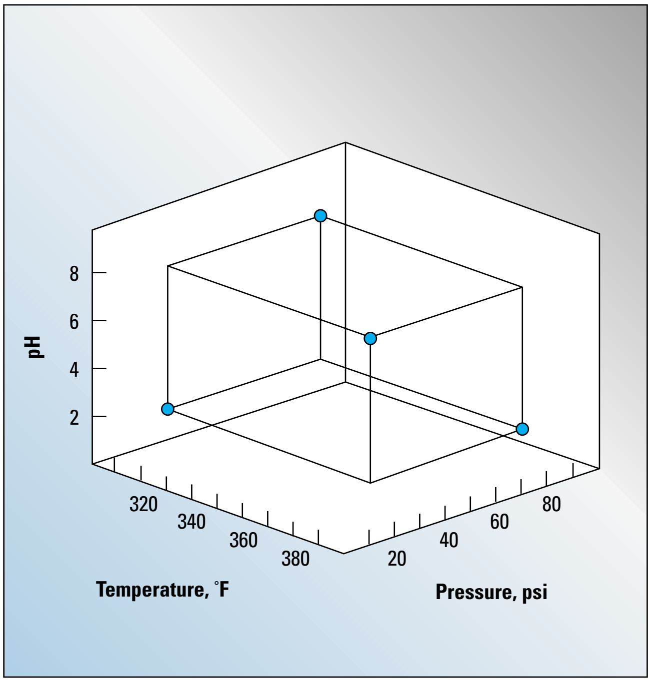



Figure 6. Fractionalized factorial design.

from further study). But, the usual statistical testing seeks to determine if a factor is *important* at a certain level of confidence (with a "Type I" error of being wrong to retain that factor for further study). Statistically, the two are not the same. A partial solution is to carry out the usual Type I statistical testing at a lower level of confidence, say, at 80% rather than the usual 95%. With this lower level of statistical confidence, more factors will pass the screen and appear to be statistically significant. Many of these factors ultimately might turn out to be unimportant, but more of those that really are important will be included in the accepted group.

*The second question.* The answer to this question involves modeling. Empirical models can be constructed with information obtained from central-composite response surface designs (as previously discussed) but, when the number of factors is large, these designs require a very large number of experiments ($2^k + 2k + 1$ experiments for $k$ dimensions). Plus, the full second-order polynomial model usually doesn't fit very well when it covers a large volume of the factor space (that is, much of the range of each of the factors) — statisticians say there is a large amount of lack of fit of the model to the data. More complicated models that fit better require additional experiments to gather the necessary information.

It is difficult to model a system over the whole domain of factor space (that is, the full range of each factor). For the practical operation of a chemical process, such a broad model is wasteful, because only that part of the model near the optimum ultimately will be used.

*The third question.* The answer to this question comes easily if the answers to the first two questions are done well — a comprehensive model that takes into account all of the important factors will reveal the optimal operating conditions. Mathematical derivative techniques (for instance, canonical analysis *(3)* or ridge analysis *(4)*) or numerical search techniques can be used for this purpose.

With this traditional approach to optimization, however, if the process changes and the response surface moves, then the process must be modeled again to reflect these changes.

## An alternative approach

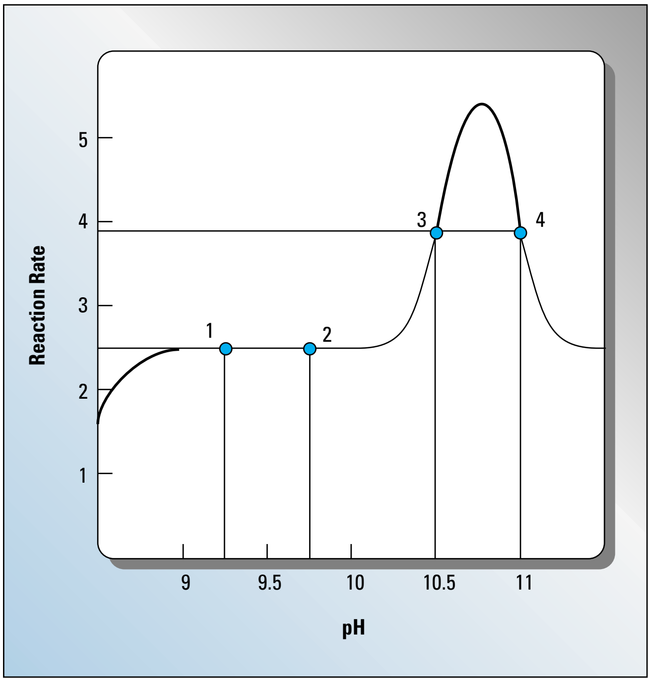
When optimization is the desired goal, questions of significant factors and functional relationships usually are of interest only in the region of the optimum. As Driver has pointed out *(1)*, in many cases statistics should be used to help answer the three questions discussed above — but in reverse order:

**3.** What are the optimum levels of the important factors?

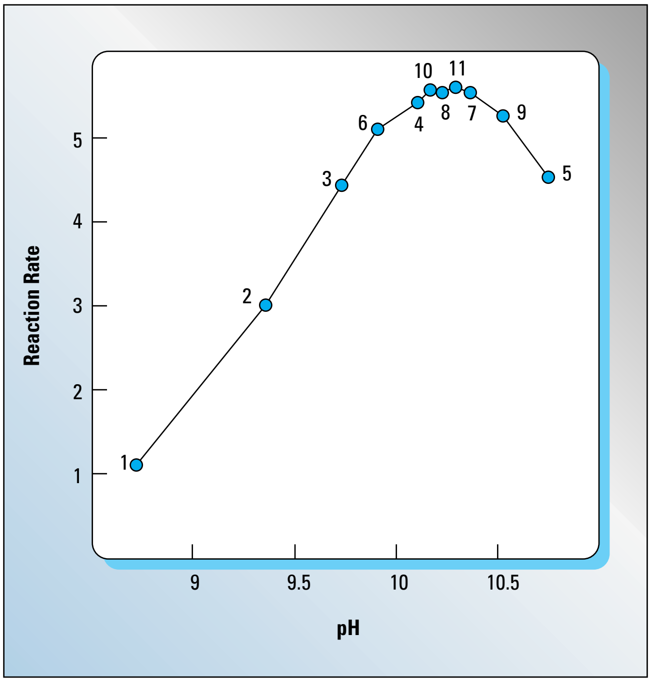
**2.** What equation does the dependence best fit?

**1.** Does an experimentally measured response depend upon certain factors?

If this alternative statistical approach to optimization is to be suc-




■ Figure 7. Effects undetected by a two-level screening design.




■ Figure 8. Fibonacci search.

cessful, then an efficient *optimization strategy* is required.

If only one factor need be optimized, a Fibonacci search is very efficient. Figure 8 shows the results of a Fibonacci search to find the optimal pH of an enzyme-catalyzed reaction. The Fibonacci algorithm is iterative, and starts with the five experiments numbered 1–5 in the figure. Of these five results, the best and the two on either side of it are retained (experiments 3, 4, and 5), and two new experiments are carried out at the midpoints of the intervals (experiments 6 and 7). Then, the procedure is repeated for the new set of five experiments (the two new experiments plus the three that were retained from the previous iteration). This leads to experiments 8 and 9 and, on the next iteration, to experiments 10 and 11. At this point, the algorithm is stopped, because the optimum pH has been found.

The Fibonacci search is *effective*: the pH giving optimal reaction rate has been found. The Fibonacci search is *efficient*: only a few experiments have been required to find the optimal pH. The Fibonacci search is *focused*: exploration has been sparser in those regions of the factor domain that give poor results, and fuller in those regions that give optimal results. Stating the last result differently, the Fibonacci search *does not get lost*: it does not waste time investigating regions of the response surface that ultimately will not be of interest. The Fibonacci search has provided a good answer to question 3 above.

The Fibonacci search usually gives enough information in the region of the optimum that an empirical parabolic model can be used to describe the behavior of the factor (pH) on the response (reaction rate) in this region (the answer to question 2 above). Because the model is used to describe a limited region of the response surface, there is little lack of fit of the model to the data. The empirical model can be used to locate the optimum more precisely.

Finally, the empirical model will reveal that pH is an important factor and should be controlled if the optimal reaction rate is to be achieved consistently (the answer to question 1 above).

Although the Fibonacci search possesses all of these desirable qualities, it still is a single factor search and will be stranded on multifactor ridges when used for single-factor-at-a-time optimization.

## An optimal strategy for optimization

In 1957, Box suggested the sequential application of small factorial designs to industrial processes to move the operating conditions closer and closer to the multifactor optimum *(5)*. This method is analogous to Darwinian evolution in that it involves natural variation and survival of the fittest, and is called "evolutionary operation" or EVOP for short. Soon after the introduction of the concept of EVOP, Spendley, Hext, and Himsworth *(6)* recommended replacing the factori-

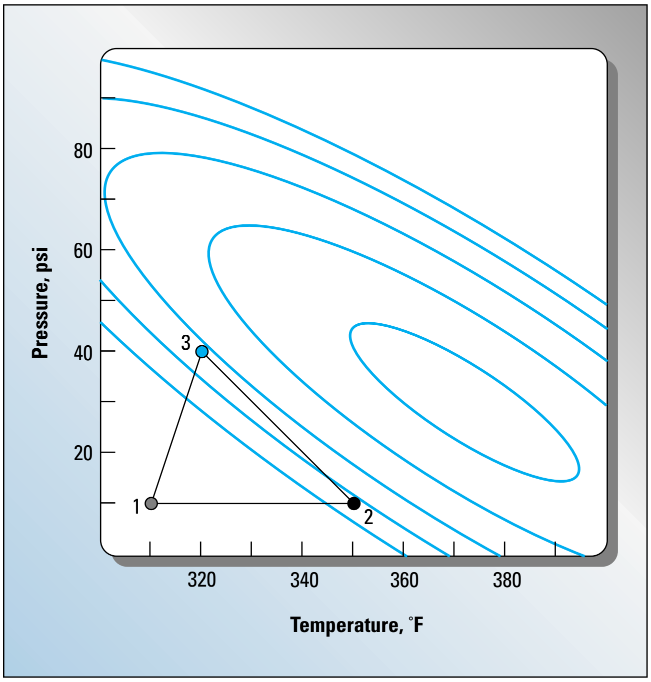



Figure 9. Simplex design.

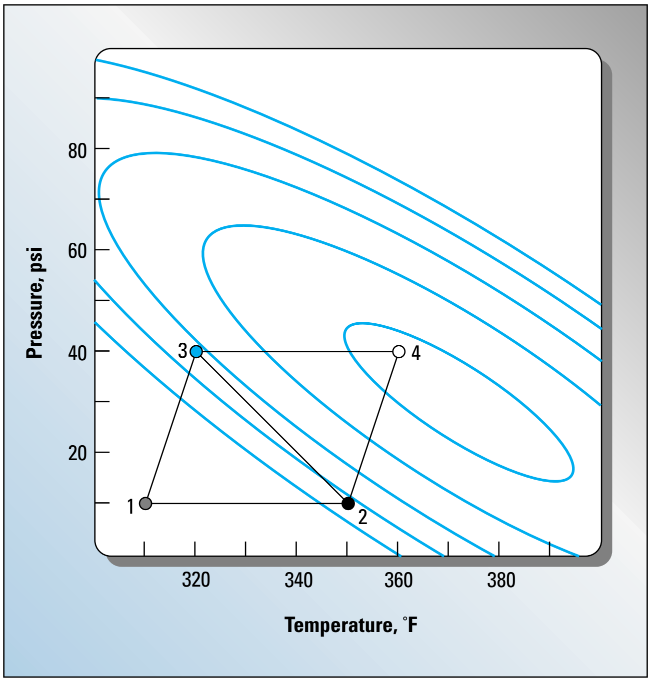



Figure 10. Movement of a simplex pattern.

al design with a more efficient pattern of experiments known as a simplex design.

A simplex is a geometric figure with its number of vertexes (corners) equal to one more than the number of dimensions of the factor space. As shown in Figure 9, a simplex in two dimensions has three vertexes and can be represented as a triangle. The vertexes represent factor levels where experiments are carried out. For example, in Figure 9, vertex 1 describes an experiment at a temperature of 310°F and a pressure of 10 psi.

Figure 10 illustrates how the simplex pattern of experiments can be moved toward the optimum by rejecting one vertex and creating another. This process of creating a new, adjacent simplex by carrying out only one new experiment holds true for any number of dimensions of the factor space. Figure 11 shows how the simplex progresses toward the optimum by the repeated application of this principle.

Nelder and Mead (7) modified the original fixed-size simplex algorithm so it could expand when it finds itself moving in desirable directions and contract when moving in undesirable directions. Figure 12 depicts the behavior of the resulting variable-size simplex.

An important application of the

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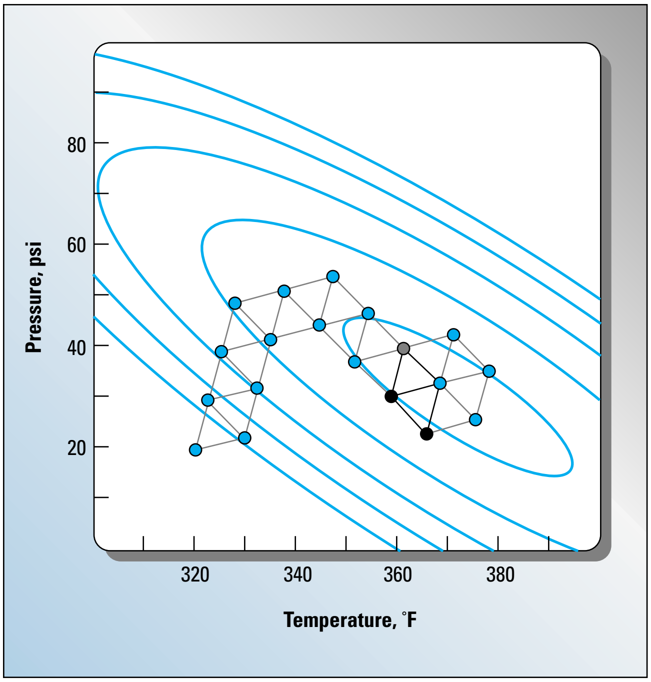
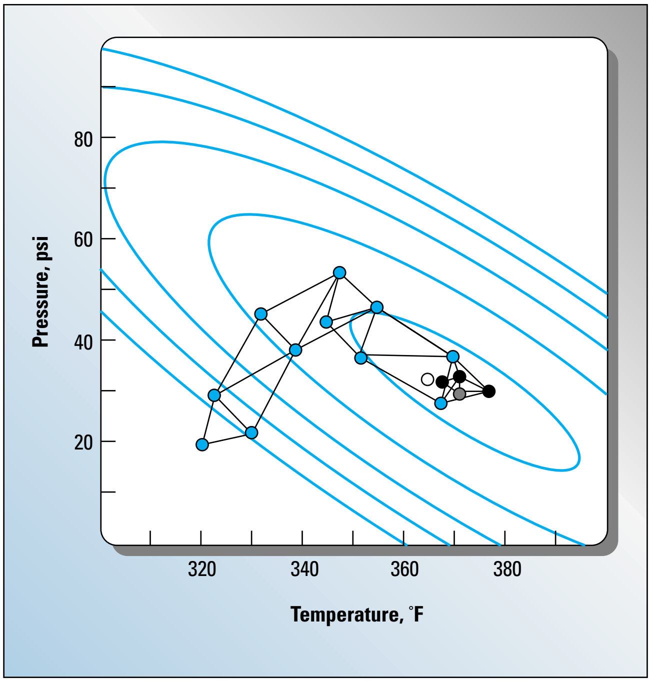



■ Figure 11. Progress of simplex towards optimum.




■ Figure 12. Variable-size simplex.

variable size simplex is for rapid optimization of processes during research and development. Here, it usually is relatively safe to make large changes in the levels of the factors. If a large simplex is used for optimization, it will collapse into the region of the optimum rather quickly, as seen in Figure 12. This has important advantages that have been discussed previously.

As illustrated in Figure 12, the simplex is *effective*: the optimum is found. The simplex is *efficient*: only a few experiments are required to reach the region of the optimum. The simplex is *focused*: exploration is sparser in those regions that give poor results, and fuller in those regions that give optimal results. The simplex *does not get lost*: it does not waste time investigating regions of the response surface that ultimately will not be of interest. These are the characteristics of *an optimal strategy for optimization*.

When processes age or when process inputs (such as feedstocks) alter, the response surface often will change and the optimal set of operating conditions will move somewhere else in the factor space. An important capability of simplex EVOP methods is that, if run continuously, they can follow a changing optimum. Whenever the simplex finds itself on the side of a hill because the optimum has shifted elsewhere, it always will try to climb the hill to find the new optimum.

## Gain the competitive edge

The simplex method of evolutionary operation is efficient, effective, focused, and does not get lost. It can rapidly optimize chemical processes, and, equally important, can follow shifting optima to keep these processes at peak performance so they maintain their competitive edge. CEP

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