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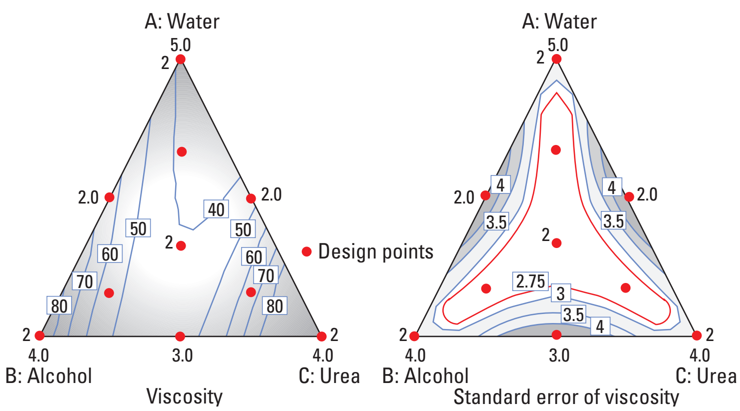
Design, Analyze, and Optimize with *Design-Expert*

Design-Expert 6.0.6
Stat-Ease, Inc.
$995, network licenses available on a concurrent usage basis
www.statease.com
Requires: *Windows 95* and up

Design-Expert 6.0.6 for design-of-experiments (DoE) can serve a variety of needs among experimental chemists, from screening to modeling and optimization. This review highlights the computational capabilities and functions of *Design-Expert 6.0.6* and some of the less obvious experimental conditions. Copies of *Design-Expert* can be downloaded from www.statease.com for a 30-day trial. The software is well supported by online help features and a printed manual, which includes 17 tutorials and 5 appendices of technical information for advanced DoE applications. Mathematical methods for DoE analysis are the focus of recent books by D. Montgomery (*1*) and C. F. Wu and M. Hamada (*2*). Users can get the educational version, *Design-Ease*, on CD-ROM with a textbook by M. Anderson and P. Whitcomb (*3*). The educational version of *Design-Expert* comes with Montgomery's textbook.

DoE methods use probability and statistics to define the minimum number of experiments needed to identify significant cause-and-effect relationships between a given number of factors and one or more responses. Mathematically, DoE methods are well developed to identify efficient experimental designs. The three major components of DoE are design, analysis, and optimization. The strength of *Design-Expert* is the ease with which these tasks can be carried out and the usefulness of information provided in the displays. *Design-Expert* organizes these tasks in subsections of a folder for each project and set of experimental data.

Most DoE operations are intuitive and seamless, supported by useful information in graphics and text. With minimum effort—and often minimal computational time (PC with 350-MHz Pentium II microprocessor, 64-Mb RAM)—virtually any part of a DoE project can be examined and modified, and the results can be evaluated. All text and graphics can be easily cut and pasted into reports, edited, and rearranged. In general, this option is much more powerful than the ability to export text.



Contour plots from a mixture design for three factors (water, 3–5%; alcohol, 2–4%; urea, 2–4%; constrained to a total of 9%) and two responses (viscosity, 35- to 144-mPa-s; turbidity, 323–1122 ntu): left, the dependence of the "viscosity" response; and right, the standard error of the "viscosity" response, as functions of the solvent composition. The 14 design points are clearly located on axes from each vertex to the midpoint of the opposite side. The axes represent the range of values for each factor: two center points, two points at each of the three vertices, three center edge points, and three axial check blend points. With very little modification, this design could easily represent the optimization of a ternary solvent mobile-phase mixture for an HPLC separation.

New designs are selected from four categories: factorial, response surface, mixture, and crossed-process mixture. Page layouts are well organized and informative. Designs are displayed on separate pages in a table format. *Design-Expert* limits many designs to a relatively small maximum number of factors, but all designs can have up to 100 responses. In contrast, the DoE module in *Statistica* by StatSoft, Inc. (www.statsoft.com) allows designs to have more than 100 factors. A large number of factors would be desirable for DoE applications in combinatorial chemistry. A large number of responses would be useful for DoE applications where there are many target analytes but relatively few instrumental conditions to optimize in high-resolution chromatography or spectroscopy, for example. Technically, several factorial designs are restricted to categorical variables, but these often can be reclassified as numeric variables without hindering the computations.

In the software's analysis section, the goal is to reduce the mathematical model to key factors controlling observed responses. Throughout this section, results of statistical analyses are automatically displayed in text and graphic formats to provide consistent, objective criteria for fitting the model to the experimental results. Frequent annotations are provided to flag statistically significant results that have bearing on subsequent choices for the model. As might be expected, the computational time for the analysis section starts to become noticeable as the complexity of the problem increases.

A notable feature of the optimization section is convenience. Responses can be calculated for any combination of allowed experimental conditions. The user also has a choice of graphic or numeric displays for optimization. Procedures to set desired values or criteria (maximum, minimum, in range) for the factors and responses are self-explanatory. A table lists values of the factors and responses for all acceptable solutions, and the results can be copied into reports. Results for each solution can be examined in a graph one at a time, but it is trivial to step through all possible solutions and see the differences. Because a large quantity of information on optimization can be produced in a very short time—for various conditions of interest—

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capabilities to visualize the results are very important.

In retrospect, several DoE conventions may be nontrivial to implement experimentally, depending on the user's circumstances. For example, *Design-Expert* follows statistical conventions to avoid bias and assigns a random order in which to conduct experiments. Moreover, DoE experimental conditions are defined to create a geometrically uniform distribution over the range of values specified by the user, as shown by the example on p. 222 A.

Response surface and mixture designs in *Design-Expert* often use five or six levels per factor: Assigned values are not just whole integers but also include one-third and two-third fractions, in or beyond a specified range, to maintain geometric symmetry. Depending on the design, suggested values in a range from 2 to 4 may be 2, 2.33, 3, 3.33, 3.67, 4 or 1.66, 2, 3, 4, 4.34. These conditions are a clear departure from the common experimental sequences, which vary logarithmically or by orders of magnitude.

It is expected that users will follow a learning curve in the application of DoE methods to their experiments. The most basic decisions are which design to use and how many levels to set for the known factors. If some experimentalists eventually find themselves searching for capabilities beyond *Design-Expert*, they will most likely still value the computational experiences that increased their understanding.

Reviewed by Katherine T. Alben, New York State Department of Health, Albany, NY.

References

(1) Montgomery, D. *Design & Analysis of Experiments,* 5th ed.; John Wiley: New York, 2001.

(2) Wu, C. F.; Hamada, M. *Experiments: Planning, Analysis, and Parameter Design Optimization;* John Wiley: New York, 2000.

(3) Anderson, M.; Whitcomb, P. *DoE Simplified: Practical Tools for Effective Experimentation;* Productivity, Inc.: Portland, OR, 2000.