

Get pumped up for:

Design of Experiments (DOE) Made Easy and More Powerful via Design-Expert® Software

Part 3 – Mixture Design for Optimal Formulation

*Posted at www.statease.com/webinar.html

Feel free to press the raise hand 🙋 feature on GotoWebinar, which I will watch for at intervals during my presentation. To avoid disrupting the Voice over Internet Protocol (VoIP) system, I will mute all. If I do not get to you, please accept my apology in advance. Then I'd appreciate you sending me an email after the talk so we can discuss your issue(s) 'off-line.' -- Mark



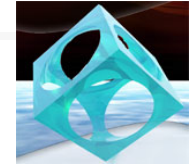
By Mark J. Anderson, PE, CQE
Stat-Ease, Inc., Minneapolis, MN

DOE made easy with Design-Expert
software by Stat-Ease



Timer by Hank Anderson

mark@statease.com 1



Objective:

Show-and-tell what DOE can do with the aid of dedicated software from Stat-Ease and support of its experts.

Agenda of Webinars:

- ~~1. Factorials for discovery, breakthrough and verification (✓*)~~
- ~~2. Response surface methods (RSM) for process optimization (✓*)~~
3. Mixture design for optimal formulation

"Theory guides, experiment decides."

-- I. M. Kolthoff

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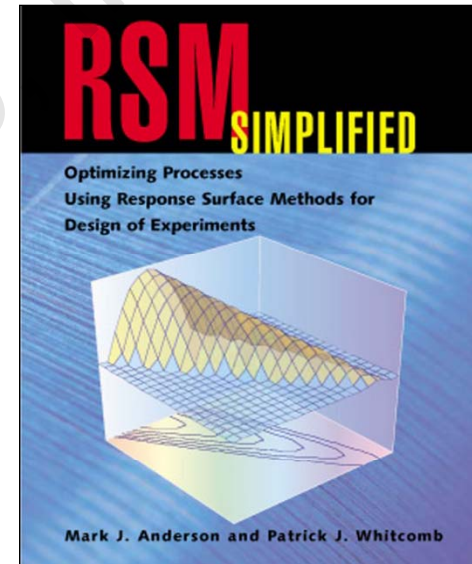
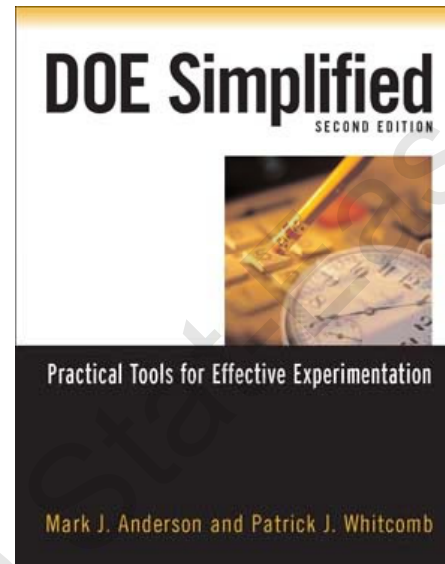
- Tablet-sticking solved - [*Pharmaceutical Formulation & Quality \(PFQ\)*](#)
- Mixture design develops predictive model for estimating an entire range of glaze colors with far fewer test tiles - [*Ceramics Technical*](#)
- High sensory rating achieved for “extra virgin” blend of olive oils - [*ASQ Chemical Process Industries Division newsletter*](#)
- Elastomeric formulation optimized - [*Rubber & Plastics News*](#)
- Sweet spot discovered for coating composition - [*Paint and Coatings Industry*](#)
- Optimal formulation removed a coating in only 45 minutes versus 8 hours for the old recipe - [*Aerospace Engineering & Manufacturing*](#)
- Pound cake recipe fine-tuned - [*Today's Chemist at Work*](#)
- Diet optimized for shrimp - [*Aquaculture*](#)
- Blend of rayon fibers formulated to produce maximal absorbency
- Multiple specifications for plasma etch met in a most desirable way - [*Fab Engineering & Operations \(FEO\)*](#)
- Mixture design creates thinner, whiter keypad backlighting - [*Product Design & Development*](#)

Contact mark@statease.com for these and other pubs – *likely some relevant for you.*

Now in 2nd edition*!



Co-author Pat



New -- a free intro to *Formulation Simplified* book (under development):

A Primer on Mixture Design: What's In It for Formulators?

www.statease.com/pubs/MIXprimer.pdf

Considerations:

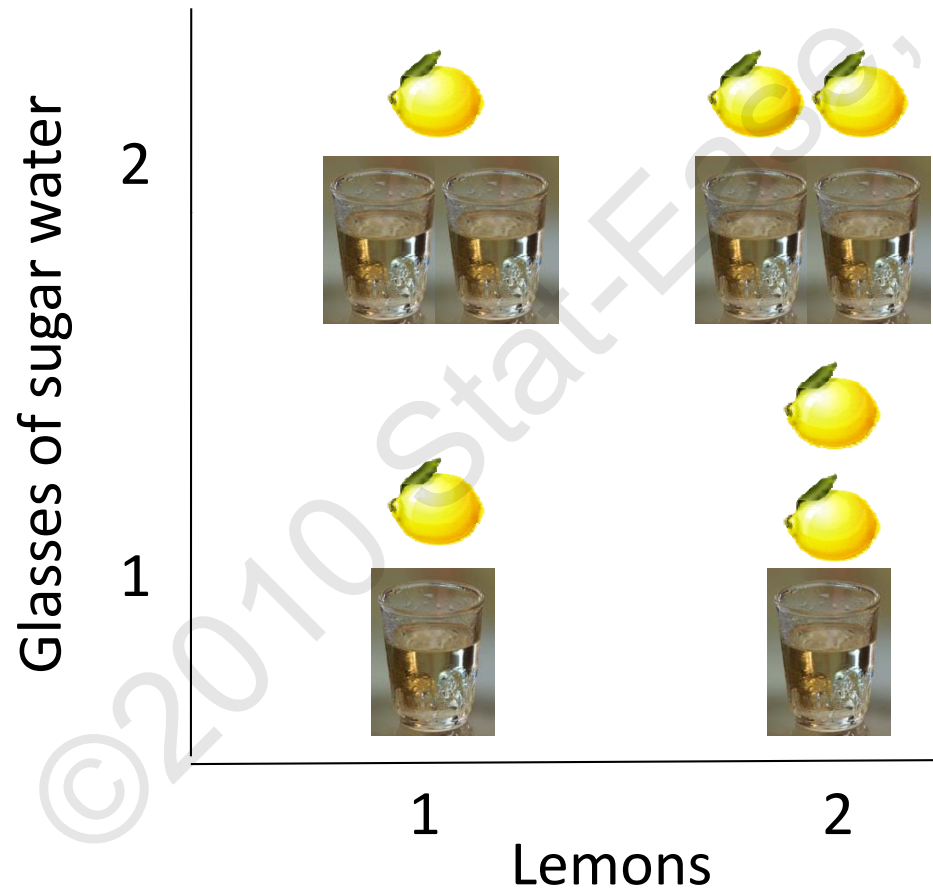
- Factors are ingredients of a mixture.
- The response is a function of proportions, not amounts.
- ❖ Given these two conditions, fixing the total (an equality constraint) facilitates modeling of the response as a function of component proportions.



Let's try forcing a factorial design onto a mixture.

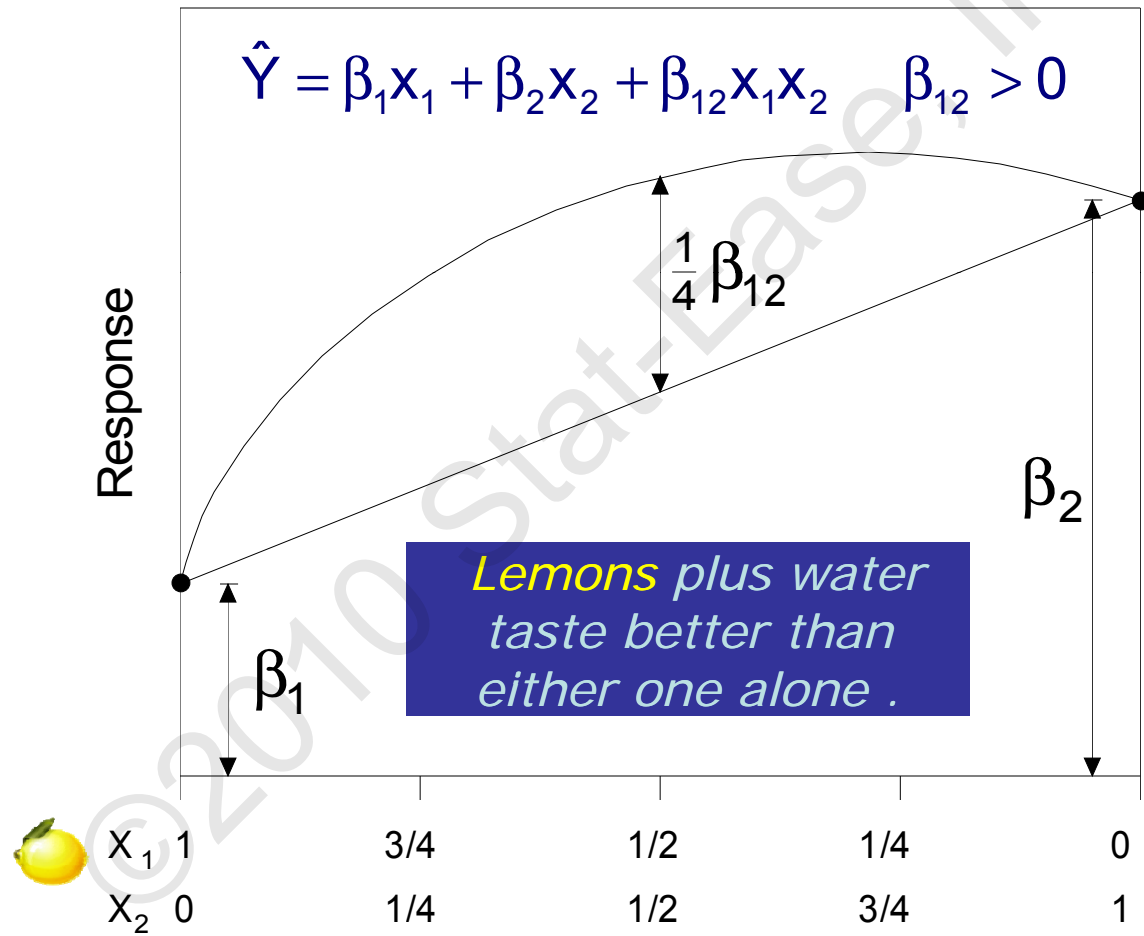
*(Pioneered by Henry Scheffé, U Cal., 1957)

Forcing (squeezing?) factorial design on a mixture: Lemonade

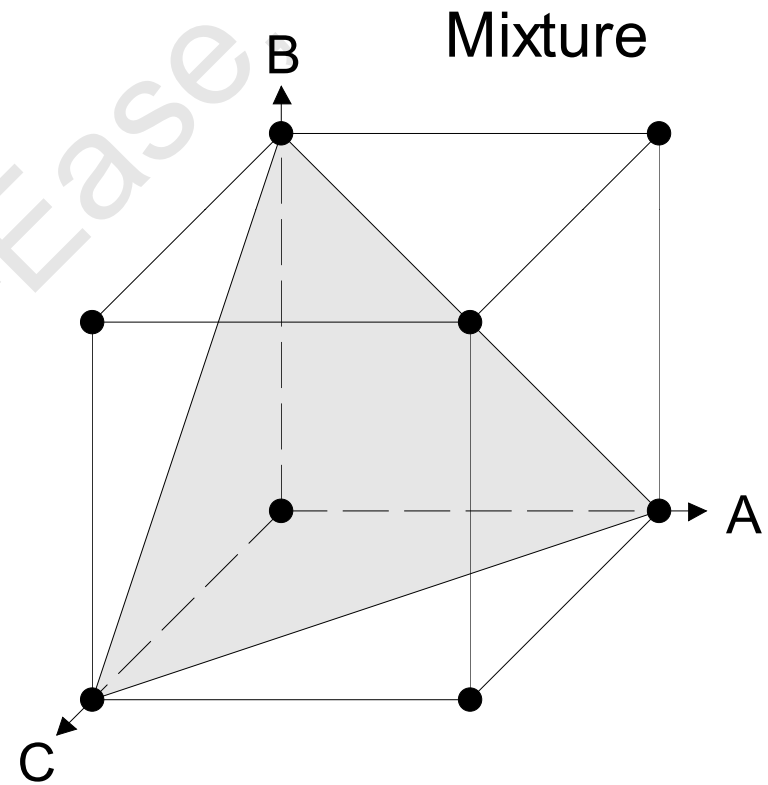
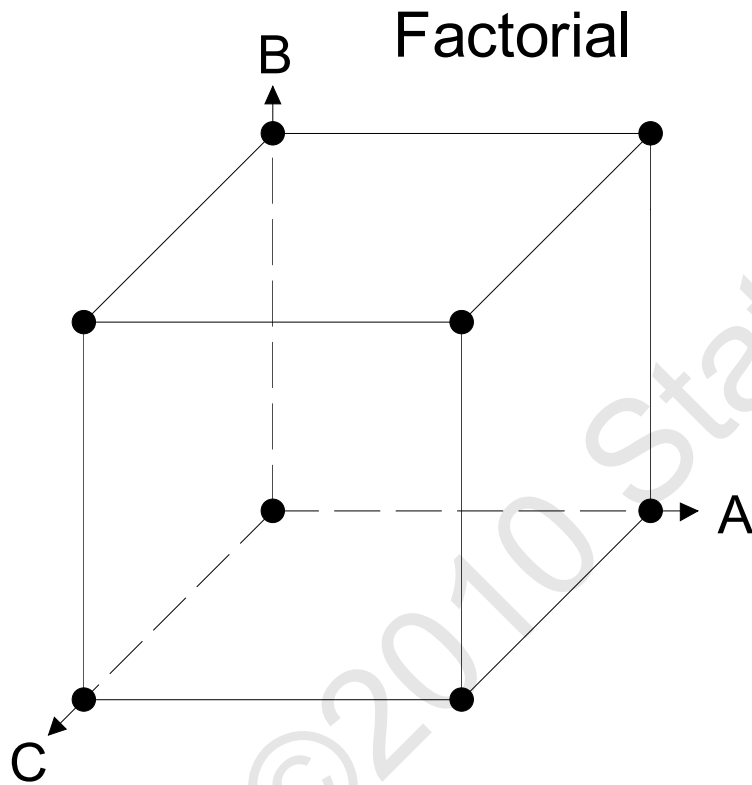


Mixture Design and Modeling (sweet!)

Two components: Quadratic (synergistic)



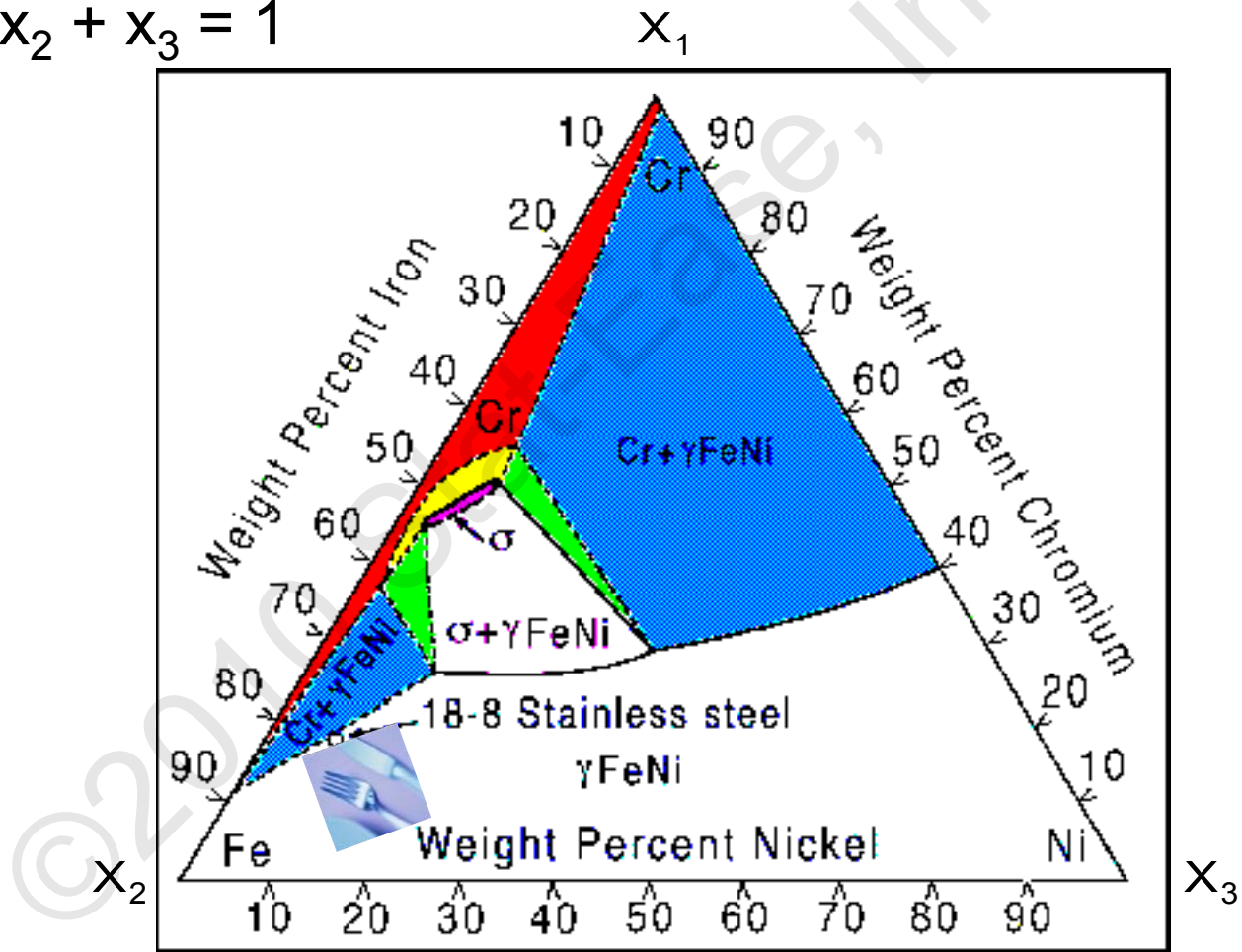
Three-Component Mixture

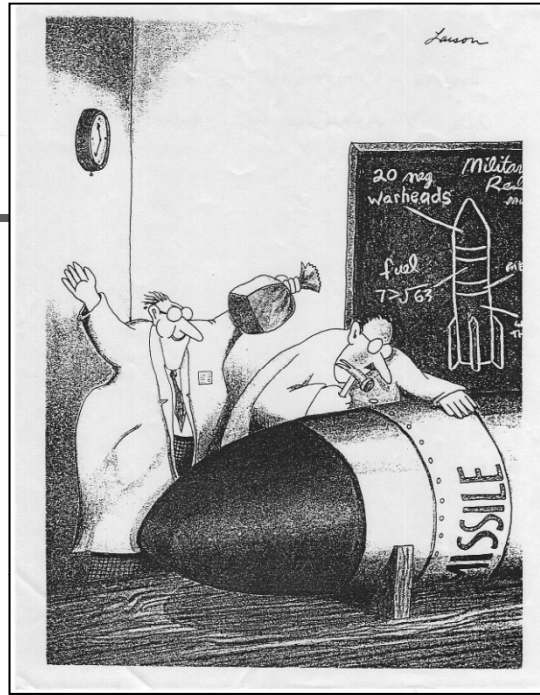


Ternary Diagram for Mixture Composition

(for example, stainless steel flatware)

$$X_1 + X_2 + X_3 = 1$$

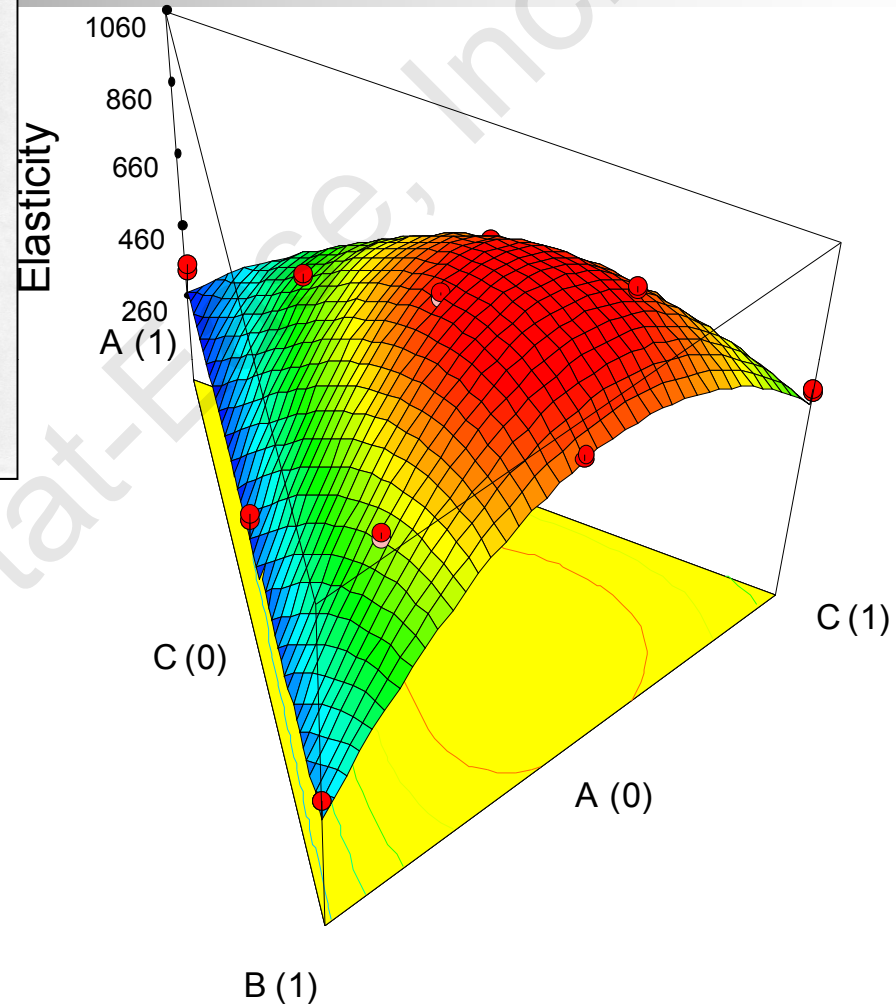




Mixture Design: Solid Rocket Fuel

Special cubic model:

$$\begin{aligned} \text{Elasticity} = & \\ & + 351 * A \\ & + 446 * B \\ & + 653 * C \\ & - 6 * AB \\ & + 1008 * AC \\ & + 1597 * BC \\ & + 6141 * ABC \end{aligned}$$





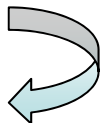
➤ Partial quadratic mixture (PQM) analysis:

Model non-linear blending behavior more simply.

Starting with a complete Scheffé quadratic (CSQ) model there are now two options with Design-Expert v8 software:

1. Reduce it via backward (or other algorithmic) regression.
2. Form a PQM model** via “stepwise” (forward-backward) selection that chooses nonlinear blending terms from the CSQ plus squared terms. See a few details on next slide.

*** (Enabled via Edit, Advanced Preferences, Math tab in v8.05)*



* See Piepel, et al, “Augmenting Scheffé Linear Mixture Models with Squared and/or Crossproduct Terms,” *Journal of Quality Technology*, Vol. 34, No. 3, July 2002.



For the complete Scheffé quadratic (CSQ) model

$$\hat{y} = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

assume that x_2 and x_3 exhibit the same nonlinear blending with x_1 , that is: $\beta_{12} = \beta_{13}$.

Then replace $x_1 x_2$ and $x_1 x_3$ with x_1^2 to form a partial quadratic mixture (PQM) model:

$$\hat{y} = \beta'_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta'_{11} x_1^2 + \beta_{23} x_2 x_3$$

PQM models may fit better with fewer terms and less prediction variance than a reduced CSQ!



*“Waste Glass Durability”
(Log transform)*



- Design for linear plus squared (“L+S”) terms:
Reduce model points required for optimal builds for screening with checkpoints on non-linear blending.

The L+S option* provides a better check for curvature when doing screening (versus simply blending a number of replicate centroids). However, L+S requires far fewer blends than a complete Scheffé quadratic (CSQ) model. For example, with a dozen components, L+S needs only 24 blends ($2q$) vs 78 for CSQ.

**(Enabled via Edit, Advanced Preferences, Math tab)*



*“Liquidus”
Rebuild.
See trace*

Other New Features for Mixture Design



- Blocking expanded to simplex mixture designs: *Blend your cake and bake it in two oven batches, for example.*

Make a simplex (0-100) cake =>



- Increased limit on components for screening and historical designs: *Design-Expert now handles up to 50 individual ingredients – up from 40 and 24; respectively.*

- Design and analyze for special quartic and full quartic mixture models: *Capture extremely non-linear relationships among the components.*



*“Gloss”
See 3d Graph*

New Features for Mixture Design

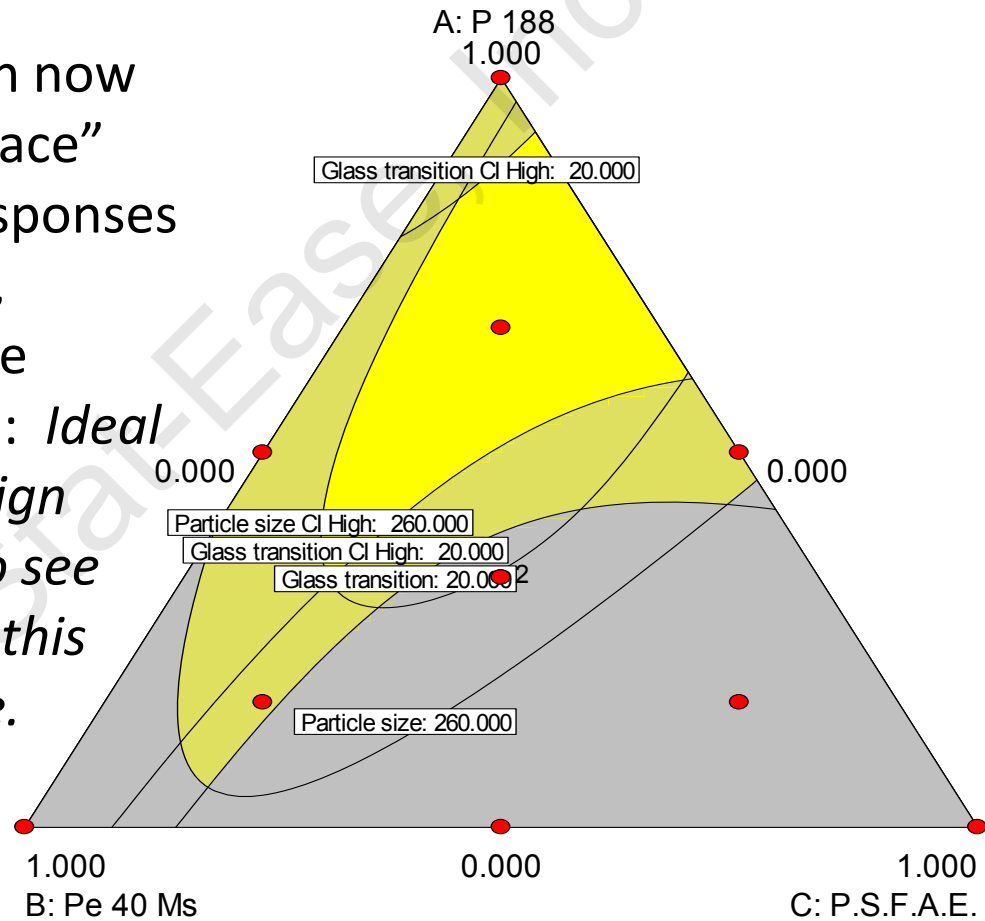
Bonus with free update to v8.04



- Graphical optimization now frames the “design space” where all modeled responses fall within confidence, prediction or tolerance intervals (user choice): *Ideal tool for quality by design (QbD), for example, to see the real sweet spot in this pharmaceutical recipe.*



File: CEP-Mix



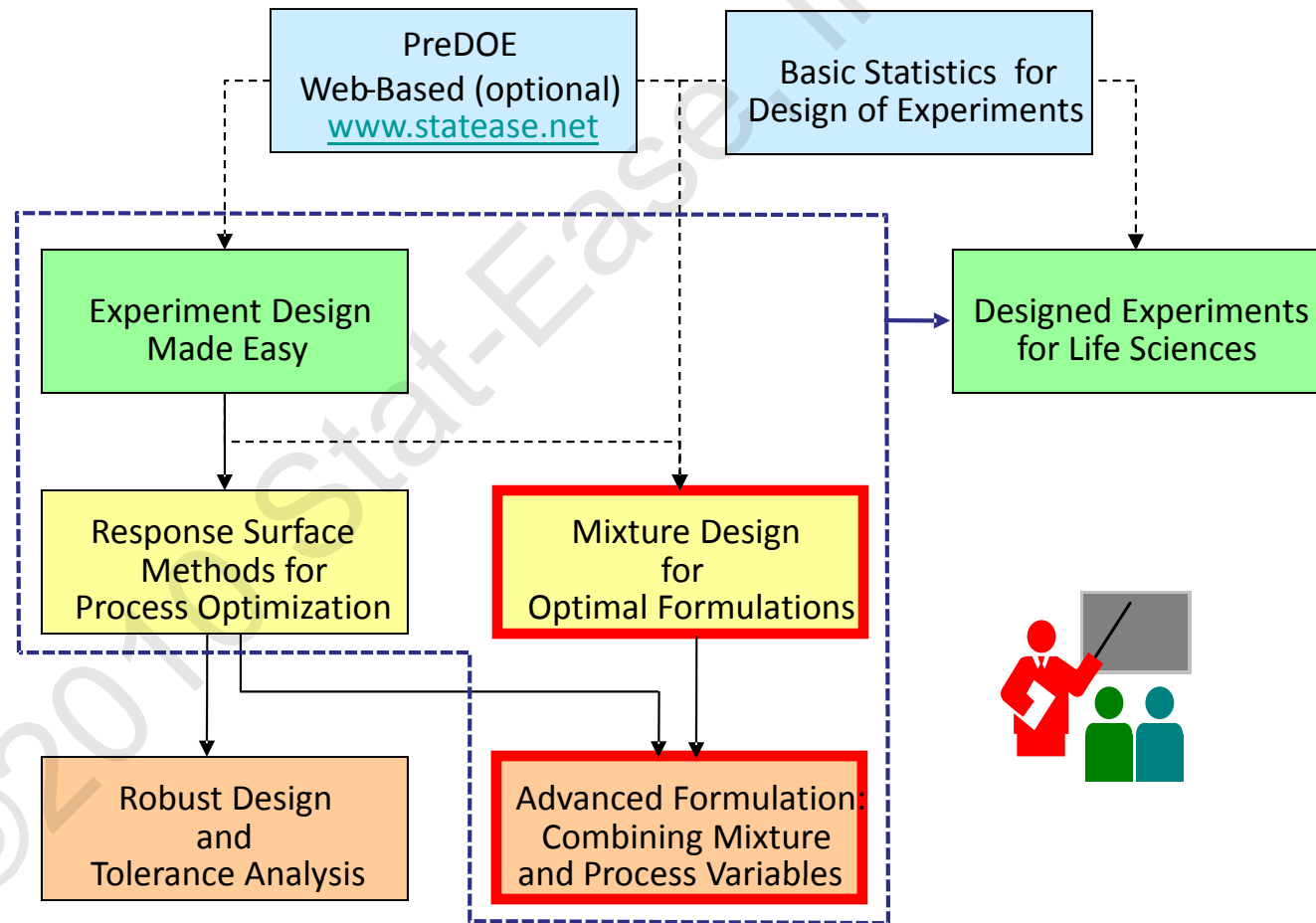
Overlay Plot



Computer-Intensive Statistical Workshops



Shari Kraber,
Workshop Manager
& Master Statistician
shari@statease.com



How to get help



- Search publications posted at www.statease.com.
- In Stat-Ease software press for Screen Tips, view reports in annotated mode, look for context-sensitive Help (right-click) or search the main Help system.
- Explore Experiment Design Forum <http://forum.statease.com> and post your question (if not previously answered).
- E-mail stathelp@statease.com for answers from Stat-Ease's staff of statistical consultants.
- Call 612.378.9449 and ask for "statistical help."

For all the new features in v8 of Design-Expert software, see
www.statease.com/dx8descr.html



*Best of luck for your
experimenting!*

Thanks for listening!

-- Mark

Mark J. Anderson, PE, CQE
Stat-Ease, Inc.

mark@statease.com

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