Supplement to Chapter 11 of *Formulation Simplified*: <u>Augmenting Mixture Designs</u>

In Chapter 11 we provided a strategy for experiments with mixtures. However, one big question remained unaddressed: What if you set your component constraints too tightly and just miss the sweet spot? No worries—this supplement provides an optimal procedure for adding further blends to expand your region of experimentation.

A case where the initial constraints come up short

To demonstrate the need for augmenting mixture experiments, consider a design on three components, all ranging from 0.2 to 0.6 and a scale of 0 to 1. Ideally this region of experimentation would encompass an optimum such as the one seen in Figure S11.1a—the maximum result being at the centroid. However, for the sake of making the case for augmentation, assume the response surface points outside of the boundaries as illustrated by Figure S11.1b.

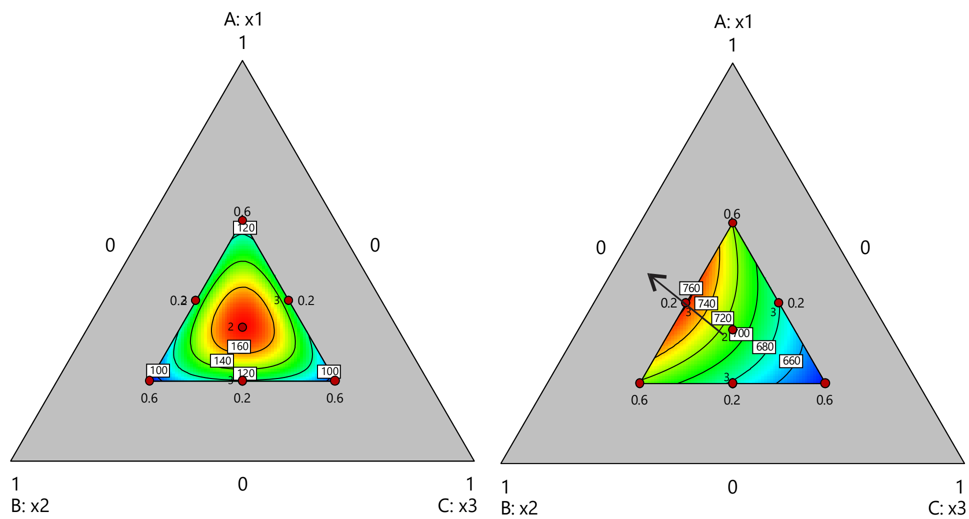

Figure S11.1a,b: Ideal experimental outcome (left) versus less desirable results (right)

The arrow in Figure S11.1b provides the driving force for augmenting the design with new blends that, hopefully, expand the experimental region to a better place. But before you press ahead with a new series of blends in previously untested regions of composition, consider these caveats:

- Resist the temptation to extrapolate the model—it's only an empirical approximation within the current ranges.
- Consider whether it's worth the work—perhaps the current optimum may be good enough given your limits of material, budget or time.
- Assess the risk of going out of current bounds—if not utterly unsafe, mix up some pilot blends under carefully controlled conditions.

Augmenting a mixture DOE space

Having cleared all the caveats above and, given that the true optimum appears to be very close to an existing boundary, it pays to keep the existing data and augment it with further experimentation rather than start over. This requires re-defining of the limits for some, or all, of the mixture components. Then a new block of blends must be laid out. This can be done via optimal design.

To illustrate the process, let's again do a three-component experiment, but this time a more realistic one whose boundaries do not form a simplex. Figure S11.2 shows the initial mixture DOE space, the layout of blends and the response contours. Notice that the optimum evidently occurs outside of the current region for a formulation with more of ingredient A than possible with its current upper limit of 0.5 units.

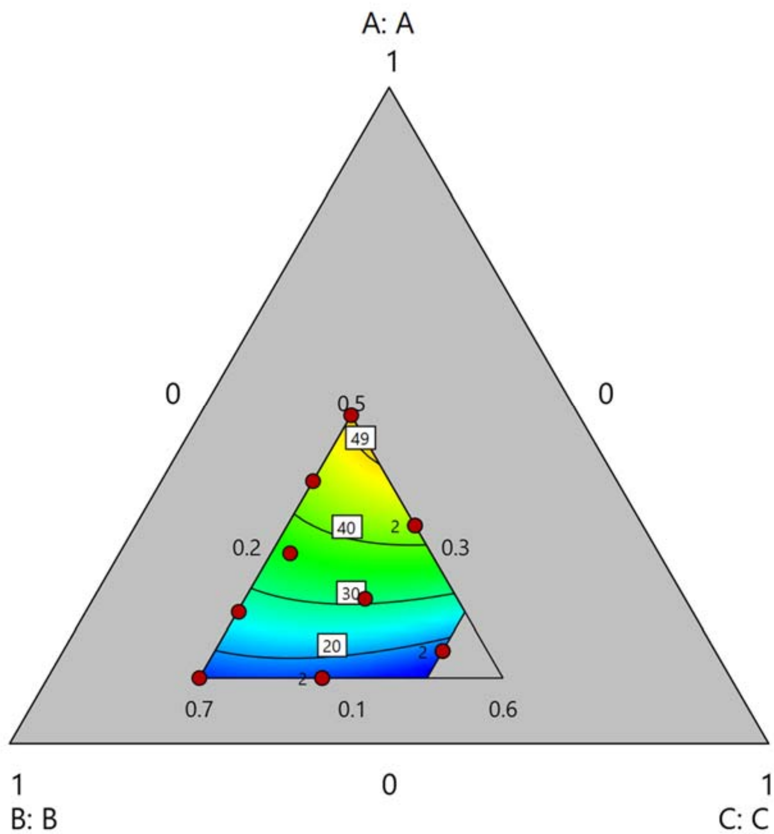

Figure S11.2: A new experiment that will benefit by being augmented

The formulators decide to expand component A to 0.8 units. To make room for the added 0.3 units, they reduce the lower limits of B by 0.2 units and C by 0.1 units. This maintains the total constraint at 1 unit. Figure S11.3 shows the new region shaded by standard error of prediction—dark due to being devoid of experimental blends.

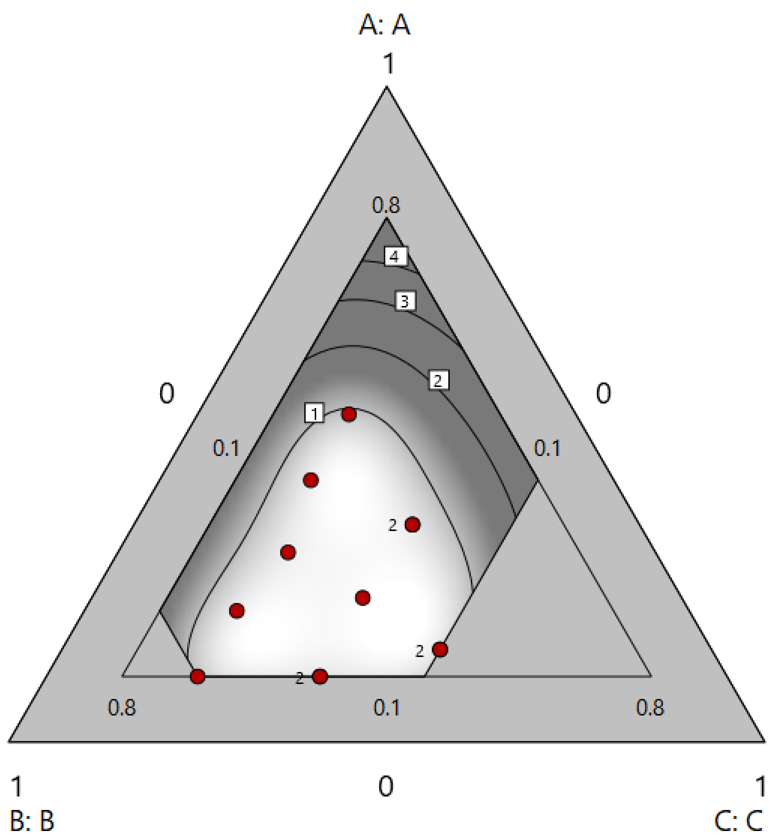

Figure S11.3: Mixture DOE space expanded—shaded by standard error of prediction

The final step is to shed light on the newly expanded regions by selecting additional blends I-optimally to run in a second block. In this case the experimenters decided to run 6 more mixtures—this providing a precision of estimation commensurate with their initial design. Figure S11.4 shows how nicely these new blends fill the gaps and enlighten all but the lower left corner—a location of little interest in any case.

Workaround for Expanding an Existing Mixture Design

Your software may not allow the expansion of component ranges. If so, rebuild the design with the new limits. Then, after resizing the design* to determine how many more blends to run, augment it using tools for optimal point selection.

*(See Chapter 11 sidebar on “Properly Sizing Your Mixture Design”.)

“Only he who keeps his eye fixed on the far horizon will find the right road.”

- Dag Hammarskjold, *Markings*, 1963

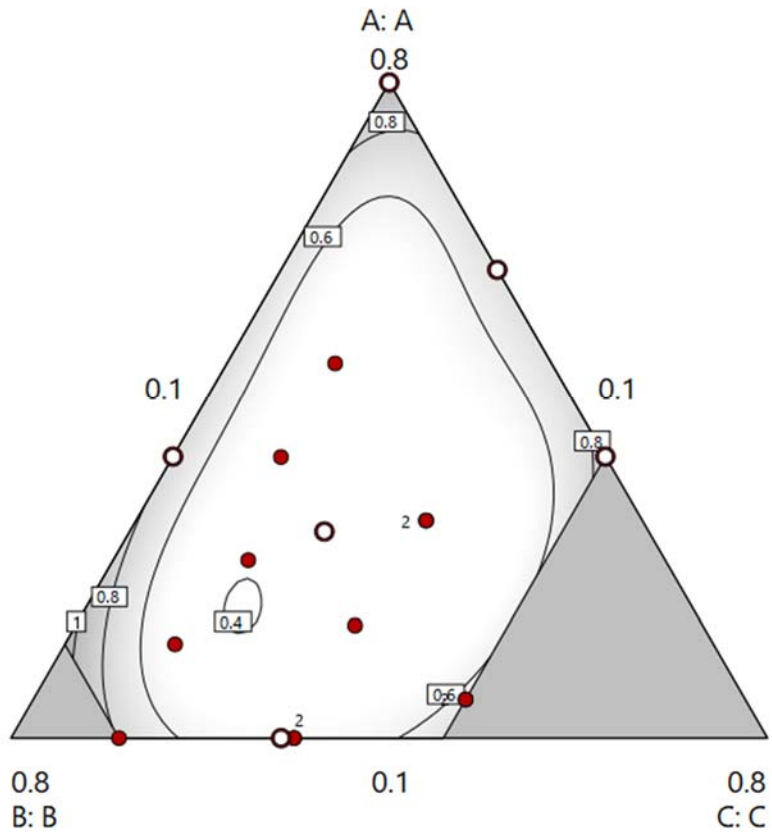

Figure S11.4: Expanded region augmented with 6 additional blends (open circles)

Notice the new point at the middle of the bottom edge coming very close to 2 other runs done in the initial experiment. This may seem redundant. However, the near overlap provides statistical strength for estimating the effect of the blocks.

Conclusion

If you set your component constraints too tightly and just miss the sweet spot, consider expanding your horizons and filling them in optimally with further blends. For experiments on two or three components, contour plots make it easy to see what path to take, as we illustrated above. If you need direction on augmenting mixture DOE spaces on four or more components, consider expanding the ones that your software shows at their limits when it searches out the multiple-response optimum.