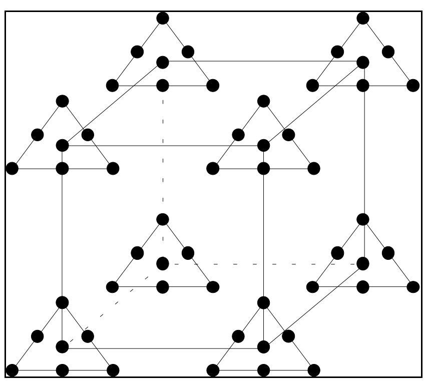
Section 8 – Crossed Mixture-Process Tutorials

Design-Expert® software offers "crossed" designs, which combine mixture components and process factors (numeric and/or categorical). (Before embarking on this tutorial, you should first complete the previous tutorials on response surface methods (RSM) and mixture design.) You will exercise this unique mixture-process design feature by investigating Cornell's famous fish patty experiment from his textbook *Experiments with Mixtures*, published by John Wiley and Sons, New York.

The food formulators hope to make something delicious from a blend of three tasty-sounding (?) fish: mullet, sheepshead and croaker. Yum! The seven blends in the design include one of each of the three fishes, plus the three binary blends and a blend of one-third each. The fish-patties can be cooked at varying deep frying time, oven temperature and oven time. Testing each of these process factors at two levels for all seven blends results in a total of 56 experiments. The diagram below shows the blends as points on triangles, repeated at each of the eight corners of a cube representing the process.



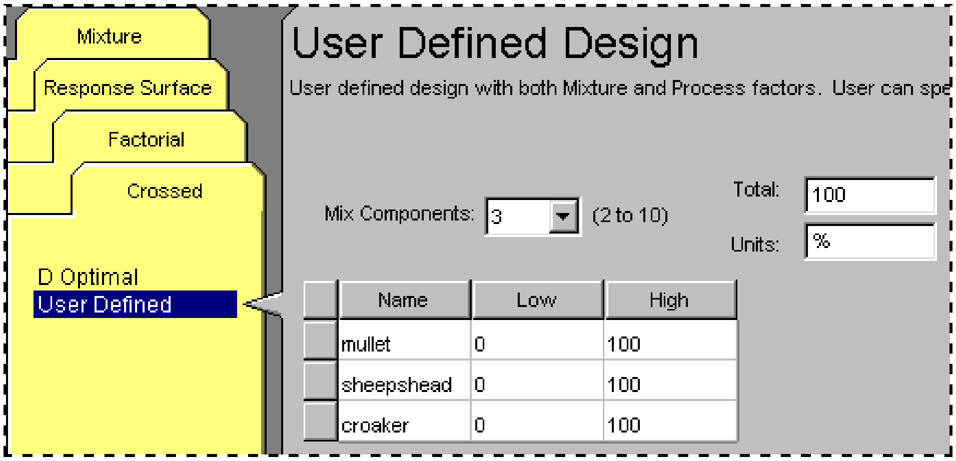
Fish Patty Design: Seven Blends (on Triangles) at Eight Process Combinations (Cube)

The response measure is patty texture. (Never mind about taste!)

The Experiments as Originally Run

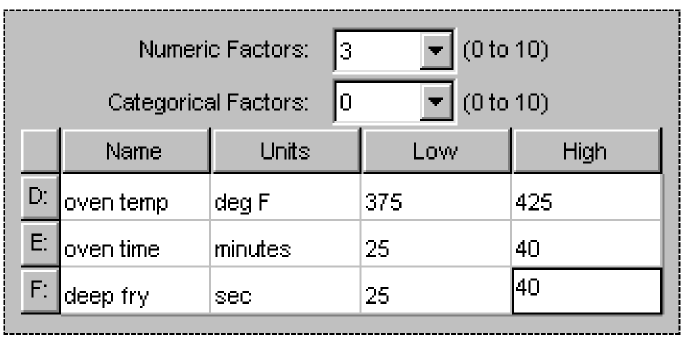
To build the design, choose **File, New Design** or click on the associated "blank sheet" icon at the left end of the toolbar. Then click on the **Crossed** tab and select the **User Defined** option. The user-defined option allows you to reproduce Cornell's design with all points chosen. Normally, to save on runs, you would want the first choice on the list, d-optimal, which will select an ideal subset of design points from a candidate set for a specified model – we'll explore this option later.

Enter **3** as the number of components (fish types). Enter the names of the fish as shown below. The low limits all remain zero. Set all the high limits to **100**. Enter the total of **100** and the units as **%**.



Defining the Mixture

Click on the **Continue** button to move on to the process design factors. Enter "**3**" as the number of numeric factors. Enter the factor names, units and levels (low and high) as shown below.

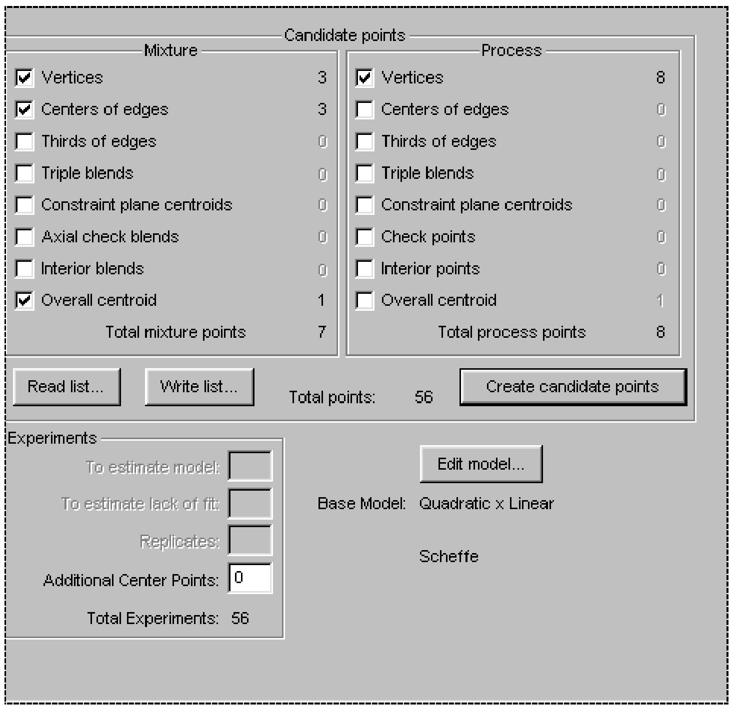


Defining the Process

Click on the **Continue** button to define the models you want to fit for the mixture and process portions of the crossed design. The default model is quadratic by quadratic. Click on the **Edit model** button and change the default for the **Process Order** to **Linear**. Click the **OK** button to implement the change.

Defining the Design Models for Process and Mixture

Now, direct your attention to the "candidate" points. Normally only some of these points would actually make it to the design, but by choosing the User Defined option, you get all of them in the design. However, there's a problem - the **Mixture** candidate set of points (at left of screen) contains more points than those chosen by Cornell. Fix this by clicking off the **Axial check blends** and **Interior blends**. Only vertices, centers of edges and the overall centroid should now be checked. The **Process** candidate set of points (at right) also contains more points than those chosen by Cornell. Click off the **Check points** and the **Overall centroid**. Click on the **Create candidate points** button to see how many points you get. As shown below, the points should total to 56 (the 7 mixtures specified by Cornell, multiplied by 8 process combinations).



Candidate Points After Deselecting Some of the Default Choices

Click on the **Continue** button to move on to the response specification. Enter **Ave Texture** with units of **gm*10^-3**. Click on the **Continue** button to complete the design. Design-Expert now displays the 56 experiments in random run order.

Analyze the Results

To get the response data, right click on the header of the response column, select **Simulate Response** and choose the file named **Fish Patties.sim**. The simulator displays its output at a readable speed so you can observe the responses. Anything outside of 2 to 3.5 is bad. To preserve the results, go to **File** and select **Save As**. Change the file name to **Fish Patties** or some other unique name of your choice.

To analyze the data, click on the node labeled **Ave Texture**. Then, click on the ***Fit Summary*** button. The software may take a while to complete the computations. You now see a unique matrix of probabilities that helps you determine the best crossed model for mixture and process. Check on-line Help for details on how to interpret this matrix. As shown below, the software provides suggestion(s) on which combination is best – in this case, a quadratic mixture model crossed with a linear process model. Either the higher orders of model terms do not significantly improve explanation of variance, or they cannot be used due to aliasing. (Remember that this design was set up for a quadratic model for the mixture components and linear model for process factors.)

Transform | Fit Summary | Model | ANOVA | Diagnostics | Model Graphs

Response: **Ave Texture**

Mixture Process Crossed Model Table

Prob > F Matrix

[Mixture Order]	**Process Order**					
	Mean	**Linear**	**2FI**	**Quadratic**	**Cubic**	
[Mean]**		< 0.0001	0.9883	*	* 0.8488	
		< 0.0001	0.6237	*	* 0.9176	
[Linear]	< 0.0001	< 0.0001	< 0.0001	* < 0.0001	* < 0.0001	
		< 0.0001	0.1129	*	* 0.7158	
[Quadratic]	0.5401	0.0003	0.0028	* 0.0028	* 0.0389	Suggested
		< 0.0001	0.1212	*	*	
[Special Cubic]	0.6426	0.4611	0.2567	* 0.2567	*	
		* < 0.0001	* 0.1212	*	*	
[Cubic]	*	*	*	*	*	

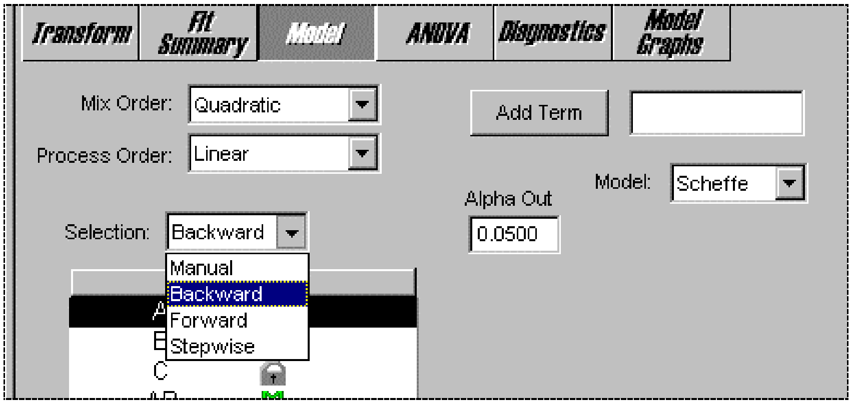
* The crossed model is aliased

** Note that Mean Mixture order can only be selected for Analysis or Evaluation models if the parameterization is changed from Scheffe to Slack.

Fit Summary for Crossed Model

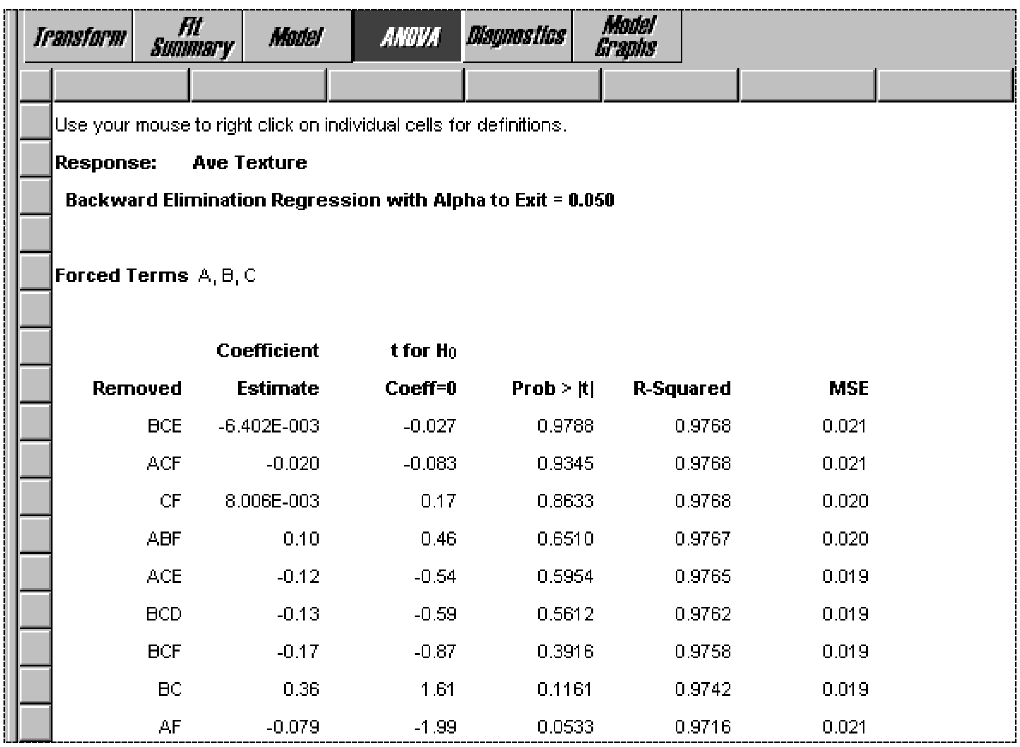
Scroll down to see more statistics on the various crossed models. Again note that the Quadratic*Linear is suggested by the software. Go ahead now and click on the ***Model*** button. Design-Expert uses the suggested model as its default. Accept these for the moment by clicking ahead to the ***ANOVA*** button. Notice that many of the model terms exhibit high Prob>F values. This is a byproduct of crossing the two models for mixture and process, which creates many superfluous higher-order terms. When analyzing designs like this, you will often find it beneficial to reduce your model to just the significant terms, subject to requirements for maintaining hierarchy (no interactions without their parent terms).

To reduce the model, go back and click on the ***Model*** button. You could manually deselect the insignificant terms observed from the ANOVA, but it will be quicker to let Design-Expert do this for you. Change the selection mode to **Backward**.



Selecting Backward Reduction

This enables automatic model reduction by a backward (stepwise) algorithm. The criteria for elimination will be a probability value of 0.05 as specified in the Alpha Out field. Click on the ***ANOVA*** button. As shown below, the software gives you a report on eliminated terms.



Use your mouse to right click on individual cells for definitions.

Response: Ave Texture

Backward Elimination Regression with Alpha to Exit = 0.050

Forced Terms A, B, C

Removed	Coefficient Estimate	t for H_0 Coeff=0	Prob > |t|	R-Squared	MSE
BCE	-6.402E-003	-0.027	0.9788	0.9768	0.021
ACF	-0.020	-0.083	0.9345	0.9768	0.021
CF	8.006E-003	0.17	0.8633	0.9768	0.020
ABF	0.10	0.46	0.6510	0.9767	0.020
ACE	-0.12	-0.54	0.5954	0.9765	0.019
BCD	-0.13	-0.59	0.5612	0.9762	0.019
BCF	-0.17	-0.87	0.3916	0.9758	0.019
BC	0.36	1.61	0.1161	0.9742	0.019
AF	-0.079	-1.99	0.0533	0.9716	0.021

Report on Removed Coefficients After Backward Elimination

The ANOVA table shows that the reduced model fits very well.

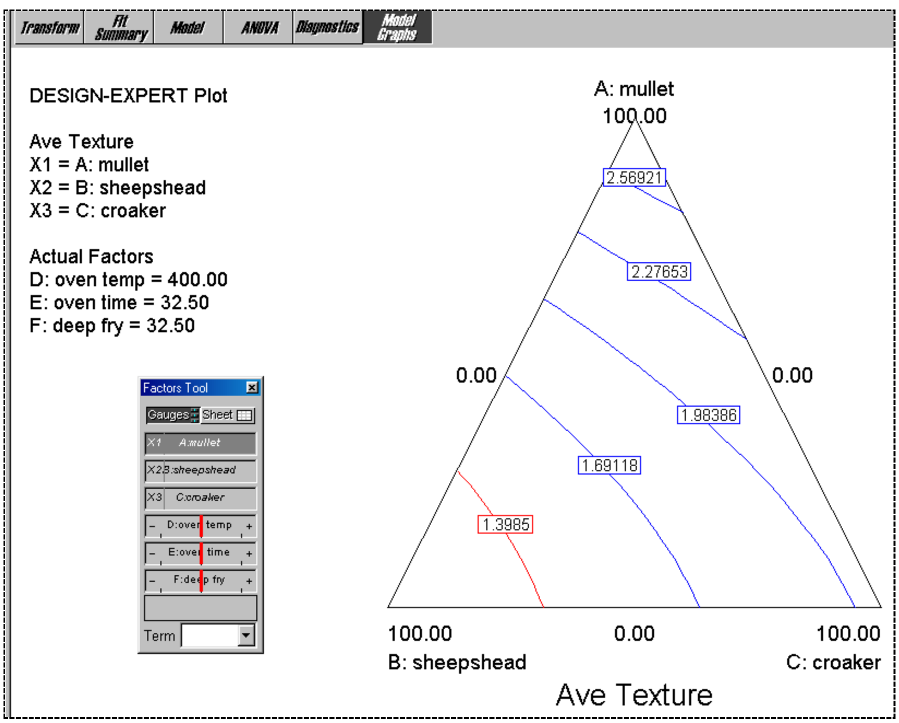
ANOVA for Crossed Reduced Quadratic x Linear Model

Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	29.26	14	2.09	100.23	< 0.0001
Linear Mixture	*14.04*	*2*	*7.02*	*336.59*	*< 0.0001*
AB	*0.38*	*1*	*0.38*	*18.00*	*0.0001*
AC	*0.28*	*1*	*0.28*	*13.27*	*0.0008*
AD	*1.92*	*1*	*1.92*	*92.27*	*< 0.0001*
AE	*4.71*	*1*	*4.71*	*226.02*	*< 0.0001*
BD	*0.26*	*1*	*0.26*	*12.71*	*0.0009*
BE	*0.64*	*1*	*0.64*	*30.62*	*< 0.0001*
BF	*0.15*	*1*	*0.15*	*6.97*	*0.0117*
CD	*0.55*	*1*	*0.55*	*26.25*	*< 0.0001*
CE	*1.81*	*1*	*1.81*	*86.94*	*< 0.0001*
ABD	*0.24*	*1*	*0.24*	*11.60*	*0.0015*
ABE	*0.16*	*1*	*0.16*	*7.90*	*0.0075*
ACD	*0.11*	*1*	*0.11*	*5.06*	*0.0299*

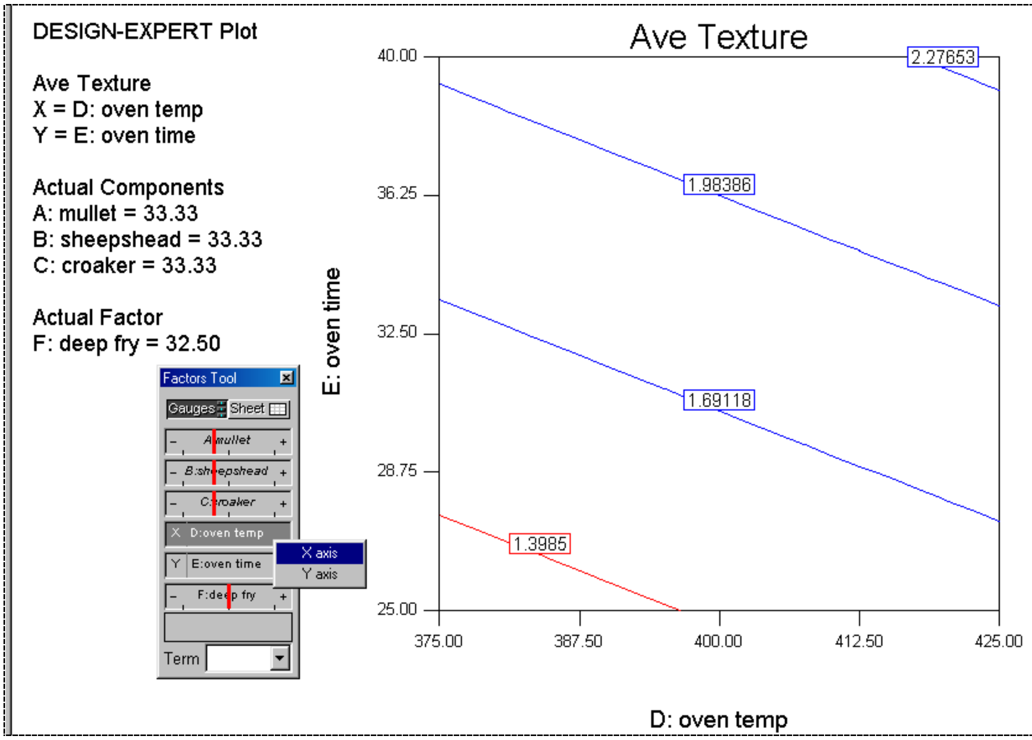
Analysis of Variance (partially shown) for Crossed Model

Click on the ***Diagnostics*** button and examine the diagnostic graphs. They look good, so move on to the ***Model Graphs*** to view the response in mixture (triangular) space.



Mixture View for Model Graph

Click or grab the various process factors on the floating tool bar and move them to see how the response changes. This requires many computations so expect somewhat of a time lag. Now right-click on the **Factors Tool** where it lists **D:oven temp** and select it for the **X axis**. As shown below, the view changes to process (rectangular) space.



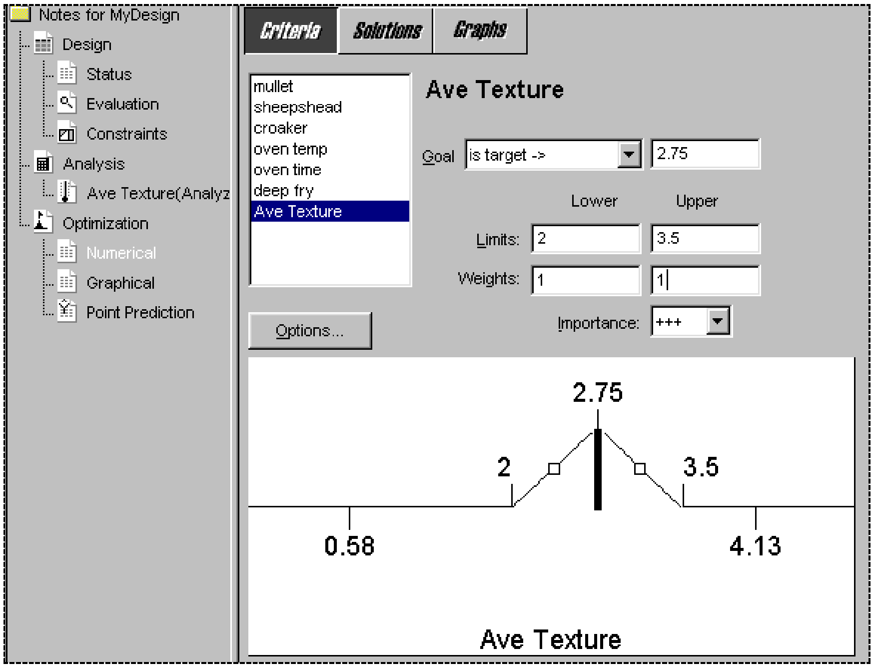
Changing to the Process View

If you want to get nicer contours with fewer significant digits, right click on the graph and select Graph preferences. Then, in the Preference area, click on Contours and change the values as well as the Format.

Continue on if you like and explore different combinations of the mixture components and the third process factor. Due to the complexity of the crossed models, the updating of the graph will be slower than normal, so be patient.

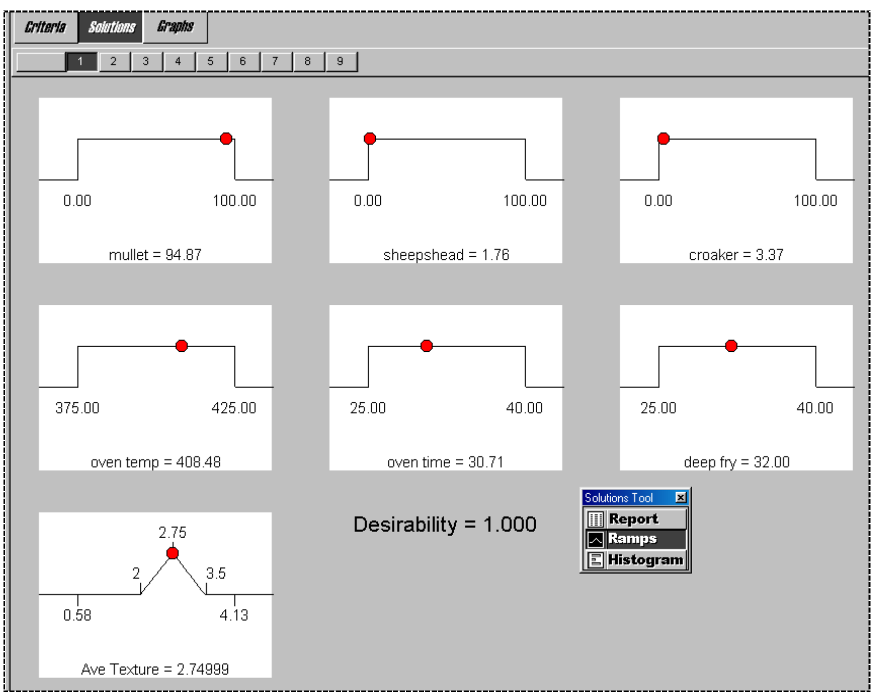
Find the Optimal Solution

The goal of the experimental program is to learn how to produce fish patties with a texture in the range of 2.00 to 3.50 x 10^3 grams. The target is 2.75. To find the optimal combinations of formulas and processing, click on the optimization node labeled **Numerical**. Then select **Ave Texture**. Select a **Goal** of **is target->** and enter **2.75**. Then for **Limits** enter a **Lower** of **2** and **Upper** of **3.5**. Leave the weights and importance settings at their default levels. Your screen should now look like that below.



Optimization Criteria for Texture

Click on the ***Solutions*** button. Then mouse to the **Solutions Tool** and select the **Ramps** option. Notice the many solutions listed at the top of your screen. (Due to the random nature of the optimization algorithm, your screen may show fewer or more solutions.) The software defaults to what it thinks may be the best solution. However, in this case, if you click solution number 2 and beyond, you will see many combinations that satisfy the texture requirements.

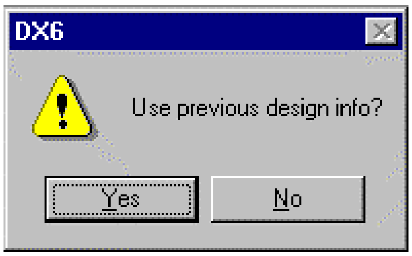


One of Many Solutions for Making Fish Patties with Proper Texture

The Experiments as D-Optimal Design

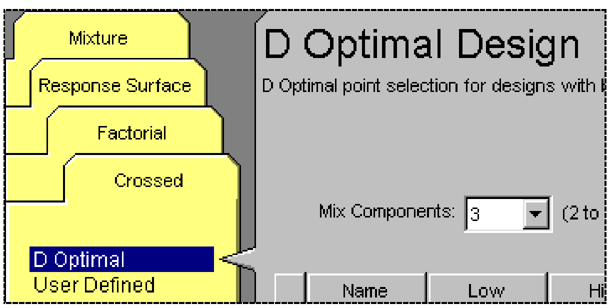
As noted in the introduction, we wanted to reproduce the fish patty case exactly as reported by Cornell in his textbook *Experiments with Mixtures*. Now let's try a d-optimal design, which will be much more efficient. We recommend you use this approach to designing your own mixture-process experiment.

Choose **File, New Design**. When asked whether to "**Save changes to Fish Pattes**," click on **No**. The software then asks whether to "**Use previous design info**." Click on **Yes**.



Re-using Previous Design Information

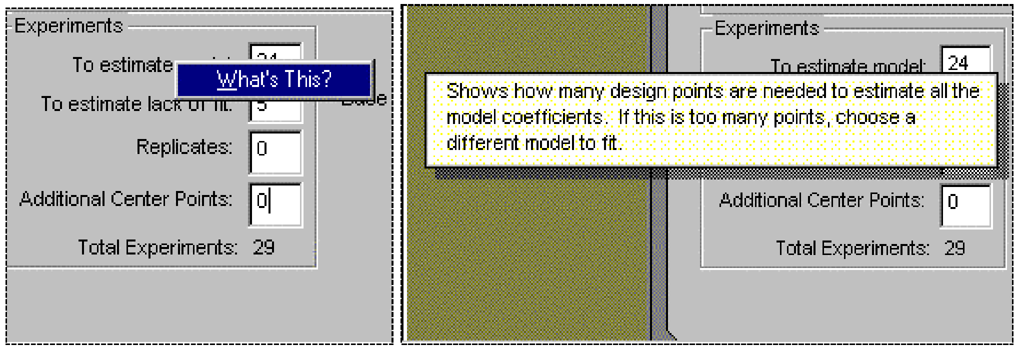
You now see the builder for Crossed designs, but with all the component names already filled in for you. Select the **D Optimal** option.



D Optimal Design Option for Crossed Design

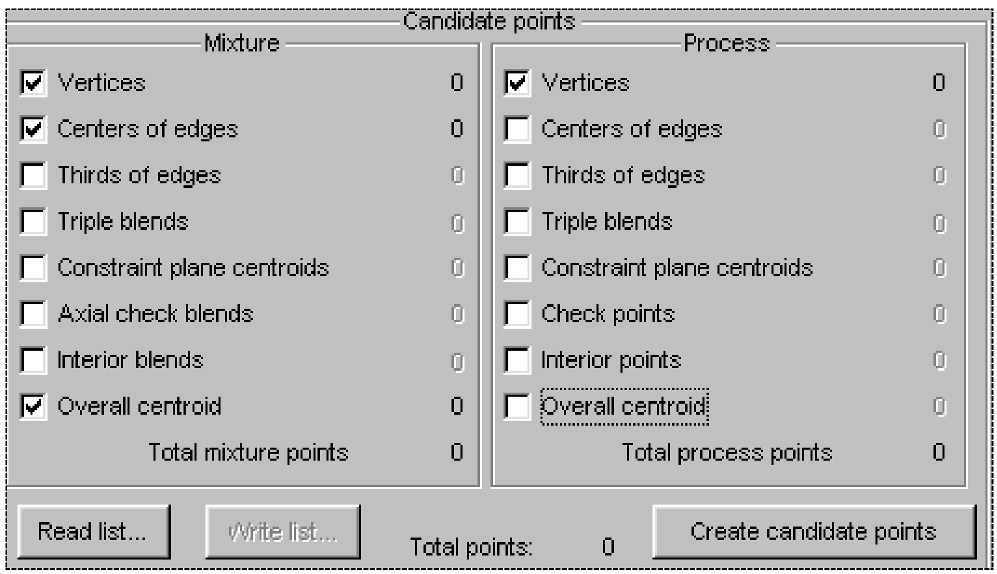
Click on the **Continue** button to see the process factor screen. This is already filled in so just click again on **Continue** to bring up the D Optimal design screen. This should already be set up for the quadratic-linear base model that you want for the process-mixture design on the fish patties.

The d-optimal algorithm will select a subset of design points from a candidate set to estimate the specified model. Look carefully at the candidate set screen. Notice the ungrayed options at the bottom for specifying the number of experiments. Since the original data has no replicates, set **Replicates** to **0**. Hit the tab key and you should see a total of 29 experiments. Leave the options for model and lack of fit at their default levels. To obtain more details on these options, for example the model points, right click over the descriptor (not the entry field) and select **What's This?**.



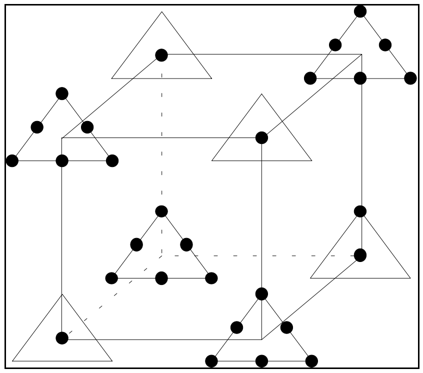
Getting Details on Options via Context-Sensitive Help System

Before moving on, you need to re-create the points originally selected by Cornell. In the **Mixture** candidate set of points (at upper left of screen), click <u>off</u> the **Axial check blends** and **Interior blends**. In the **Process** candidate set of points (at right), click <u>off</u> the **Check points** and the **Overall centroid**. Then click on the **Create candidate points** button. You should now get a total of 56 candidate points, the same as when you did earlier when you set up this case study as a User Defined design.



Candidate Points After Deselecting Some of the Default Choices

Click on the **Continue** button to move on to the response specification. Accept the default response name by clicking **Continue**. Design-Expert now builds four different d-optimal designs and selects the best. There are often several equally good subsets of the candidate points. The design you get depends on the original starting point, which is selected via a "random bootstrap" method. (For details on how this is done, see the write-up on d-optimal in the Statistical Details: Design Selection section of this manual. You can change how many designs the program builds, and other parameters of the d-optimal algorithm, via Edit, Preferences, Math Design.) The 29 experiments listed can be different each time you do a d-optimal design. The design we got is pictured below. (Sorry, but you can't get picture this with Design-Expert – yet.)

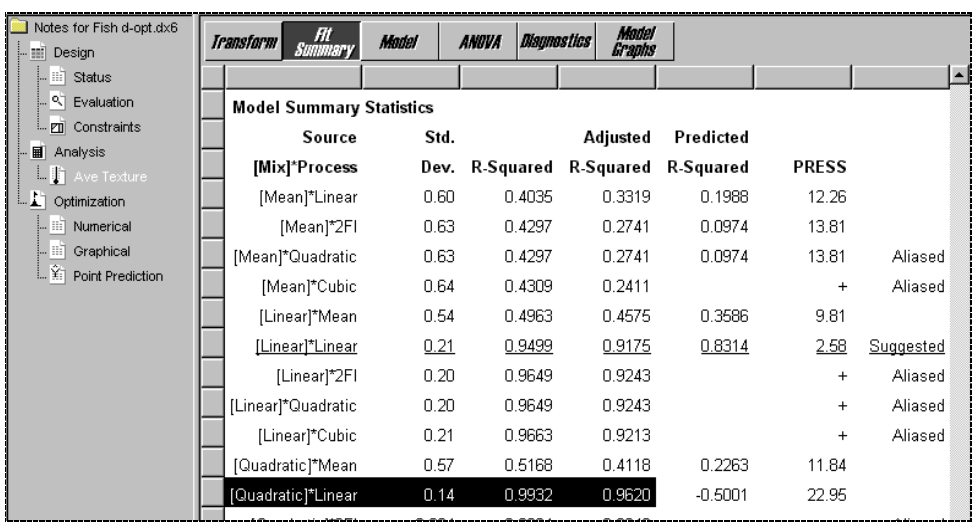


Fish Patty Design: 29 D-Optimal Combinations

Analyze the Results

To get the response data, right click on the header of the response column, select **Simulate Response** and choose the file named **Fish Patties.sim**. The program then generates data. To preserve the results, go to **File** and select **Save As**. Change the file name to "**Fish D-opt**" or some other unique name of your choice.

To analyze this data, click on the analysis node labeled **Ave Texture**. Then click on the ***Fit Summary*** button. Design-Expert suggests a linear mixture model crossed with a linear process model. Taking the recommendation at face value, one would conclude that this outcome differs from the larger User Defined design, where the suggested model was a quadratic mixture model crossed with a linear process model. However, if you scroll down, you will see that this more complex model produces a better adjusted R-squared, which indicates that the added terms provide some benefit. Unfortunately, the quadratic*linear model exhibits a negative predicted R-squared, so the program cannot suggest you use this.

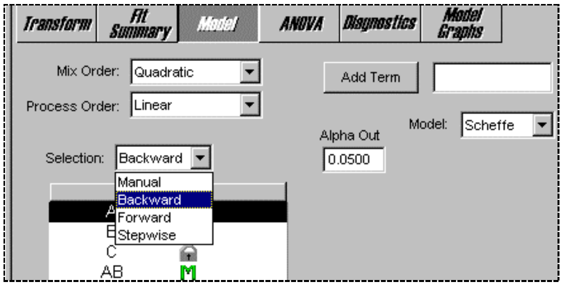


Model Summary Statistics

Source [Mix]*Process	Std. Dev.	R-Squared	Adjusted R-Squared	Predicted R-Squared	PRESS	
[Mean]*Linear	0.60	0.4035	0.3319	0.1988	12.26	
[Mean]*2FI	0.63	0.4297	0.2741	0.0974	13.81	
[Mean]*Quadratic	0.63	0.4297	0.2741	0.0974	13.81	Aliased
[Mean]*Cubic	0.64	0.4309	0.2411		+	Aliased
[Linear]*Mean	0.54	0.4963	0.4575	0.3586	9.81	
[Linear]*Linear	0.21	0.9499	0.9175	0.8314	2.58	Suggested
[Linear]*2FI	0.20	0.9649	0.9243		+	Aliased
[Linear]*Quadratic	0.20	0.9649	0.9243		+	Aliased
[Linear]*Cubic	0.21	0.9663	0.9213		+	Aliased
[Quadratic]*Mean	0.57	0.5168	0.4118	0.2263	11.84	
[Quadratic]*Linear	0.14	0.9932	0.9620	-0.5001	22.95	

Model Summary Statistics (your results may differ slightly due to random bootstrap)

Given what is known about this system from prior experimentation, and the promising adjusted R-squared value, it makes sense to click on the ***Model*** button and change the mixture model order to **Quadratic**. Then change the selection mode to **Backward**.



Modified Mix Order (Quadratic) and Selection Criteria (Backward)

This enables model reduction, which will eliminate many superfluous high-order terms generated by the crossing of models. Clicking on the ***ANOVA*** button to see what happens to the predicted R-squared value. The software gives you a report on eliminated terms. Scroll past this to the actual ANOVA and accompanying statistics. Notice that the reduced model fits very well. The predicted R-squared now exceeds that of the linear*linear model!

ANOVA for Crossed Reduced Quadratic x Linear Model

Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	15.09	13	1.16	84.37	< 0.0001
Linear Mixture	*7.59*	*2*	*3.80*	*275.89*	*< 0.0001*
AB	*0.21*	*1*	*0.21*	*15.40*	*0.0014*
AC	*0.15*	*1*	*0.15*	*10.66*	*0.0052*
AD	*0.95*	*1*	*0.95*	*69.07*	*< 0.0001*
AE	*2.92*	*1*	*2.92*	*212.34*	*< 0.0001*
AF	*0.16*	*1*	*0.16*	*11.81*	*0.0037*
BD	*0.16*	*1*	*0.16*	*11.54*	*0.0040*
BE	*0.49*	*1*	*0.49*	*35.49*	*< 0.0001*
CD	*0.38*	*1*	*0.38*	*27.83*	*< 0.0001*
CE	*0.42*	*1*	*0.42*	*30.60*	*< 0.0001*
ABD	*0.097*	*1*	*0.097*	*7.05*	*0.0180*
ABE	*0.13*	*1*	*0.13*	*9.69*	*0.0071*
Residual	0.21	15	0.014		
Cor Total	15.30	28			

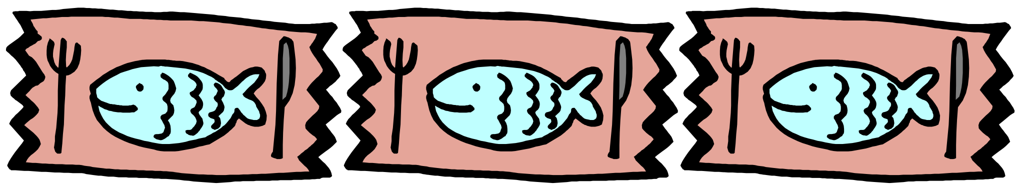
Std. Dev.	0.12	R-Squared	0.9865
Mean	1.94	Adj R-Squared	0.9748
C.V.	6.05	Pred R-Squared	0.9588
PRESS	0.63	Adeq Precision	43.583

ANOVA After Backward Reduction (Your results may differ)

Click on the ***Diagnostics*** button and examine the diagnostic graphs. They look good.

Click on the **Model Graphs** button and have a look. You will find that the outcome is essentially identical to that from the much larger User Defined design.

If you like, continue on to the numerical optimization and re-enter the target of 2.75 with limits of 2 to 3.5. The recommended formulation for ideal texture of the fish patty should be very similar to what you found before with the much larger user-defined design. Before leaving this example, you might want to try some "what ifs": Maximize or minimize various fish components (depends on relative cost), and/or minimize deep fry and oven time (to increase productivity). You can see the ultimate power of doing the crossed DOE on mixture and process.



Final comments

In all but the simplest case, a User Defined design (all possible combinations of mixture and process points) will be too large to be practical. Consider doing a d-optimal design, which provides a reasonable subset of points to estimate the model you specify.