Streamlined Models for Combined Mixture-Process Designs

KCV Models
(Kowalski, Cornell and Vining)

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KCV Model
Combining Mixture and Process Variables

- KCV models for combining mixture and process variables.
  - Example *(3M+2P)*
  - Exercise *(corndogs)*

1. Scott Kowalski , John A. Cornell & G. Geoffrey Vining (2000) A new model and class of designs for mixture experiments with process variables, *Communications in Statistics - Theory and Methods*, 29:9-10, 2255-2280.
2. Mark Anderson, Pat Whitcomb and Martin Bezener (2018), *Formulation Simplified*, Productivity Press, appendix 9A, chapter 9.

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Agenda

- **KCV models for combining mixture and process variables.**
  - Example *(3M+2P)*
  - Exercise *(corndogs)*

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Crossed Model
Combining Mixture and Process

The big reason to combine mixture components and process factors in a single DOE is to model the dependence of one on the other. The crossed model is the ultimate realization of this.

Mixture quadratic: $\eta(x) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<} \sum_{j}^{q} \beta_{ij} x_i x_j$

Process quadratic: $\eta(z) = \alpha_0 + \sum_{k=1}^{n} \alpha_k z_k + \sum_{k<} \sum_{l}^{n} \alpha_{kl} z_k z_l + \sum_{k=1}^{n} \alpha_{kk} z_k^2$

Crossed quadratic by quadratic model:

$$\eta(x,z) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<} \sum_{j}^{q} \beta_{ij} x_i x_j + \sum_{i=1}^{q} \sum_{k=1}^{n} \gamma_{ik} x_i z_k + \sum_{i<} \sum_{j}^{q} \sum_{k=1}^{n} \gamma_{ijk} x_i x_j z_k + \sum_{i}^{q} \sum_{k<} \sum_{l}^{n} \gamma_{ikl} x_i z_k z_l$$
$$+ \sum_{i<} \sum_{j}^{q} \sum_{k<} \sum_{l}^{n} \gamma_{ijkl} x_i x_j z_k z_l + \sum_{i=1}^{q} \sum_{k=1}^{n} \gamma_{ikk} x_i z_k^2 + \sum_{i<} \sum_{j}^{q} \sum_{k=1}^{n} \gamma_{ijkk} x_i x_j z_k^2$$

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Additive Model
Combining Mixture and Process

The advantage of an additive model is fewer coefficients, therefore fewer runs are required. However, the ability to model the dependence of mixture components and process factors on one another is lost.

Mixture quadratic: $\eta(x)=\sum_{i=1}^{q}\beta_i x_i+\sum_{i<}\sum_{j}^{q}\beta_{ij}x_i x_j$

Process quadratic: $\eta(z)=\alpha_0+\sum_{k=1}^{n}\alpha_k z_k+\sum_{k<}\sum_{l}^{n}\alpha_{kl}z_k z_l+\sum_{k=1}^{n}\alpha_{kk}z_k^2$

Additive quadratic and quadratic model:

$$\eta(x,z)=\sum_{i=1}^{q}\beta_i x_i+\sum_{i<}\sum_{j}^{q}\beta_{ij}x_i x_j+\sum_{k=1}^{n}\alpha_k z_k+\sum_{k<}\sum_{l}^{n}\alpha_{kl}z_k z_l+\sum_{k=1}^{n}\alpha_{kk}z_k^2$$

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Crossed vs Additive
Combining Mixture and Process

The crossed model:

- Completely links the mixture components and process factors. *I.e. all model terms are crossed.*
- This requires lots of coefficients (therefore lots of runs).

The additive model:

- Has a smaller model (requires fewer runs).
- Does not link the mixture and process factors. It does not contain any cross product terms.
- Might as well do separate designs on the mixture components and process factors.

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KCV Model
Compromise Model

A compromise model was proposed by Kowalski, Cornell and Vining[1]. In their approach the linear models are crossed and higher order terms are additive.

Cross linear models:

$$\left(\eta(x)=\sum_{i=1}^{q}\beta_i x_i \times \eta(z)=\beta_0+\sum_{k=1}^{n}\beta_i z_i\right)\rightarrow \eta(x,z)=\sum_{i=1}^{q}\beta_i x_i+\sum_{i=1}^{q}\sum_{k=1}^{n}\gamma_{ik}x_i z_k$$

Add second order terms:

$$\text{Mix: }\sum_{i<}\sum_{j}^{q}\beta_{ij}x_i x_j \quad \text{Process: }\sum_{k<}\sum_{l}^{n}\alpha_{kl}z_k z_l+\sum_{k=1}^{n}\alpha_{kk}z_k^2$$

KVC combined model:

$$\eta(x,z)=\sum_{i=1}^{q}\beta_i x_i+\sum_{i<}\sum_{j}^{q}\beta_{ij}x_i x_j+\sum_{i=1}^{q}\sum_{k=1}^{n}\gamma_{ik}x_i z_k+\sum_{k<}\sum_{l}^{n}\alpha_{kl}z_k z_l+\sum_{k=1}^{n}\alpha_{kk}z_k^2$$

Red terms from crossed linear models, **Blue** terms are additive.

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KCV Model
Compromise Model (3-Mix + 2-Process)

E.g.: If we had three mixture components and two process factors, the quadratic by quadratic KCV model is:

$$\eta(x)=\beta_1x_1+\beta_2x_2+\beta_3x_3+\beta_{12}x_1x_2+\beta_{13}x_1x_3+\beta_{23}x_2x_3$$

$$\eta(z)=\beta_0+\beta_1z_4+\beta_1z_5+\beta_{45}z_4z_5+\beta_{44}z_4^2+\beta_{55}z_5^2$$

$$\begin{aligned}\eta(x,z)=\;&\left.\begin{matrix}\beta_1x_1+\beta_2x_2+\beta_3x_3\\ +\beta_{14}x_1z_4+\beta_{24}x_2z_4+\beta_{34}x_3z_4\\ +\beta_{15}x_1z_5+\beta_{25}x_2z_5+\beta_{35}x_3z_5\end{matrix}\right\}\text{Red crossed linear models}\\ &\left.\begin{matrix}+\beta_{12}x_1x_2+\beta_{13}x_1x_3+\beta_{23}x_2x_3\\ +\beta_{45}z_4z_5+\beta_{44}z_4^2+\beta_{55}z_5^2\end{matrix}\right\}\text{Blue terms are additive}\end{aligned}$$

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KCV versus Additive Model

Compromise Model (3-Mix + 2-Process)

KCV Model

15 terms

$$\eta(x,z) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$
$$+\beta_{14} x_1 z_4 + \beta_{24} x_2 z_4 + \beta_{34} x_3 z_4$$
$$+\beta_{15} x_1 z_5 + \beta_{25} x_2 z_5 + \beta_{35} x_3 z_5$$
$$+\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$
$$+\beta_{45} z_4 z_5 + \beta_{44} z_4^2 + \beta_{55} z_5^2$$

Additive Model

11 terms

$$\eta(x,z) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$
$$+\beta_{12} x_1 x_2 + \beta_{12} x_1 x_3 + \beta_{23} x_2 x_3$$
$$+\alpha_1 z_1 + \alpha_2 z_2$$
$$+\alpha_{12} z_1 z_2 + \alpha_{11} z_1^2 + \alpha_{22} z_2^2$$

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KCV versus Crossed Model

Compromise Model (3-Mix + 2-Process)

KCV Model

15 terms

$$\eta(x,z) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$
$$+\beta_{14} x_1 z_4 + \beta_{24} x_2 z_4 + \beta_{34} x_3 z_4$$
$$+\beta_{15} x_1 z_5 + \beta_{25} x_2 z_5 + \beta_{35} x_3 z_5$$
$$+\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$
$$+\beta_{45} z_4 z_5 + \beta_{44} z_4^2 + \beta_{55} z_5^2$$

Crossed Model

36 terms

$$\eta(x,z) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<} \sum_{j}^{q} \beta_{ij} x_i x_j$$
$$+\sum_{i=1}^{q} \sum_{k=1}^{n} \gamma_{ik} x_i z_k + \sum_{i<} \sum_{j}^{q} \sum_{k=1}^{n} \gamma_{ijk} x_i x_j z_k$$
$$+\sum_{i}^{q} \sum_{k<} \sum_{l}^{n} \gamma_{ikl} x_i z_k z_l + \sum_{i<} \sum_{j}^{q} \sum_{k<} \sum_{l}^{n} \gamma_{ijkl} x_i x_j z_k z_l$$
$$+\sum_{i=1}^{q} \sum_{k=1}^{n} \gamma_{ikk} x_i z_k^2 + \sum_{i<} \sum_{j}^{q} \sum_{k=1}^{n} \gamma_{ijkk} x_i x_j z_k^2$$

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Kowalski, Cornell and Vining
KCV Combined Models

Mixture Components	Process Factors	Crossed Q by Q	Q by Q max cubic	KCV Q by Q	Additive Q plus Q
2	2	18	15	**10**	8
3	2	36	27	**15**	11
4	2	60	42	**21**	15
3	3	60	42	**21**	15
4	3	100	64	**28**	19
5	3	150	90	**36**	24
4	4	150	90	**36**	24
5	4	225	125	**45**	29
6	4	315	165	**55**	35

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KCV Model
Alternative to Ratios

KCV Model

$$\eta(x,z) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$
$$+\beta_{14} x_1 z_4 + \beta_{24} x_2 z_4 + \beta_{34} x_3 z_4$$
$$+\beta_{15} x_1 z_5 + \beta_{25} x_2 z_5 + \beta_{35} x_3 z_5$$
$$+\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$
$$+\beta_{45} z_4 z_5 + \beta_{44} z_4^2 + \beta_{55} z_5^2$$

Ratio Model

$$\eta(R,z) = \beta_0 + \beta_1 R_1 + \beta_2 R_2 + \beta_3 z_3 + \beta_4 z_4$$
$$+\beta_{13} R_1 z_3 + \beta_{14} R_1 z_4$$
$$+\beta_{23} R_2 z_3 + \beta_{24} R_2 z_4$$
$$+\beta_{12} R_1 R_2 + \beta_{11} R_1^2 + \beta_{22} R_2^2$$
$$+\beta_{34} z_3 z_4 + \beta_{33} z_3^2 + \beta_{44} z_4^2$$

Models have the same number of coefficients and similar **linear by linear links** between the components and factors.

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Agenda

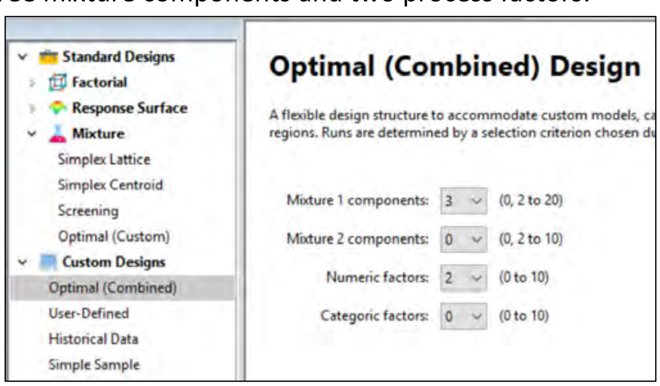
- **KCV models for combining mixture and process variables.**
  - ***Example*** ***(3M+2P)***
  - Exercise *(corndogs)*

3 Mixture + 2 Process Variables

KCV Model - Build *(page 1 of 4)*

Build a three component mixture with two process using a KCV model:

1. Three mixture components and two process factors:



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3 Mixture + 2 Process Variables

KCV Model - Build *(page 2 of 4)*

2. Enter the mixture components:

Mixture 1 components: 3 — Total: 1 — Units: — (●) Horizontal ( ) Vertical

	Name	Change	Low	High
A [Mixture]	A	Easy	0.25	0.6
B [Mixture]	B	Easy	0.1	0.4
C [Mixture]	C	Easy	0.2	0.6

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3 Mixture + 2 Process Variables

KCV Model - Build *(page 3 of 4)*

3. Enter the process factors:

Numeric factors: 2 (●) Horizontal

Categoric factors: 0 ( ) Vertical

	Name	Units	Change	Type	Levels	L[1]	L[2]
D [Numeric]	D		Easy	Continuous	N/A	-1	1
D [Numeric]	E		Easy	Continuous	N/A	-1	1

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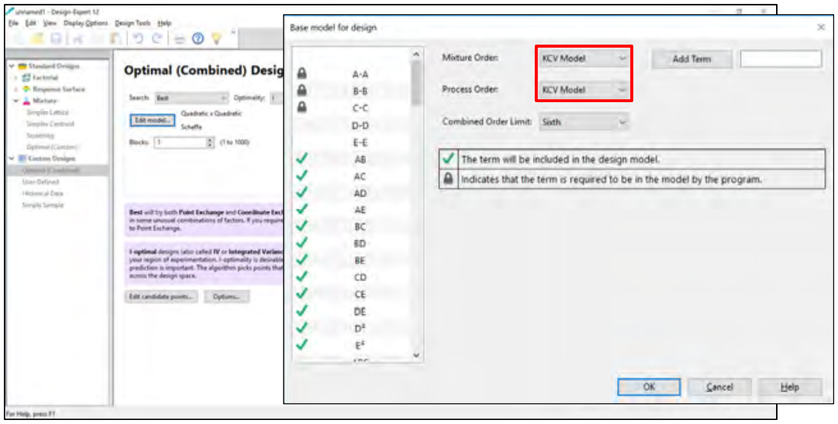
3 Mixture + 2 Process Variables
KCV Model - Build *(page 4 of 4)*

4. Change the model, "**Edit model…**", to "**KCV Model**" by "**KCV Model**":



OK | Next >> | Finish

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3 Mixture + 2 Process Variables
KCV Model – Simulate and Analyze

1. Right click on the response (R1) column header then "**Simulate…**" to "**Load an existing simulation**" and open "**KCV MP combined.simx**".

2. Analyze and model octane.

3. Find the composition and the process factor settings that maximize R1.

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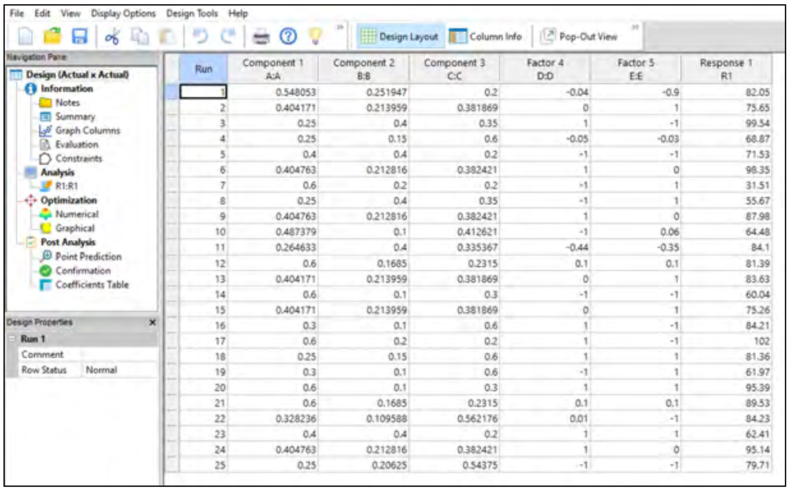
3 Mixture + 2 Process Variables
KCV Model – Design



Run	Component 1 A:A	Component 2 B:B	Component 3 C:C	Factor 4 D:D	Factor 5 E:E	Response 1 R1
1	0.548053	0.251947	0.2	-0.04	-0.9	82.05
2	0.404171	0.213959	0.381869	0	1	75.65
3	0.25	0.4	0.35	1	-1	99.54
4	0.25	0.15	0.6	-0.05	-0.03	68.87
5	0.4	0.4	0.2	-1	-1	71.53
6	0.404763	0.212816	0.382421	1	0	98.35
7	0.6	0.2	0.2	-1	1	31.51
8	0.25	0.4	0.35	-1	1	55.67
9	0.404763	0.212816	0.382421	1	0	87.98
10	0.487379	0.1	0.412621	-1	0.06	64.48
11	0.264633	0.4	0.335367	-0.44	-0.35	84.1
12	0.6	0.1685	0.2315	0.1	0.1	81.39
13	0.404171	0.213959	0.381869	0	1	83.63
14	0.6	0.1	0.3	-1	-1	60.04
15	0.404171	0.213959	0.381869	0	1	75.26
16	0.3	0.1	0.6	1	-1	84.21
17	0.6	0.2	0.2	1	-1	102
18	0.25	0.15	0.6	1	1	81.36
19	0.3	0.1	0.6	-1	1	61.97
20	0.6	0.1	0.3	1	1	95.39
21	0.6	0.1685	0.2315	0.1	0.1	89.53
22	0.328236	0.109588	0.562176	0.01	-1	84.23
23	0.4	0.4	0.2	1	1	62.41
24	0.404763	0.212816	0.382421	1	0	95.14
25	0.25	0.20625	0.54375	-1	-1	79.71

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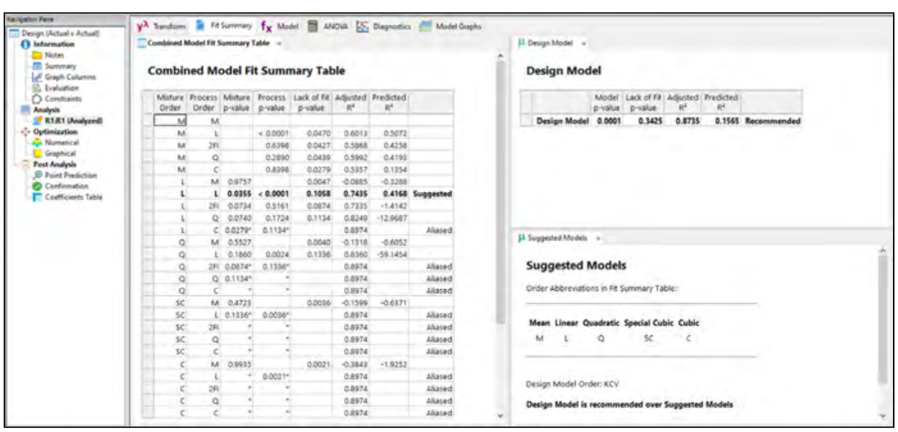
3 Mixture + 2 Process Variables
KCV Model – Fit Summary



Combined Model Fit Summary Table

Mixture Order	Process Order	Mixture p-value	Process p-value	Lack of Fit p-value	Adjusted R^2	Predicted R^2	
M	M						
M	L		< 0.0001	0.0470	0.6013	0.5072	
M	2FI		0.6398	0.0427	0.5868	0.4258	
M	Q		0.2890	0.0439	0.5992	0.4193	
M	C		0.8398	0.0279	0.5357	0.1354	
L	M	0.9757		0.0047	-0.0885	-0.3288	
L	**L**	**0.0355**	**< 0.0001**	**0.1058**	**0.7435**	**0.4168**	**Suggested**
L	2FI	0.0734	0.5161	0.0874	0.7335	-1.4142	
L	Q	0.0740	0.1724	0.1134	0.8249	-12.9687	
L	C	0.0279*	0.1134*		0.8974		Aliased
Q	M	0.5527		0.0040	-0.1318	-0.6052	
Q	L	0.1860	0.0024	0.1336	0.8360	-59.1454	
Q	2FI	0.0874*	0.1336*		0.8974		Aliased
Q	Q	0.1134*	*		0.8974		Aliased
Q	C	*	*		0.8974		Aliased
SC	M	0.4723		0.0036	-0.1599	-0.6371	
SC	L	0.1336*	0.0036*		0.8974		Aliased
SC	2FI	*	*		0.8974		Aliased
SC	Q	*	*		0.8974		Aliased
SC	C	*	*		0.8974		Aliased
C	M	0.9935		0.0021	-0.3843	-1.9252	
C	L	*	0.0021*		0.8974		Aliased
C	2FI	*	*		0.8974		Aliased
C	Q	*	*		0.8974		Aliased
C	C	*	*		0.8974		Aliased

Design Model

	Model p-value	Lack of Fit p-value	Adjusted R^2	Predicted R^2	
Design Model	**0.0001**	**0.3425**	**0.8735**	**0.1565**	**Recommended**

Suggested Models

Order Abbreviations in Fit Summary Table:

Mean	Linear	Quadratic	Special Cubic	Cubic
M	L	Q	SC	C

Design Model Order: KCV

Design Model is recommended over Suggested Models

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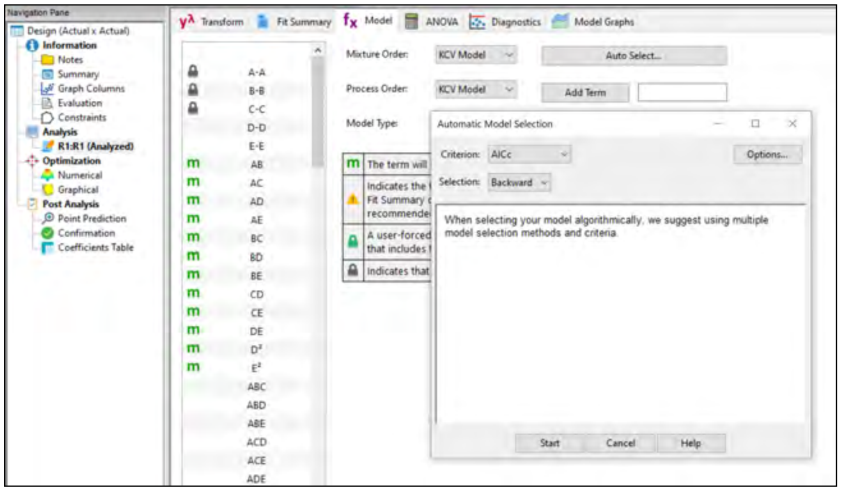
3 Mixture + 2 Process Variables

KCV Model – Model Reduction



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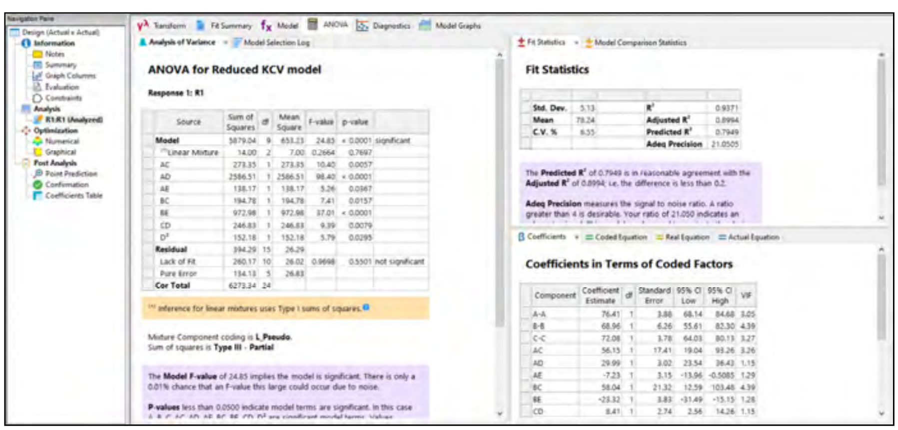
3 Mixture + 2 Process Variables

KCV Model – ANOVA



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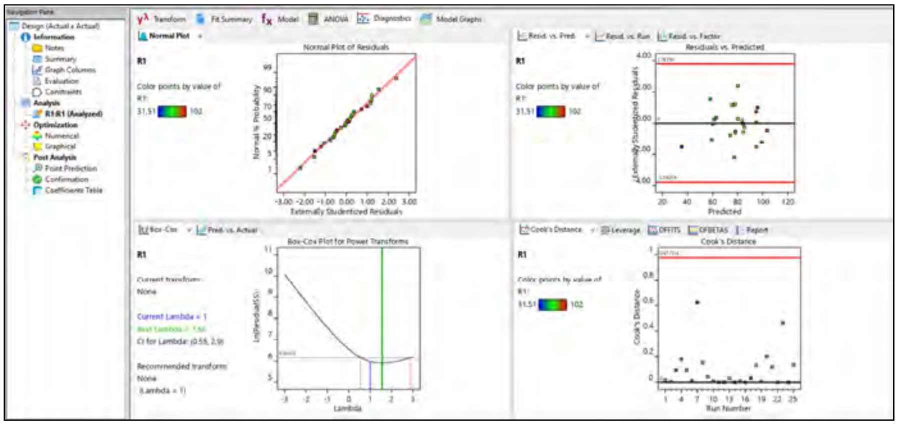
3 Mixture + 2 Process Variables
KCV Model – Diagnostics



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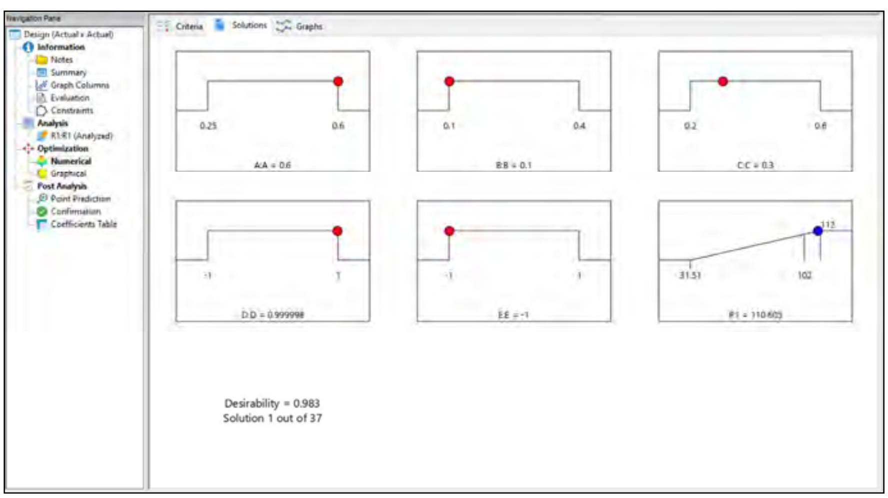
3 Mixture + 2 Process Variables
KCV Model – Numerical Optimization



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3 Mixture + 2 Process Variables
Designing for KCV Model

- The additive quadratic model has 11 coefficients.
  NO linkage between mixture components and process factors.
- The KCV quadratic model has 15 coefficients.
  The linkage between mixture components and process factors is the component by factor interactions.
- The quadratic crossed model has 36 coefficients.
  The linkage between mixture components and process factors is complete; i.e. all terms are crossed.
- The quadratic crossed model limited to cubic terms to has 27 terms.
  The linkage between mixture components and process factors is intermediate between KCV and crossed.

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Agenda

- **KCV models for combining mixture and process variables.**
  - Example *(3M+2P)*
  - **Exercise *(corndogs)***

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Corn Dogs
Combined Mixture Process Design

Vary four of the ingredients:

Components	Varied	Ingredients	Fixed
Flour	7 to 9 oz.	Baking powder	1½ teaspoons
Cornmeal	4 to 7 oz.	Salt	1 teaspoon
Sugar	1.5 to 2.5 oz.	Egg (beaten)	1
Buttermilk	9 to 11 oz.	Baking soda	½ teaspoon

Vary three process factors:

Process factors	Range
Temperature *(oven)*	175 to 195 degrees C
Time *(oven)*	3 to 5 minutes
Deep fry	45 to 75 seconds

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Corn Dogs
Combined Mixture Process Design

Model Choices

Mixture	Process	Type	Coefficients
Quadratic	Quadratic	Crossed	100
Quadratic	Quadratic	Crossed (max cubic)	64
Quadratic	2FI	Crossed	70
Quadratic	Linear	Crossed	40
Quadratic	**Quadratic**	**KCV**	**28**
Quadratic	Quadratic	Additive	20 (10+10)

Choose KCV model

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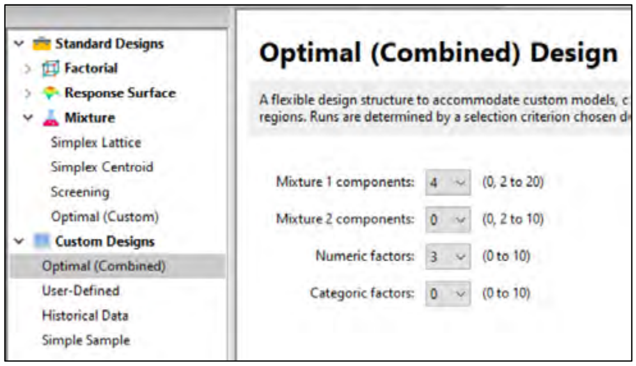
Building a Design *(KCV model)*
Corn Dogs *(page 1 of 5)*

1. Set up an Optimal combined design with 4 mixture components and 3 numeric factors:



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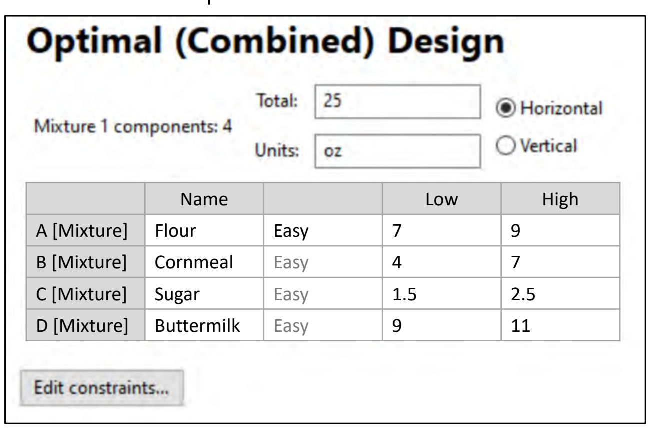
Building a Design *(KCV model)*
Corn Dogs *(page 2 of 5)*

2. Enter the mixture components:



Optimal (Combined) Design

Mixture 1 components: 4 — Total: 25 — Units: oz — (•) Horizontal ( ) Vertical

	Name		Low	High
A [Mixture]	Flour	Easy	7	9
B [Mixture]	Cornmeal	Easy	4	7
C [Mixture]	Sugar	Easy	1.5	2.5
D [Mixture]	Buttermilk	Easy	9	11

Edit constraints...

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Building a Design *(KCV model)*
Corn Dogs *(page 3 of 5)*

3. Enter the numeric factors

Optimal (Combined) Design

Numeric factors: 3 ◉ Horizontal

Categoric factors: 0 ○ Vertical

	Name	Units	Change	Type	Levels	L[1]	L[2]
E [Numeric]	Temperature	deg C	Easy	Continuous	N/A	175	195
F [Numeric]	Time	minutes	Easy	Continuous	N/A	3	5
G [Numeric]	Deep fry	Seconds	Easy	Continuous	N/A	45	75

Edit constraints...

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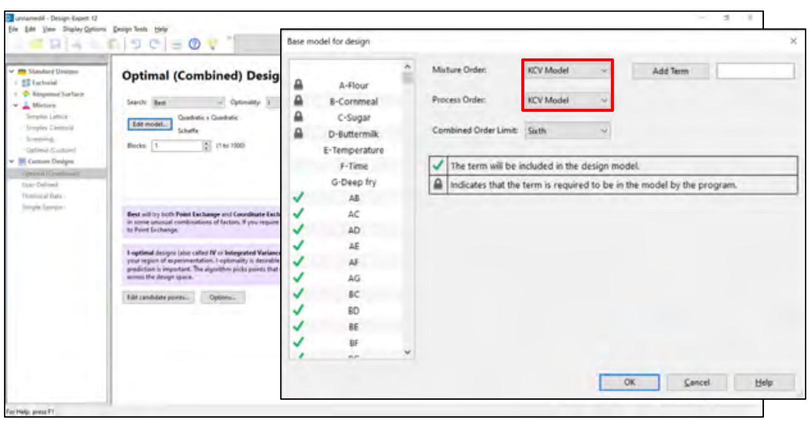
Building a Design *(KCV model)*
Corn Dogs *(page 4 of 5)*

4. Change the model, "**Edit model…**", to "**KCV Model**" by "**KCV Model**":



OK and then Next >>

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Building a Design *(KCV model)*
Corn Dogs *(page 5 of 5)*

8. Enter the responses:

Responses: 2 (1 to 999)

	Name	Units
	Taste	1 - 5
	Texture	1 - 5

Finish

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Corn Dogs
Analyze and Optimize

1. Right click on the column header of the response and "**Simulate…**" to "**Load an existing simulation**" and open "**corn dog KCV.simx**".
2. Analyze – *Hint: Use "AICc" with "Backward" selection.*
3. Optimize:
   - Maximize Taste: lower limit = 3, upper limit = 5
   - Maximize Texture : lower limit = 3, upper limit = 5

   Scale for responses (compared to competitor's corn dog):
   1. worse
   2. somewhat worse
   3. same as competition
   4. somewhat better
   5. better

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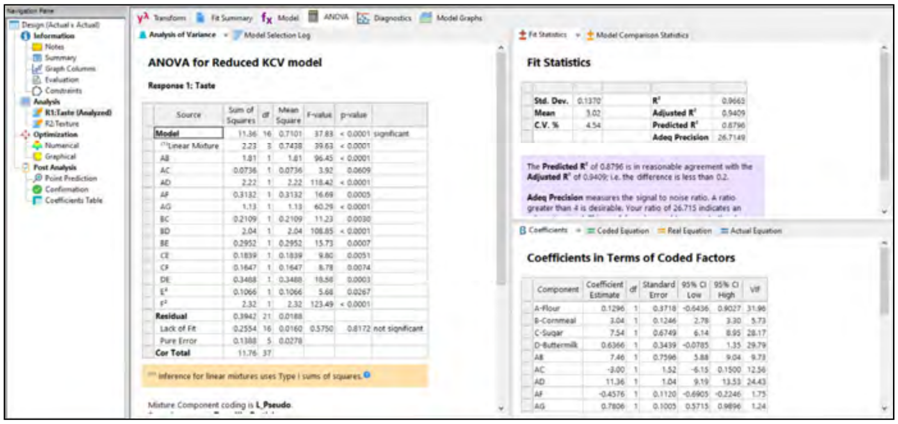
Corn Dogs
Reduced KCV Model – Taste



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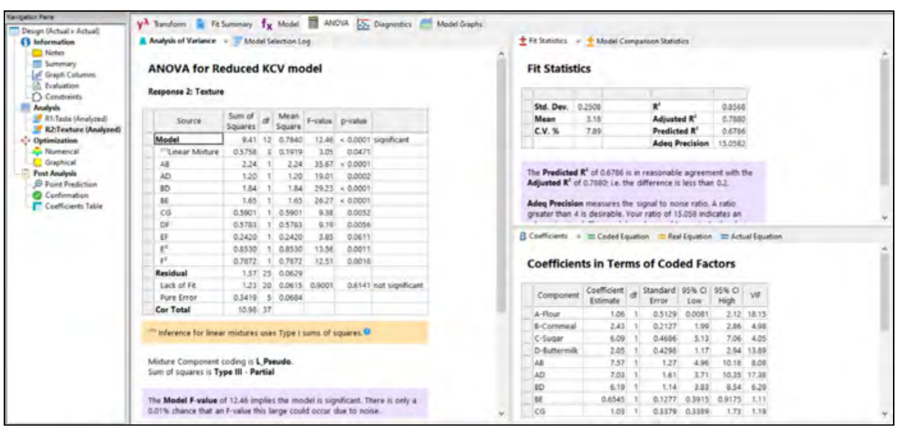
Corn Dogs
Reduced KCV Model – Texture



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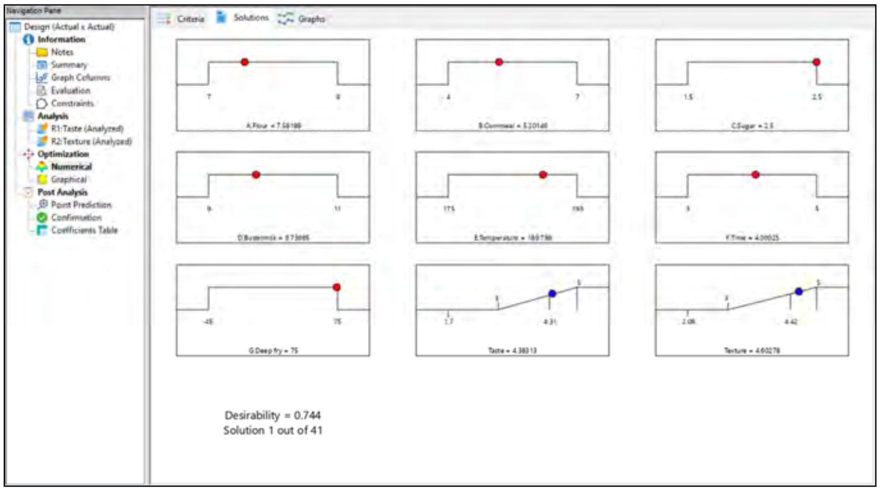
Corn Dogs
KCV Model – Numerical Optimization



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Corn Dogs
KCV Model – Summary

- The additive quadratic model has 20 coefficients.
  NO linkage between mixture components and process factors.
- The KCV quadratic model has 28 coefficients.
  The linkage between mixture components and process factors is the component by factor interactions.
- The quadratic crossed model has 100 coefficients.
  The linkage between mixture components and process factors is complete; i.e. all terms are crossed.
- The quadratic crossed model limited to cubic terms to has 64 terms.
  The linkage between mixture components and process factors is intermediate between KCV and crossed.

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What's Next?

- ✓ Next Up: Webinar on "Multiple Response Optimization" in May 2020
- ✓ Watch previously recorded webinars from our website *(see next slide for some of my favorite topics)*
- ✓ Attend a public workshop, or bring us on-site!

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Recorded Webinars
Existing DX features

- Sizing for precision.
  Webinars: *Sizing Mixture (RSM) Designs for Adequate Precision via Fraction of Design Space (FDS)* and *Unleashing Evaluation: Giving Perspective to Power, Precision, and Problems*.
- Multilinear constraints (MLCs) and non-linear constraints.
  Webinar: *Advanced Tools for Building Designs for Irregularly Shaped DOE Spaces.*
- Propagation of error (POE).
  Webinar: *Overview of Robust Design, Propagation of Error, and Tolerance Analysis.*
- Optimization using Cpk and Ppk.
  Webinar: *Practical DOE – "Tricks of the Trade"*.
- Using intervals to frame your operating space.
  Webinar: *Quality by Design (QbD) Space for Pharmaceuticals and Beyond*.

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Thank You for Attending!
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