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7-Component Mixture Design with Additional Constraints

The 7 components come in 3 types of material; A, B, & C
3 of type A, 2 of type B, and 2 of type C. (perhaps A is three solvents, or three sugars, etc.)

All of type A must make up between 20% and 36% of the final blend. Less than 20% and maybe the viscosity is too low. Because we are interested in minimizing the number of components in the final blend (cheaper to blend/stock fewer components), we want to allow formulations that consist of just one type of A component and so ranges will all be from 0% to 36%. Combinations of two or three types of A are to be considered because combinations may lead to improved product properties.

Ranges on a proportion scale for A1, A2, and A3 are:

A1:	0	0.36
A2	0	0.36
A3:	0	0.36

Additional constraints are A1 + A2 + A3 >= 0.20
A1 + A2 + A3 <= 0.36

The amount of type B must be between 10% and 24% of the final blend. Once again we want to consider trials that consist of just one type of B and so a low limit of 0% will be used for both B component types. Knowledge of the chemistry (or maybe safety guidelines) requires that the ratio of B1 to B2 be less than or equal to 3 to 1.

Ranges for B1 and B2 are:

B1:	0	0.24
B2	0	0.24

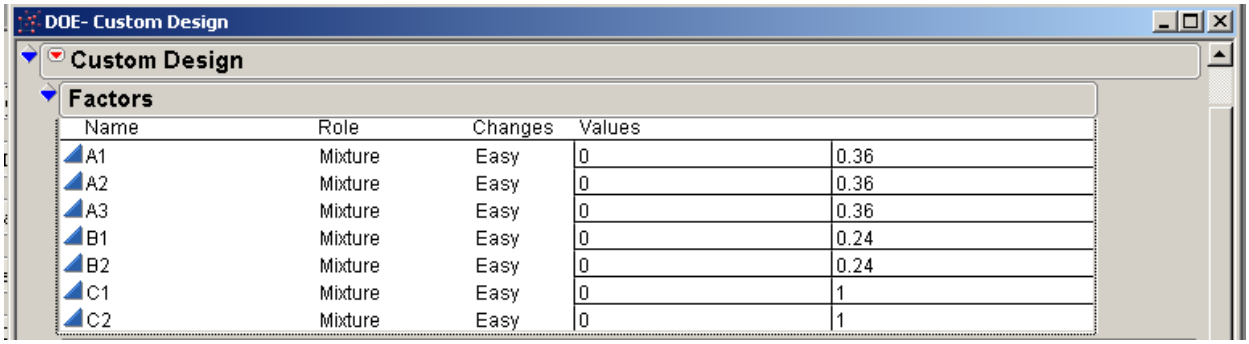
Additional constraints are: B1 + B2 >= 0.10
B1 + B2 <= 0.24
B1/B2 <= 3/1
This third constraint can be rewritten as B1 <= 3*B2 or B1 - 3*B2 <= 0

The amounts of type C have no additional constraints and are materials that are more or less used to take up the slack in the design. They may be fillers or diluents, etc. The ranges for C1 and C2 are set to 0 to 1 even though we know we could calculate that the high end must be no more than 70% since the minimum sum of the type A is 20% and the minimum sum of the type B is 10%.

Ranges for C1 and C2 are:

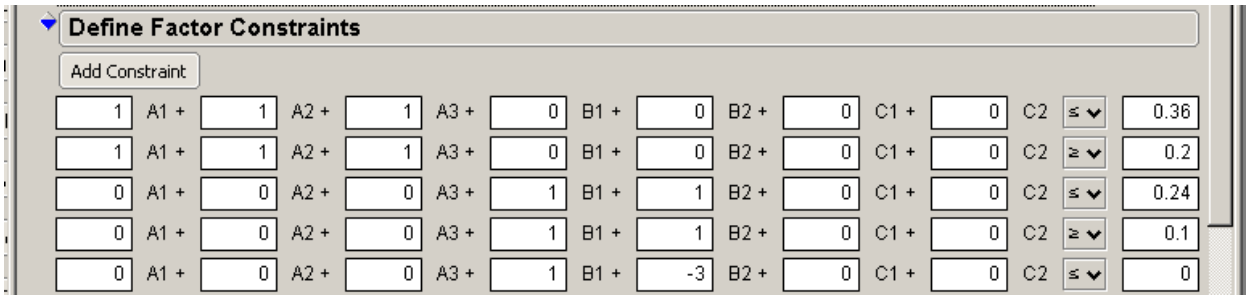
C1:	0	1
C2:	0	1

In JMP the ranges go in as below:

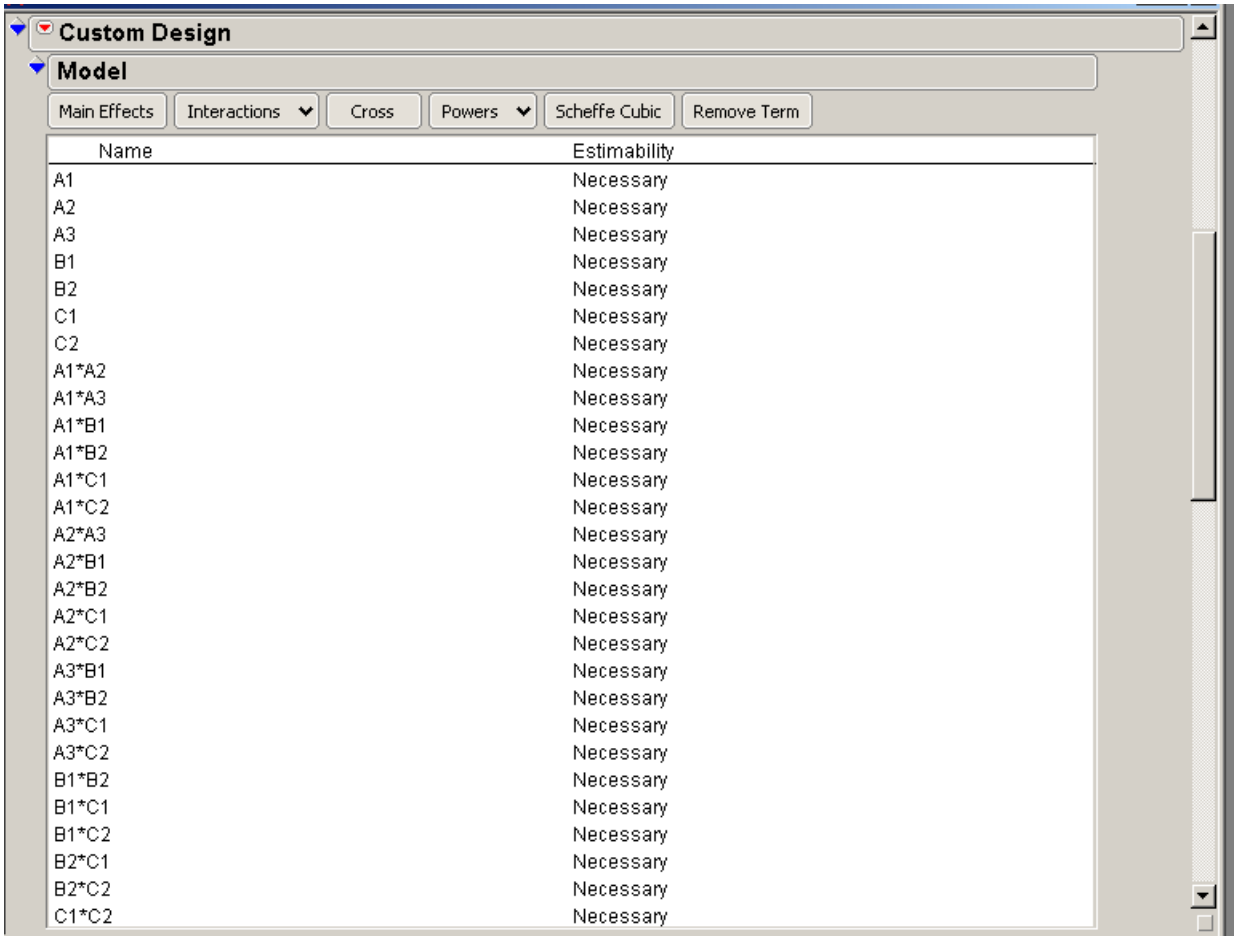


Name	Role	Changes	Values	
A1	Mixture	Easy	0	0.36
A2	Mixture	Easy	0	0.36
A3	Mixture	Easy	0	0.36
B1	Mixture	Easy	0	0.24
B2	Mixture	Easy	0	0.24
C1	Mixture	Easy	0	1
C2	Mixture	Easy	0	1

The constraints go in as below:



The full mixture interaction model (also known as the Scheffe quadratic model) is shown below:



Name	Estimability
A1	Necessary
A2	Necessary
A3	Necessary
B1	Necessary
B2	Necessary
C1	Necessary
C2	Necessary
A1*A2	Necessary
A1*A3	Necessary
A1*B1	Necessary
A1*B2	Necessary
A1*C1	Necessary
A1*C2	Necessary
A2*A3	Necessary
A2*B1	Necessary
A2*B2	Necessary
A2*C1	Necessary
A2*C2	Necessary
A3*B1	Necessary
A3*B2	Necessary
A3*C1	Necessary
A3*C2	Necessary
B1*B2	Necessary
B1*C1	Necessary
B1*C2	Necessary
B2*C1	Necessary
B2*C2	Necessary
C1*C2	Necessary

Four rows of JMP's 33-unique trial custom design for a mixture interaction model with 5 constraints are shown below:

	A1	A2	A3	B1	B2	C1	C2
1	0.2	0	0	0	0.24	0	0.56
2	0.30659522	0.0445548	0.00884998	0.07284811	0.02715189	0.27557107	0.26442893
3	0	0.15303804	0.20696196	0.18	0.06	0.12428611	0.27571389
4	0	0	0.36	0.18	0.06	0.4	0

NOTE:

1) all trials sum to 1.0000
2) trial #1 has only three components; 1 each of type A, B, & C (low cost to manufacture?)
3) trial #1 has at least 20% of A and no more than 24 % of B
4) trial #2 has all 7 components in the blend
5) trial #3 has two of the three type A components
6) trial #4 has no more than 36% of type A, and no more than 24% of type B, AND B1 is no more than 3 times B2

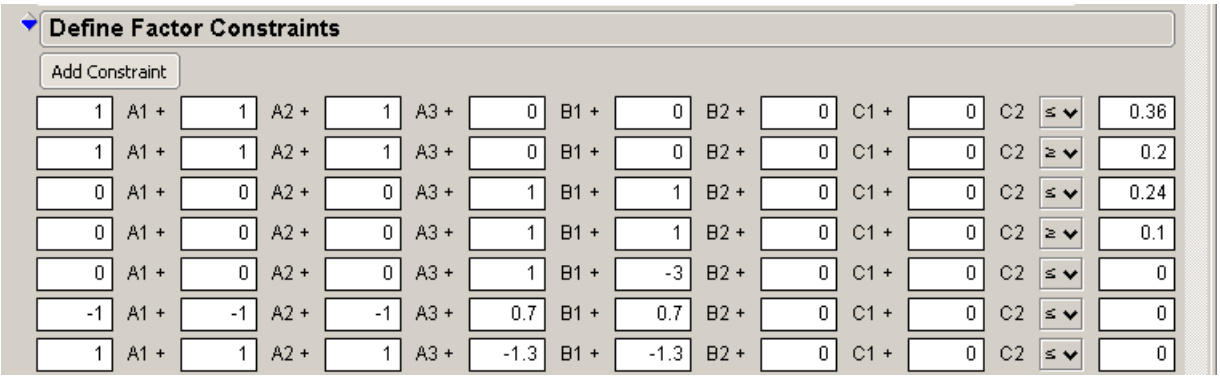
Examining the design someone notes that some trials fall outside the set of conditions that the ratio of the TOTAL "A" over the TOTAL "B" must be between 0.7 and 1.3. Again, knowledge of the chemistry leads you to want the design trials to meet these constraints. These two constraints can be written as:

(A1 + A2 + A3)/(B1 + B2) >= 0.7
(A1 + A2 + A3)/(B1 + B2) <= 1.3

By clearing fractions and rearranging sides of the inequality, these can be rewritten as:

-(A1 + A2 + A3) + 0.7*(B1 + B2) <= 0
(A1 + A2 + A3) - 1.3*(B1 + B2) < = 0

and added to the previous five constraints as shown below:



A new design is created with the additional two constraints. Four rows of JMP's 33 unique trial custom design for a quadratic model are shown below:

	A1	A2	A3	B1	B2	C1	C2
1	0.2	0	0	0	0.24	0.56	0
2	0.25793285	0.01416455	0.0399026	0.00159526	0.23840474	0.20748221	0.24051779
3	0.14431949	0	0.16768051	0.18	0.06	0	0.448
4	0	0.2	0	0.18	0.06	0	0.56
5	0.312	0	0	0.18	0.06	0.448	0
6	0	0	0.2	0	0.15384615	0	0.64615385
7	0.25852287	0	0	0.11609223	0.08277152	0	0.54261338

NOTE: As before (albeit with different trial numbers this time) we see:

1) all trials sum to 1.0000
2) trial #1 has only three components; 1 each of type A, B, & C (low cost to manufacture?)
3) trial #1 has at least 20% of A and no more than 24 % of B
4) trial #2 has all 7 components in the blend
5) trial #3 has two of the three type A components
6) trial #4 has no less than 20% of type A, and no more than 24% of type B, AND B1 is no more than 3 times B2

BUT ALSO because of the two new constraints

7) trial #6 has A3 no more than 1.3 times B2
8) trial #7 has A1 no more than 1.3 times (B1 + B2)

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