Création & analyse d'information
Conseil, études & formation en statistique

Philippe **Pagès**
19 rue Pasteur
94170 Le Perreux
Tel : 06.72.95.49.11
philippe.pages@neuf.fr
SIRET : 449 514 355 00014
APE: 8559A
TVA Intracommunautaire :
FR 92 449 514 355
Agrément formation continue :
11 94 06 444 94

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Evaluating a perturbated and evolving Design

An experimenter wants to study the effects of six numerical factors:

Factor name	Unit	Min(initial)	Max (initial)
X – G percent	%	0.45	0.65
R – Y ratio	%	75.5	76.0
R – Mw	g/mol	To be defined	To be defined
Acid amount	µL	300	700
Stirring speed	rpm	650	750
X – Add time	minutes	3	6

R & X are to materials to be used.
Other Factors are obvious.

- "X – G percent" is the percent of gas "G" in "X"
  It's obtained by a gasification process which isn't perfectly mastered so it will vary in an unknown range with regard to the target.
- "X – Add time" is the time necessary to introduce "X" into the final product.
  It's also not perfectly mastered so it will vary in an unknown range with regard to the target.
- "Stirring speed" is also not perfectly mastered so it will vary in an unknown range with regard to the target.
- ✓ "Acid amount" is perfectly mastered and will not vary at all.

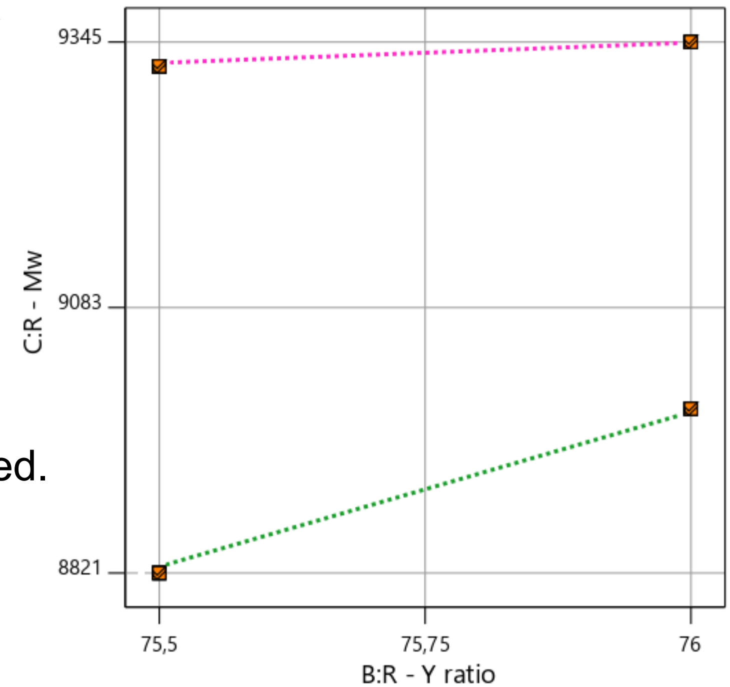
The variations of the three first Factors with regard to their targets will be known at the end only.

An experimenter wants to study the effects of six numerical factors:

"R – Y ratio" is the ratio of a "Y" component in "R".
"R – Mw" is the Molecular Weight of "R".

Those two Factors aren't independent of each other : they will be defined using four available batches of "R" presenting "extreme" combinations of the two characteristics:

- "R – Y ratio" : two batches present a precise value of 75.5 and the two other one of 76.0; this small variation range is suspected to be very influent
- "R – Mw":
  - for the two batches with "R – Y ratio" = 75.5, the "extreme" values are respectively 8821 (Min) & 9321 (Max)
  - for the two batches with "R – Y ratio" = 76.0, the "extreme" values are respectively 8983 (Min) & 9345 (Max)



This situation generates a correlation between both Factors (r = 0.281); thus a classical orthogonal design cannot be used.

Moreover:

- the available quantity of batch [75.5 / 8821] is greater than the one of the three other batches thus it would be more interesting to use a "unbalanced" design than a "balanced" one.
- there is not a fifth batch with intermediate values of "R – Y ratio" and "R – Mw" (something around [75.75 / 9100]) so it's impossible to run "Centre Points".
  It was decided to include "Verification Points" spread out in the design, one for every "R" batch at the theoretical Centre of the four other Factors.

An experimenter wants to study the effects of six numerical factors:

This experimenter suspects that at least some order 2 interactions (2FI) will exist but don't know which ones. So, it would like to estimate all of them.
But it also wishes to realize a number of runs as small as possible.

For six factors the number of coefficients of the 2FI model is 22 (constant: 1 – Main Effects: 6 – 2FI:(6*(6-1)/2)=15) thus the minimum of different runs to perform is 22, to which possible Centre or Verification points can be added.

In its "Factorial" entry Design Expert proposes a "Min-Run Characterize" design ("Minimum Run Resolution V Characterization Design" ; called "Min-Run Res V" in former versions) that comprises 22 Runs for six Factors and thus addresses the need.
"Resolution V" means that 2FI will only be aliased with three-factor (3FI) and higher interactions.
This design is "equireplicated" ("balanced"): both levels of every factor are tested the same number of time (11 in this case).
One can also find in the literature a "Rechtschaffner matrix" that also comprises 22 Runs for six Factors and thus also addresses the need.
It's also "Resolution V" but isn't "equireplicated" (it's "unbalanced"): one level of every factor is tested 10 times and the other one 12. So it might be possible with this "RS matrix" to built a design in which more try would be done with the batch [75.5 / 8821] than with the other ones.

An experimenter wants to study the effects of six numerical factors:

As 22 isn't a power of 2, both the "Min-Run Characterize" design and the "Rechtschaffner matrix" cannot be orthogonal and are thus "imperfect".

This raises one question **before** running the experiment :

- which of those two matrices is **a priori** the closest to orthogonality?
  To reduce the presentation we will not discuss this point.

In those standard matrices the high and low levels of every Factor are the same for all runs.
So it will be necessary to correct the "R – Mw" levels according to the "R – Y ratio" ones.
This raises two questions **before** running the experiment :

- which of those two matrices is the closest to orthogonality **after correction**?
- does the fact of modifying the Norm of the corrected Factor alleviate this problem?

It was decided to add "Verification points" to the corrected design.
This raises one more questions **before** running the experiment :

- does the fact of taking those "Verification points" into account for fitting the model (consider them as "Normal points") modifies orthogonality and is it for the better or for the worse?

Moreover don't forget that three of the remaining Factors ("X – G percent" ; "X – Add time" ; "Stirring speed"). aren't correctly mastered and will probably vary regarding the targets.
This raises three additional questions **after** running the experiment :

- how much do those (possible) variations perturbate orthogonality for the selected design?
- is it for the better or for the worse?
- is it possible to compensate those (possible) perturbations?

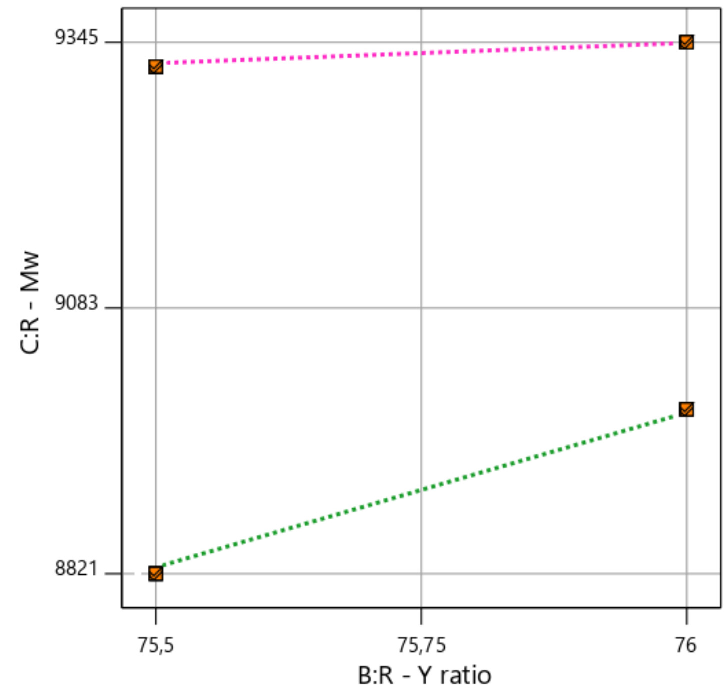
An experimenter wants to study the effects of six numerical factors:

Instead of correcting some levels of an existing matrix and even if the dotted lines drawn on the graph beside aren't actual "Constraints" (*) they can be used "as if" to generate a D-Optimal design with 22 runs, if possible with more runs with the batch [75.5 / 8821] than with the other ones.

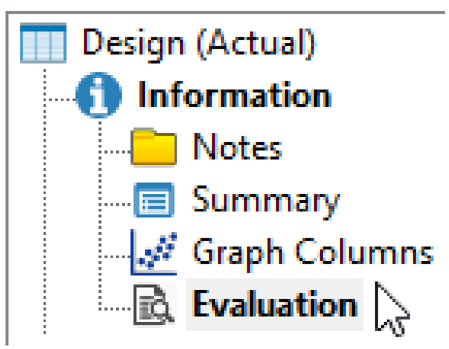
(*) future "R" batches can exhibit "Y ratio" and "Mw" outside those lines and it's interesting to be able to predict values, even imperfectly, in the unexplored corners of the design space and beyond.

This raises one question **before** running the experiment :

- is this D-Optimal design closer to orthogonality than a corrected standard matrix?



All those questions can get an answer by the use of the "**Evaluation**" procedure of "**Design Expert**".



Creating and correcting a

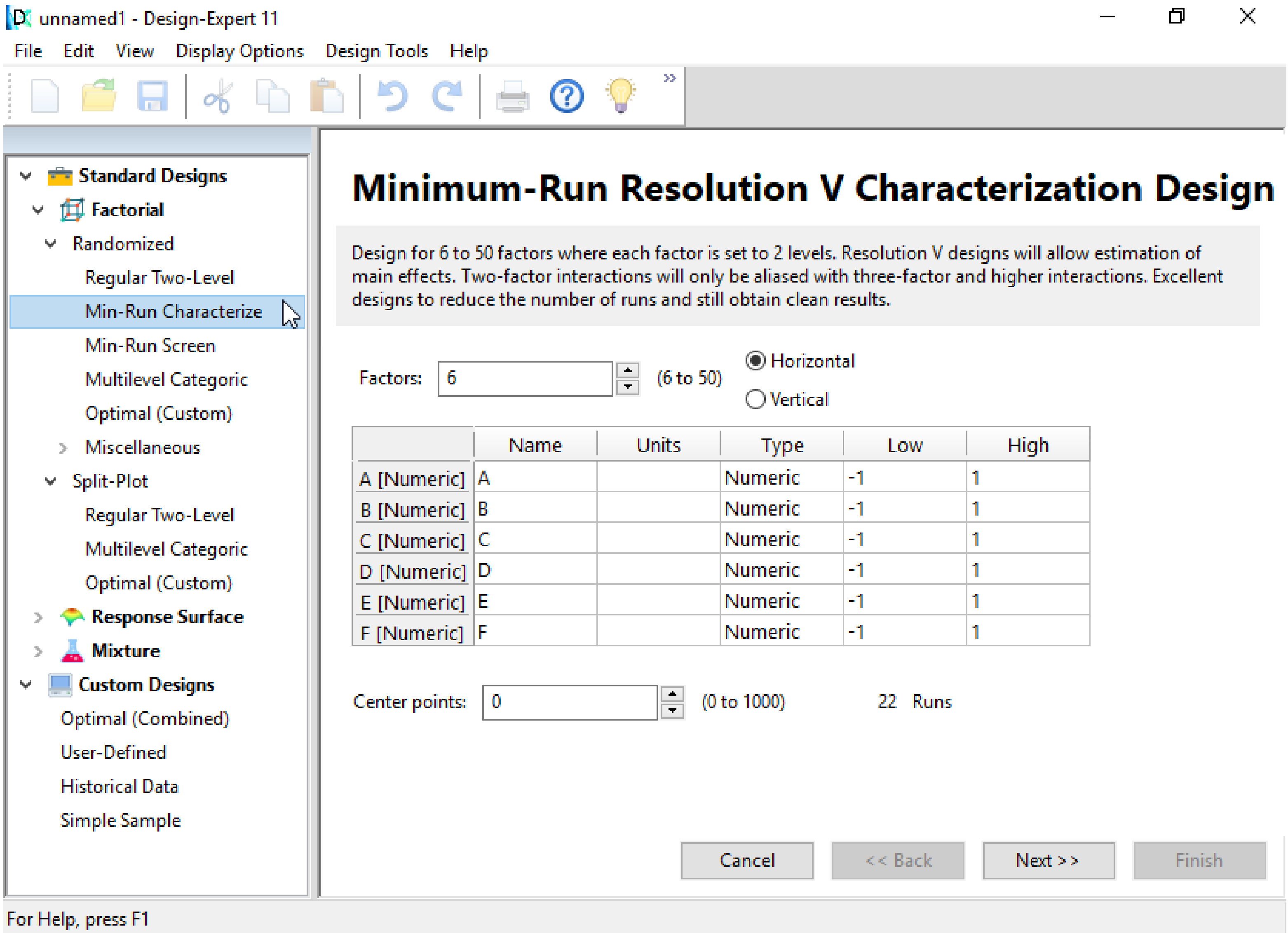
Minimum Run Resolution V Characterization Design

Evaluating it

<u>after “R – Mw” correction</u>

including and excluding Verification Points

Minimum Run Resolution V Characterization Design
Design Creation



Minimum Run Resolution V Characterization Design

Design Creation – Factors definition

Factors: 6 (6 to 50)

Horizontal

Vertical

	Name	Units	Type	Low	High
A [Numeric]	X - G percent	%	Numeric	0,45	0,65
B [Numeric]	R - Y ratio	%	Numeric	75,5	76
C [Numeric]	R - Mw	g/mol	Numeric	8821	9345
D [Numeric]	Acid amount	µL	Numeric	300	700
E [Numeric]	Stirring speed	rpm	Numeric	650	750
F [Numeric]	X - Add time	minutes	Numeric	3	6

Initial limits for “R _ Mw” set to extreme Min. & Max.
They will be changed afterwards as well as the “Norm”

Next >>

Center points: 4 (0 to 1000) 26 Runs

“Center points” will be modified to become “Verification points”.

The “Factorial Effects Aliases” panel expresses the fact that :

- every “Main Effect” is correlated with the same coefficient with all “3FIs” (order 3 Interactions) in which it is not involved
- …

Factorial Effects Aliases

Factorial Effects Aliases

Estimated Term	Aliased Terms
Intercept	= Intercept
A	= A + 0,333 * BCD + 0,333 * BCE + 0,333 * BCF - 0,333 * BDE - 0,333 * BDF - 0,333 * BEF
	- 0,333 * CDE - 0,333 * CDF - 0,333 * CEF + 0,333 * DEF
B	= B + 0,333 * ACD + 0,333 * ACE + 0,333 * ACF - 0,333 * ADE - 0,333 * ADF - 0,333 * AEF
	- 0,333 * CDE - 0,333 * CDF - 0,333 * CEF + 0,333 * DEF
C	= C + 0,333 * ABD + 0,333 * ABE + 0,333 * ABF - 0,333 * ADE - 0,333 * ADF - 0,333 * AEF
	- 0,333 * BDE - 0,333 * BDF - 0,333 * BEF + 0,333 * DEF
D	= D + 0,333 * ABC - 0,333 * ABE - 0,333 * ABF - 0,333 * ACE - 0,333 * ACF + 0,333 * AEF
	- 0,333 * BCE - 0,333 * BCF + 0,333 * BEF + 0,333 * CEF
E	= E + 0,333 * ABC - 0,333 * ABD - 0,333 * ABF - 0,333 * ACD - 0,333 * ACF + 0,333 * ADF
	- 0,333 * BCD - 0,333 * BCF + 0,333 * BDF + 0,333 * CDF
F	= F + 0,333 * ABC - 0,333 * ABD - 0,333 * ABE - 0,333 * ACD - 0,333 * ACE + 0,333 * ADE

Minimum Run Resolution V Characterization Design

Design Creation – Factorial Effects Aliases

AB	= AB - 0,333 * ACD - 0,333 * ACE - 0,333 * ACF + 0,333 * ADE + 0,333 * ADF
	+ 0,333 * AEF - 0,333 * BCD - 0,333 * BCE - 0,333 * BCF + 0,333 * BDE
	+ 0,333 * BDF + 0,333 * BEF - 0,333 * CDE - 0,333 * CDF - 0,333 * CEF
	+ 0,333 * DEF
AC	= AC - 0,333 * ABD - 0,333 * ABE - 0,333 * ABF + 0,333 * ADE + 0,333 * ADF
	+ 0,333 * AEF - 0,333 * BCD - 0,333 * BCE - 0,333 * BCF - 0,333 * BDE
	- 0,333 * BDF - 0,333 * BEF + 0,333 * CDE + 0,333 * CDF + 0,333 * CEF
	+ 0,333 * DEF
AD	= AD - 0,333 * ABC + 0,333 * ABE + 0,333 * ABF + 0,333 * ACE + 0,333 * ACF
	- 0,333 * AEF + 0,333 * BCD - 0,333 * BCE - 0,333 * BCF - 0,333 * BDE
	- 0,333 * BDF + 0,333 * BEF - 0,333 * CDE - 0,333 * CDF + 0,333 * CEF
	+ 0,333 * DEF
AE	= AE - 0,333 * ABC + 0,333 * ABD + 0,333 * ABF + 0,333 * ACD + 0,333 * ACF
	- 0,333 * ADF - 0,333 * BCD + 0,333 * BCE - 0,333 * BCF - 0,333 * BDE
	+ 0,333 * BDF - 0,333 * BEF - 0,333 * CDE + 0,333 * CDF - 0,333 * CEF
	+ 0,333 * DEF
AF	= AF - 0,333 * ABC + 0,333 * ABD + 0,333 * ABE + 0,333 * ACD + 0,333 * ACE
	- 0,333 * ADE - 0,333 * BCD - 0,333 * BCE + 0,333 * BCF + 0,333 * BDE
	- 0,333 * BDF - 0,333 * BEF + 0,333 * CDE - 0,333 * CDF - 0,333 * CEF
	+ 0,333 * DEF
BC	= BC - 0,333 * ABD - 0,333 * ABE - 0,333 * ABF - 0,333 * ACD - 0,333 * ACE
	- 0,333 * ACF - 0,333 * ADE - 0,333 * ADF - 0,333 * AEF + 0,333 * BDE
	+ 0,333 * BDF + 0,333 * BEF + 0,333 * CDE + 0,333 * CDF + 0,333 * CEF
	+ 0,333 * DEF
BD	= BD - 0,333 * ABC + 0,333 * ABE + 0,333 * ABF + 0,333 * ACD - 0,333 * ACE
	- 0,333 * ACF - 0,333 * ADE - 0,333 * ADF + 0,333 * AEF + 0,333 * BCE
	+ 0,333 * BCF - 0,333 * BEF - 0,333 * CDE - 0,333 * CDF + 0,333 * CEF
	+ 0,333 * DEF
BE	= BE - 0,333 * ABC + 0,333 * ABD + 0,333 * ABF - 0,333 * ACD + 0,333 * ACE
	- 0,333 * ACF - 0,333 * ADE + 0,333 * ADF - 0,333 * AEF + 0,333 * BCD
	+ 0,333 * BCF - 0,333 * BDF - 0,333 * CDE + 0,333 * CDF - 0,333 * CEF
	+ 0,333 * DEF
BF	= BF - 0,333 * ABC + 0,333 * ABD + 0,333 * ABE - 0,333 * ACD - 0,333 * ACE
	+ 0,333 * ACF + 0,333 * ADE - 0,333 * ADF - 0,333 * AEF + 0,333 * BCD
	+ 0,333 * BCE - 0,333 * BDE + 0,333 * CDE - 0,333 * CDF - 0,333 * CEF
	+ 0,333 * DEF
CD	= CD - 0,333 * ABC + 0,333 * ABD - 0,333 * ABE - 0,333 * ABF + 0,333 * ACE
	+ 0,333 * ACF - 0,333 * ADE - 0,333 * ADF + 0,333 * AEF + 0,333 * BCE
	+ 0,333 * BCF - 0,333 * BDE - 0,333 * BDF + 0,333 * BEF - 0,333 * CEF
	+ 0,333 * DEF
CE	= CE - 0,333 * ABC - 0,333 * ABD + 0,333 * ABE - 0,333 * ABF + 0,333 * ACD
	+ 0,333 * ACF - 0,333 * ADE + 0,333 * ADF - 0,333 * AEF + 0,333 * BCD
	+ 0,333 * BCF - 0,333 * BDE + 0,333 * BDF - 0,333 * BEF - 0,333 * CDF
	+ 0,333 * DEF
CF	= CF - 0,333 * ABC - 0,333 * ABD - 0,333 * ABE + 0,333 * ABF + 0,333 * ACD
	+ 0,333 * ACE + 0,333 * ADE - 0,333 * ADF - 0,333 * AEF + 0,333 * BCD
	+ 0,333 * BCE + 0,333 * BDE - 0,333 * BDF - 0,333 * BEF - 0,333 * CDE
	+ 0,333 * DEF

DE	= DE - 0,333 * ABC - 0,333 * ABD - 0,333 * ABE + 0,333 * ABF - 0,333 * ACD
	- 0,333 * ACE + 0,333 * ACF + 0,333 * ADF + 0,333 * AEF - 0,333 * BCD
	- 0,333 * BCE + 0,333 * BCF + 0,333 * BDF + 0,333 * BEF + 0,333 * CDF
	+ 0,333 * CEF
DF	= DF - 0,333 * ABC - 0,333 * ABD + 0,333 * ABE - 0,333 * ABF - 0,333 * ACD
	+ 0,333 * ACE - 0,333 * ACF + 0,333 * ADE + 0,333 * AEF - 0,333 * BCD
	+ 0,333 * BCE - 0,333 * BCF + 0,333 * BDE + 0,333 * BEF + 0,333 * CDE
	+ 0,333 * CEF
EF	= EF - 0,333 * ABC + 0,333 * ABD - 0,333 * ABE - 0,333 * ABF + 0,333 * ACD
	- 0,333 * ACE - 0,333 * ACF + 0,333 * ADE + 0,333 * ADF + 0,333 * BCD
	- 0,333 * BCE - 0,333 * BCF + 0,333 * BDE + 0,333 * BDF + 0,333 * CDE
	+ 0,333 * CDF

Watch for aliases among terms you need to estimate.

The “Factorial Effects Aliases” panel expresses the fact that :

- …
- every “2FI” (order 2 Interaction) is correlated with the same coefficient with all “3FIs” (order 3 Interactions) in which it is not involved

There are also correlations between “Main Effects” and “2FIs” which aren’t displayed in this panel.
“Evaluation” will allow to discover them.

Next >>

Minimum Run Resolution V Characterization Design
Design Creation – Responses definition & Power calculation

Optional Power Wizard: For each response, you may enter the minimum change the design should detect as statistically significant and the estimated standard deviation (generally obtained from historical data). The ratio will then be calculated in the Delta/Sigma field. Press **Next** to see the calculated power for each response.

Responses: 1 (1 to 999) Edit Model... ☐ Edit response types

Name	Units	Diff. to detect Delta("Signal")	Est. Std. Dev. Sigma("Noise")	Delta/Sigma (Signal/Noise Ratio)
R1		2	1	2

Let suppose there are 3 Responses

Responses: 3 (1 to 999) Edit Model... ☐ Edit response types

Name	Units	Diff. to detect Delta("Signal")	Est. Std. Dev. Sigma("Noise")	Delta/Sigma (Signal/Noise Ratio)
Particles Size	nm	1	1	1
EE	%	2	1	2
Impurities	%	3	1	3

Let define them.

Model for Power Evaluation

Intercept
A-X - G percent
B-R - Y ratio
C-R - Mw
D-Acid amount
E-Stirring speed
F-X - Add time
AB

Process Order: Main Effects

The term will be included in the power calculation.

Indicates that the term is required to be in the model by the program.

This panel allows Power calculation.

As defined it asks the questions:

What is the Power of this design if :

- "Signal" (Effect) is the same size as "Noise" (Residual Sigma)?
- "Signal" is twice the "Noise"?
- "Signal" is three times the "Noise"?

for the default "Main Effects" model.
(Remind that this design is intended to estimate "2FI" also)

Next >>

Minimum Run Resolution V Characterization Design
Design Creation – Power calculation

Warning: Italicized signal to noise information was not changed from the default. The power reported for this response may not accurately reflect your process.

Design Power

Name	Units	Delta (Signal)	Sigma (Noise)	Signal/Noise	Power for A	Power for B	Power for C	Power for D	Power for E	Power for F
Particles Size	nm	1	1	1	59,2%	59,2%	59,2%	59,2%	59,2%	59,2%
EE	%	*2*	*1*	*2*	99,2%	99,2%	99,2%	99,2%	99,2%	99,2%
Impurities	%	3	1	3	99,9%	99,9%	99,9%	99,9%	99,9%	99,9%

Power is reported at a 5,0% alpha level to detect the specified signal/noise ratio.

Power should be approximately 80% or greater for the effects you want to detect.

If we do **not** estimate “2FIs” this design will perfectly detect as significant “Main Effects” greater than twice the Residual Sigma or more (which would be based on “Centre points” **and** “2FIs” …)

What about Power if the model includes “2FIs”?

<< Back

Minimum Run Resolution V Characterization Design
Design Creation – Power calculation

Model for Power Evaluation

- Intercept
- A-X - G percent
- B-R - Y ratio
- C-R - Mw
- D-Acid amount
- E-Stirring speed
- F-X - Add time
- AB
- AC
- AD
- AE
- AF
- BC
- BD
- BE
- BF
- CD

Process Order: 2FI

✓	The term will be included in the power calculation.
🔒	Indicates that the term is required to be in the model by the program.

What about Power if the model includes "2FIs"?

Next >>

Warning: Italicized signal to noise information was not changed from the default. The power reported for this response may not accurately reflect your process.

Design Power

Name	Units	Delta (Signal)	Sigma (Noise)	Signal/Noise	Power for A	Power for B	Power for C	Power for D	Power for E	Power for F	Power for AB	Power for AC	Power for AD	Power for AE	Power for AF	Power for BC	Power for BD
Particles Size	nm	1	1	1	27,7%	27,7%	27,7%	27,7%	27,7%	27,7%	31,7%	31,7%	31,7%	31,7%	31,7%	31,7%	31,7%
EE	%	*2*	*1*	*2*	75,4%	75,4%	75,4%	75,4%	75,4%	75,4%	81,9%	81,9%	81,9%	81,9%	81,9%	81,9%	81,9%
Impurities	%	3	1	3	97,2%	97,2%	97,2%	97,2%	97,2%	97,2%	98,7%	98,7%	98,7%	98,7%	98,7%	98,7%	98,7%

Power is reported at a 5,0% alpha level to detect the specified signal/noise ratio.

Power should be approximately 80% or greater for the effects you want to detect.

Power for BE	Power for BF	Power for CD	Power for CE	Power for CF	Power for DE	Power for DF	Power for EF
31,7%	31,7%	31,7%	31,7%	31,7%	31,7%	31,7%	31,7%
81,9%	81,9%	81,9%	81,9%	81,9%	81,9%	81,9%	81,9%
98,7%	98,7%	98,7%	98,7%	98,7%	98,7%	98,7%	98,7%

If we **do** estimate "2FIs" this design will detect as significant :

- "2FIs" better than "Main Effects"
- both "Main Effects" and "2FIs" if there are greater than twice the Residual Sigma
  (which would be based on "Centre points" **only**)

If there are no "Centre points" (only the 22 base runs) Power calculation isn't possible.

Minimum Run Resolution V Characterization Design
Design Creation – Resulting Design

Finish

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Factorial	0,65	75,5	8821	700	650	6			
6	2	Factorial	0,65	76	9345	300	650	6			
4	3	Factorial	0,65	76	9345	700	650	3			
23	4	Center	0,55	75,75	9083	500	700	4,5			
10	5	Factorial	0,65	75,5	9345	700	750	6			
24	6	Center	0,55	75,75	9083	500	700	4,5			
22	7	Factorial	0,45	75,5	9345	300	750	6			
14	8	Factorial	0,65	76	9345	300	650	3			
12	9	Factorial	0,65	76	8821	700	750	6			
13	10	Factorial	0,45	76	8821	300	750	6			
1	11	Factorial	0,45	75,5	9345	700	650	6			
5	12	Factorial	0,45	76	8821	700	650	6			
18	13	Factorial	0,45	75,5	8821	300	650	6			
19	14	Factorial	0,45	75,5	8821	700	650	3			
16	15	Factorial	0,65	75,5	8821	300	750	6			
15	16	Factorial	0,45	75,5	9345	700	750	3			
25	17	Center	0,55	75,75	9083	500	700	4,5			
9	18	Factorial	0,65	75,5	9345	300	650	3			
17	19	Factorial	0,45	76	9345	300	650	3			
26	20	Center	0,55	75,75	9083	500	700	4,5			
11	21	Factorial	0,65	75,5	8821	700	750	3			
21	22	Factorial	0,65	76	9345	300	750	3			
2	23	Factorial	0,65	76	8821	300	650	3			
8	24	Factorial	0,45	76	8821	700	750	3			
20	25	Factorial	0,45	76	9345	700	750	6			
3	26	Factorial	0,45	75,5	8821	300	750	3			

- Randomize...
- Re-Order as Currently Displayed
- Hide Run Order
- Sort Ascending
- Sort Descending

It can be useful to "Randomize" the runs again several times to get an accurate "Run Order" particularly to correctly distribute "Centre points".

File saved as : ***MinRun6F4CP_Initial.dxpx***

This design is not feasible.
Let's correct the extreme values of "R – Mw" to get a feasible one.

Minimum Run Resolution V Characterization Design
Design Creation – Corrected Design

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Factorial	0,65	75,5	8821	700	650	6			
6	2	Factorial	0,65	76	9345	300	650	6			
4	3	Factorial	0,65	76	9345	700	650	3			
23	4	Unknown	0,55	75,5	9321	500	700	4,5			
10	5	Unknown	0,65	75,5	9321	700	750	6			
24	6	Unknown	0,55	76	8983	500	700	4,5			
22	7	Unknown	0,45	75,5	9321	300	750	6			
14	8	Factorial	0,65	76	9345	300	650	3			
12	9	Unknown	0,65	76	8983	700	750	6			
13	10	Unknown	0,45	76	8983	300	750	6			
1	11	Unknown	0,45	75,5	9321	700	650	6			
5	12	Unknown	0,45	76	8983	700	650	6			
18	13	Factorial	0,45	75,5	8821	300	650	6			
19	14	Factorial	0,45	75,5	8821	700	650	3			
16	15	Factorial	0,65	75,5	8821	300	750	6			
15	16	Unknown	0,45	75,5	9321	700	750	3			
25	17	Unknown	0,55	75,5	8821	500	700	4,5			
9	18	Unknown	0,65	75,5	9321	300	650	3			
17	19	Factorial	0,45	76	9345	300	650	3			
26	20	Unknown	0,55	76	9345	500	700	4,5			
11	21	Factorial	0,65	75,5	8821	700	750	3			
21	22	Factorial	0,65	76	9345	300	750	3			
2	23	Unknown	0,65	76	8983	300	650	3			
8	24	Unknown	0,45	76	8983	700	750	3			
20	25	Factorial	0,45	76	9345	700	750	6			
3	26	Factorial	0,45	75,5	8821	300	750	3			

When "R – Y ratio" = 75,5
maximum for "R – Mw"
must be changed
from 9345 to 9321.

When "R – Y ratio" = 76,0
minimum for "R – Mw"
must be changed
from 8821 to 8983.

The unique combination of
"R – Y ratio" & "R – Mw"
of the four "Centre points"
are changed to
the four combinations
of their possible extreme values.

Those modifications
have to be made by typing new
values in the appropriate cells.
Beware : mistakes not allowed!

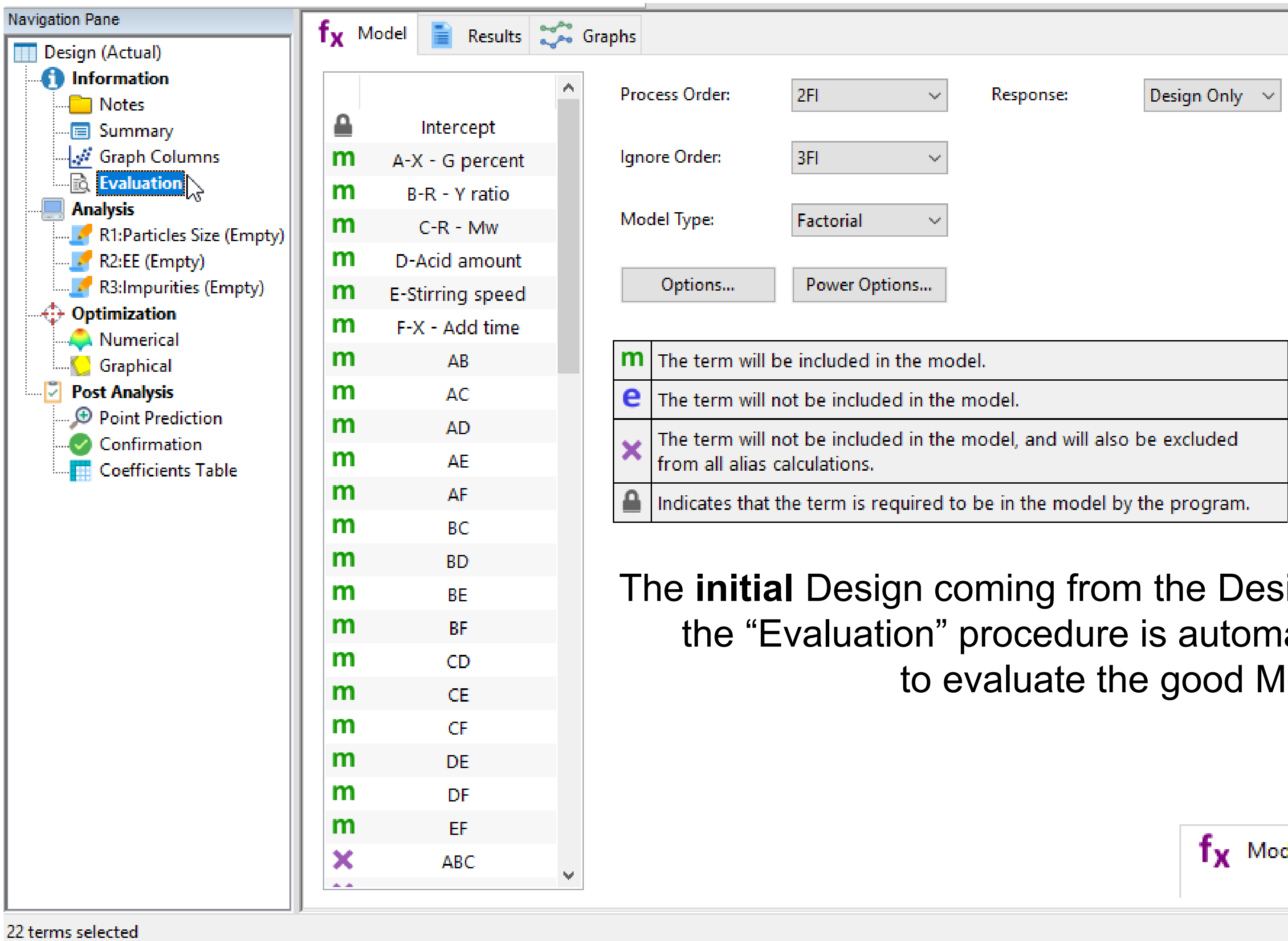
The "Space Type"
of the modified runs
becomes "Unknown".

File saved as : ***MinRun6F4VP_Cor.dxpx***

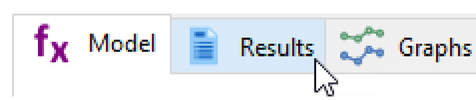
Minimum Run Resolution V Characterization Design

Design Evaluation of : **MinRun6F4VP_Cor**

“Verification points” included



The **initial** Design coming from the Design Expert Catalogue
the “Evaluation” procedure is automatically organized
to evaluate the good Model



Minimum Run Resolution V Characterization Design **corrected**

Design Evaluation of : **MinRun6F4VP_Cor** – "Verification points" included

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,3039	2,03224	0,5079	69,5 %
B	0,2469	1,58457	0,3689	85,2 %
C	0,2980	1,72587	0,4206	71,1 %
D	0,3039	2,03224	0,5079	69,5 %
E	0,3039	2,03224	0,5079	69,5 %
F	0,3039	2,03224	0,5079	69,5 %
AB	0,2604	1,48127	0,3249	81,5 %
AC	0,3204	1,72197	0,4193	65,2 %
AD	0,2490	1,35406	0,2615	84,6 %
AE	0,2490	1,35406	0,2615	84,6 %
AF	0,2490	1,35406	0,2615	84,6 %
BC	0,2792	1,42812	0,2998	76,3 %
BD	0,2604	1,48127	0,3249	81,5 %
BE	0,2604	1,48127	0,3249	81,5 %
BF	0,2604	1,48127	0,3249	81,5 %
CD	0,3204	1,72197	0,4193	65,2 %
CE	0,3204	1,72197	0,4193	65,2 %
CF	0,3204	1,72197	0,4193	65,2 %
DE	0,2490	1,35406	0,2615	84,6 %
DF	0,2490	1,35406	0,2615	84,6 %
EF	0,2490	1,35406	0,2615	84,6 %

* For a standard deviation of 1.

Power calculations are performed using response type "Continuous" and parameters:
Delta=2, Sigma=1
Power is evaluated over the -1 to +1 coded factor space.

Standard errors should be similar to each other in a balanced design. Lower standard errors are better.

The ideal VIF value is 1.0. VIFs above 10 are cause for concern. VIFs above 100 are cause for alarm, indicating coefficients are poorly estimated due to multicollinearity.

Ideal R_i^2 is 0.0. High R_i^2 means terms are correlated with each other, possibly leading to poor models.

Power should be approximately 80% or greater for the effects you want to detect.

Be sure that the model you selected contains only terms you expect to be significant.

In the **initial** Min Run :

- for "Main Effects" :
  all VIFs = 1,75376
  all Ri² = 0,4298
  all Power = 75,4%
- for "2FIs":
  all VIFs = 1,46652
  all Ri² = 0,3181
  all Power = 81,9%

Thus correcting "R - Mw" values logically worsens the Design quality.

The three indicators are not too far from targets.
They are globally worse for "Main Effects" than for "2FIs".

This means that :

- every effect isn't too strongly correlated to all the other ones
- "Main Effects" will be less precisely estimated than "2FIs"

$$\mathrm{VIF} = \frac{1}{1 - Ri^2}$$

Minimum Run Resolution V Characterization Design **corrected**
Design Evaluation of : **MinRun6F4VP_Cor** – "Verification points" included

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	27,23
Maximum Variance Mean	8,73
Average Variance Mean	0,3610
Minimum Variance Mean	0,0481
G Efficiency	9,69
Scaled D-optimality Criterion	1,48
Determinant of $(X'X)^{-1}$	3,90293E-28
Trace of $(X'X)^{-1}$	1,71
I (Cuboidal)	0,3611

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

This panel summarizes all the preceding.

A perfectly **orthogonal** design presents :
(defined on Numerical Factors or Categorical Factors with two levels)
Condition number = 1
Scaled D-optimality Criterion = 1.

Except **G Efficiency** a smaller value is better for all those indicators.
G Efficiency of 10 (%) means that the prediction error will be very heterogenous in the experimental domain.
An ideal **G Efficiency** has to be as close as possible to 100% and a good one at least greater than 50%.

The most interesting is the **Scaled D-optimality Criterion** because it allows to compare designs with different numbers of runs.

$$\text{G Efficiency}(\%) \cong 100\left(\frac{\sqrt{p/N}}{Max.Var.Mean}\right)$$

P : number of coefficients ; N : number of runs

This feasible Design is far from perfection but is satisfactory.

It could be a good solution.

Minimum Run Resolution V Characterization Design
Design Evaluation of : **MinRun6F4VP_Cor**
"Centre points" excluded

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Factorial	0,65	75,5	8821	700	650	6			
6	2	Factorial	0,65	76	9345	300	650	6			
4	3	Factorial	0,65	76	9345	700	650	3			
23	4	Unknown	0,55	75,5	9321	500	700	4,5			
10	5	Unknown	0,65	75,5	9321	700	750	6			
24	6	Unknown	0,55	76	8983	500	700	4,5			
			0,45	75,5	9321	300	750	6			
				76	9345	300	650	3			
				76	8983	700	750	6			
				76	8983	300	750	6			
				75,5	9321	700	650	6			
5	12	Unknown	0,45	76	8983	700	650	6			
18	13	Factorial	0,45	75,5	8821	300	650	6			
19	14	Factorial	0,45	75,5	8821	700	650	3			
16	15	Factorial	0,65	75,5	8821	300	750	6			
15	16	Unknown	0,45	75,5	9321	700	750	3			
25	17	Unknown	0,55	75,5	8821	500	700	4,5			
9	18	Unknown	0,65	75,5	9321	300	650	3			
17	19	Factorial	0,45	76	9345	300	650	3			
26	20	Unknown	0,55	76	9345	500	700	4,5			
11	21	Factorial	0,65	75,5	8821	700	750	3			
21	22	Factorial	0,65	76	9345	300	750	3			
2	23	Unknown	0,65	76	8983	300	650	3			
8	24	Unknown	0,45	76	8983	700	750	3			
20	25	Factorial	0,45	76	9345	700	750	6			
3	26	Factorial	0,45	75,5	8821	300	750	3			

Insert Row(s) >
Set Row Status >
Delete Row(s)
Duplicate
Edit Comment

Normal
Ignore
Highlight
Verification

To exclude runs:

- Select them in **Design (Actual)**
- Right click mouse
- Select : **Set Row Status**
  - either **Ignore**
  - or **Verification**

Using **Ignore** or **Verification** is equivalent for **Evaluation.**

For **Analysis** both **Verification** and **Ignore** runs will not be used for fitting the Model but they will be displayed on graphs if **Verification** and not displayed if **Ignore**.

Minimum Run Resolution V Characterization Design
Design Evaluation of : **MinRun6F4VP_Cor** - “Centre points” excluded

Runs set to : **Ignore**

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Factorial	0,65	75,5	8821	700	650	6			
6	2	Factorial	0,65	76	9345	300	650	6			
4	3	Factorial	0,65	76	9345	700	650	3			
~~23~~	~~4~~	~~Unknown~~	~~0,55~~	~~75,5~~	~~9321~~	~~500~~	~~700~~	~~4,5~~			
10	5	Unknown	0,65	75,5	9321	700	750	6			
~~24~~	~~6~~	~~Unknown~~	~~0,55~~	~~76~~	~~8983~~	~~500~~	~~700~~	~~4,5~~			
22	7	Unknown	0,45	75,5	9321	300	750	6			
14	8	Factorial	0,65	76	9345	300	650	3			
12	9	Unknown	0,65	76	8983	700	750	6			
13	10	Unknown	0,45	76	8983	300	750	6			
1	11	Unknown	0,45	75,5	9321	700	650	6			
5	12	Unknown	0,45	76	8983	700	650	6			
18	13	Factorial	0,45	75,5	8821	300	650	6			
19	14	Factorial	0,45	75,5	8821	700	650	3			
16	15	Factorial	0,65	75,5	8821	300	750	6			
15	16	Unknown	0,45	75,5	9321	700	750	3			
~~25~~	~~17~~	~~Unknown~~	~~0,55~~	~~75,5~~	~~8821~~	~~500~~	~~700~~	~~4,5~~			
9	18	Unknown	0,65	75,5	9321	300	650	3			
17	19	Factorial	0,45	76	9345	300	650	3			
~~26~~	~~20~~	~~Unknown~~	~~0,55~~	~~76~~	~~9345~~	~~500~~	~~700~~	~~4,5~~			
11	21	Factorial	0,65	75,5	8821	700	750	3			
21	22	Factorial	0,65	76	9345	300	750	3			
2	23	Unknown	0,65	76	8983	300	650	3			
8	24	Unknown	0,45	76	8983	700	750	3			
20	25	Factorial	0,45	76	9345	700	750	6			
3	26	Factorial	0,45	75,5	8821	300	750	3			

Minimum Run Resolution V Characterization Design
Design Evaluation of : **MinRun6F4VP_Cor** - "Centre points" excluded

Runs set to : **Verification**

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Factorial	0,65	75,5	8821	700	650	6			
6	2	Factorial	0,65	76	9345	300	650	6			
4	3	Factorial	0,65	76	9345	700	650	3			
23	**4**	**Unknown**	**0,55**	**75,5**	**9321**	**500**	**700**	**4,5**			
10	5	Unknown	0,65	75,5	9321	700	750	6			
24	**6**	**Unknown**	**0,55**	**76**	**8983**	**500**	**700**	**4,5**			
22	7	Unknown	0,45	75,5	9321	300	750	6			
14	8	Factorial	0,65	76	9345	300	650	3			
12	9	Unknown	0,65	76	8983	700	750	6			
13	10	Unknown	0,45	76	8983	300	750	6			
1	11	Unknown	0,45	75,5	9321	700	650	6			
5	12	Unknown	0,45	76	8983	700	650	6			
18	13	Factorial	0,45	75,5	8821	300	650	6			
19	14	Factorial	0,45	75,5	8821	700	650	3			
16	15	Factorial	0,65	75,5	8821	300	750	6			
15	16	Unknown	0,45	75,5	9321	700	750	3			
25	**17**	**Unknown**	**0,55**	**75,5**	**8821**	**500**	**700**	**4,5**			
9	18	Unknown	0,65	75,5	9321	300	650	3			
17	19	Factorial	0,45	76	9345	300	650	3			
26	**20**	**Unknown**	**0,55**	**76**	**9345**	**500**	**700**	**4,5**			
11	21	Factorial	0,65	75,5	8821	700	750	3			
21	22	Factorial	0,65	76	9345	300	750	3			
2	23	Unknown	0,65	76	8983	300	650	3			
8	24	Unknown	0,45	76	8983	700	750	3			
20	25	Factorial	0,45	76	9345	700	750	6			
3	26	Factorial	0,45	75,5	8821	300	750	3			

Minimum Run Resolution V Characterization Design **corrected**
Design Evaluation of : **MinRun6F4VP_Cor** – "Verification points" excluded

Model Terms | Factorial Effects Aliases

Warning: Power not defined when the residual degrees of freedom are 0.

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,3265	2,34514	0,5736	
B	0,2893	1,84176	0,4570	
C	0,3495	2,01987	0,5049	
D	0,3265	2,34514	0,5736	
E	0,3265	2,34514	0,5736	
F	0,3265	2,34514	0,5736	
AB	0,2691	1,57999	0,3671	
AC	0,3372	1,90526	0,4751	
AD	0,2619	1,49689	0,3319	
AE	0,2619	1,49689	0,3319	
AF	0,2619	1,49689	0,3319	
BC	0,3179	1,56179	0,3597	
BD	0,2691	1,57999	0,3671	
BE	0,2691	1,57999	0,3671	
BF	0,2691	1,57999	0,3671	
CD	0,3372	1,90526	0,4751	
CE	0,3372	1,90526	0,4751	
CF	0,3372	1,90526	0,4751	
DE	0,2619	1,49689	0,3319	
DF	0,2619	1,49689	0,3319	
EF	0,2619	1,49689	0,3319	

VIF (up to 2,34) and Ri² (up to 0,57) are very slightly higher without taking "Verification points" into account :

- we could consider that excluding them worsens the fitting
- but the design becomes saturated and Power cannot be calculated

This contrasted situation means that :

- globally all Effects will be rather correctly estimated
- "Main Effects" will be less precisely estimated than "2FIs"

$$VIF = \frac{1}{1 - Ri^2}$$

Minimum Run Resolution V Characterization Design **corrected**
Design Evaluation of : **MinRun6F4VP_Cor** – “Verification points” excluded

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	37,94
Maximum Variance Mean	12,22
Average Variance Mean	0,4384
Minimum Variance Mean	0,0567
G Efficiency	8,18
Scaled D-optimality Criterion	1,31
Determinant of $(X'X)^{-1}$	1,13551E-27
Trace of $(X'X)^{-1}$	1,98
I (Cuboidal)	0,4392

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

As the **Scaled D-optimality Criterion** is smaller than with “Verification points” included (1,31 instead of 1,48) exclude them will improve the fitting.

It’s a little bit contradictory with the VIF & Ri² conclusions.

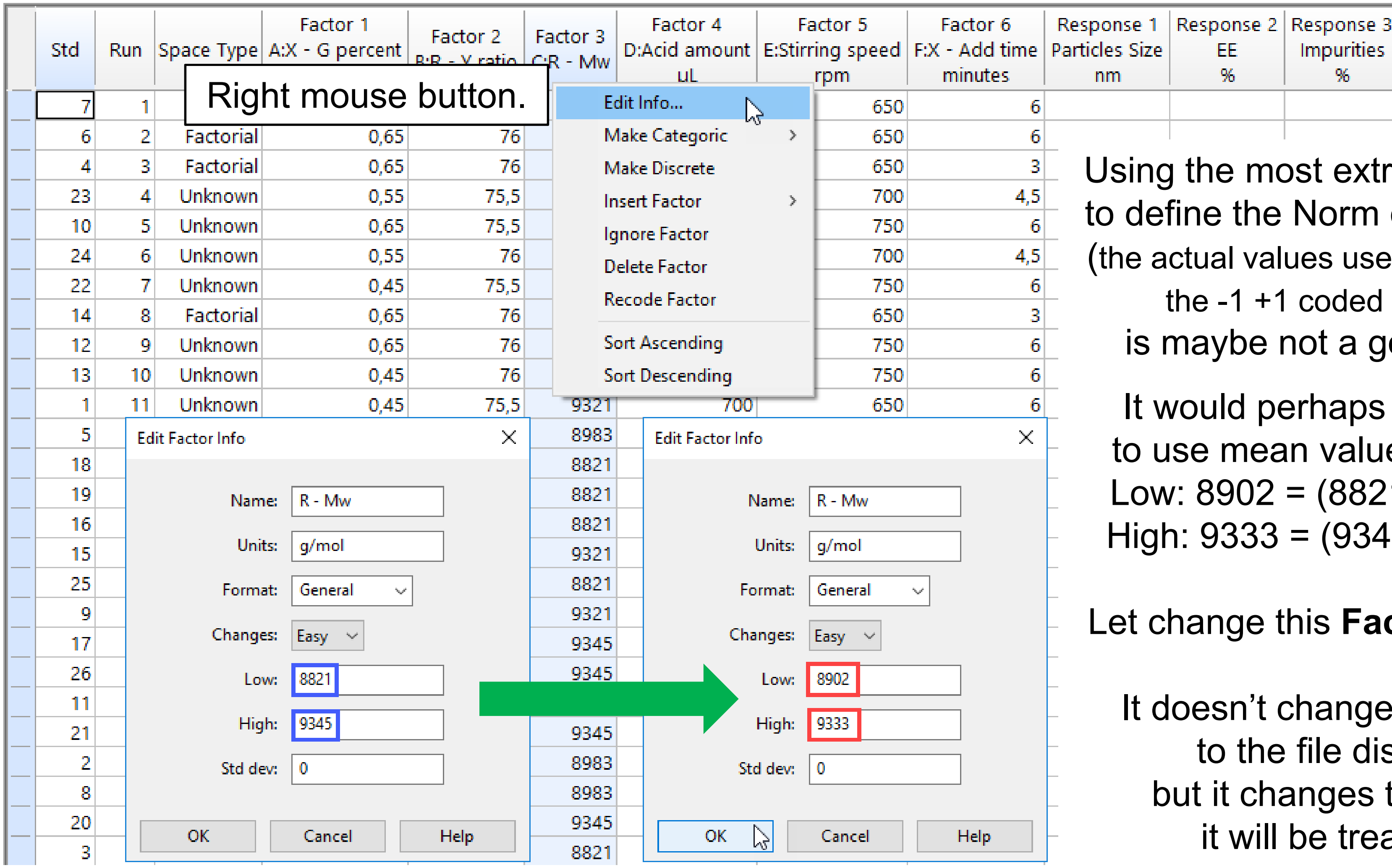
This Design is feasible and satisfactory.

It could be a good solution.

$$\text{G Efficiency}(\%) \cong 100\left(\frac{\sqrt{p/N}}{Max.Var.Mean}\right)$$

P : number of coefficients ; N : number of runs

Minimum Run Resolution V Characterization Design
Design Creation – Corrected Design – Modification of “R – Mw” Norm



Using the most extreme values to define the Norm of “R – Mw” (the actual values used to compute the -1 +1 coded values) is maybe not a good idea.

It would perhaps be better to use mean values instead
Low: 8902 = (8821+8983)/2
High: 9333 = (9345+9321)/2

Let change this **Factor Info** …

It doesn’t change anything to the file display but it changes the way it will be treated.

File saved as : ***MinRun6F4VP_Cor_Norm.dxpx***

Minimum Run Resolution V Characterization Design **corrected**

Design Evaluation of : **MinRun6F4VP_Cor_Norm** – “Verification points” included

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2894	1,84202	0,4571	73,5 %
B	0,2376	1,46795	0,3188	87,5 %
C	0,2451	1,72587	0,4206	85,6 %
D	0,2894	1,84202	0,4571	73,5 %
E	0,2894	1,84202	0,4571	73,5 %
F	0,2894	1,84202	0,4571	73,5 %
AB	0,2604	1,48127	0,3249	81,5 %
AC	0,2636	1,68992	0,4083	80,6 %
AD	0,2490	1,35406	0,2615	84,6 %
AE	0,2490	1,35406	0,2615	84,6 %
AF	0,2490	1,35406	0,2615	84,6 %
BC	0,2297	1,39838	0,2849	89,5 %
BD	0,2604	1,48127	0,3249	81,5 %
BE	0,2604	1,48127	0,3249	81,5 %
BF	0,2604	1,48127	0,3249	81,5 %
CD	0,2636	1,68992	0,4083	80,6 %
CE	0,2636	1,68992	0,4083	80,6 %
CF	0,2636	1,68992	0,4083	80,6 %
DE	0,2490	1,35406	0,2615	84,6 %
DF	0,2490	1,35406	0,2615	84,6 %
EF	0,2490	1,35406	0,2615	84,6 %

Compared to the corrected situation **before Norm change**:

- VIF & Ri^2 are still globally higher for “Main Effects” than for “FIs”
- Ten Effects have lower VIF & Ri^2 :
  - Four clearly (A D E F)
  - One rather clearly (B)
  - Five less clearly (AC BC CD CE CF)
- The eleven remaining Effects present no change (C AB AD AE AF BD BE BF DE DF EF)

VIF don’t overpass 1,85 an Ri^2 0,46 which is better.

This contrasted situation means that :

- Globally Effects would be correctly estimated
- “Main Effects” will be less precisely estimated than “2FIs”

$$VIF = \frac{1}{1 - Ri^2}$$

Minimum Run Resolution V Characterization Design **corrected**
Design Evaluation of : **MinRun6F4VP_Cor_Norm** – “Verification points” included

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	22,59
Maximum Variance Mean	7,04
Average Variance Mean	0,3261
Minimum Variance Mean	0,0480
G Efficiency	12,02
Scaled D-optimality Criterion	1,33
Determinant of $(X'X)^{-1}$	3,74234E-29
Trace of $(X'X)^{-1}$	1,49
I (Cuboidal)	0,3239

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

All indicators have better values
(a little bit higher for **G Efficiency**
more or less lower for the other ones):
the “R – Mw” Norm modification
will improve the fitting

This corrected Norm-modified Design is a better solution.

$$\text{G Efficiency}(\%) \cong 100\left(\frac{\sqrt{p/N}}{Max.Var.Mean}\right)$$

P : number of coefficients ; N : number of runs

Beware :
The “R – Mw” Norm is different, so it’s variation range is smaller and the global design space volume also.
As the Maximum Variance Mean is usually observed in a corner of the design space it’s value and thus the G Efficiency one can be fallacious.

Minimum Run Resolution V Characterization Design **corrected**
Design Evaluation of : **MinRun6F4VP_Cor_Norm** – “Verification points” excluded

Model Terms | Factorial Effects Aliases

Warning: Power not defined when the residual degrees of freedom are 0.

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,3081	2,0879	0,5211	
B	0,2763	1,6798	0,4047	
C	0,2874	2,01987	0,5049	
D	0,3081	2,0879	0,5211	
E	0,3081	2,0879	0,5211	
F	0,3081	2,0879	0,5211	
AB	0,2691	1,57999	0,3671	
AC	0,2774	1,86977	0,4652	
AD	0,2619	1,49689	0,3319	
AE	0,2619	1,49689	0,3319	
AF	0,2619	1,49689	0,3319	
BC	0,2615	1,53025	0,3465	
BD	0,2691	1,57999	0,3671	
BE	0,2691	1,57999	0,3671	
BF	0,2691	1,57999	0,3671	
CD	0,2774	1,86977	0,4652	
CE	0,2774	1,86977	0,4652	
CF	0,2774	1,86977	0,4652	
DE	0,2619	1,49689	0,3319	
DF	0,2619	1,49689	0,3319	
EF	0,2619	1,49689	0,3319	

VIF and Ri^2 are higher without taking “Verification points” into account : we could consider that they improve the fitting.

Compared to the corrected situation **before Norm change**:

- VIF & Ri^2 are still globally higher for “Main Effects” than for “FIs”
- Ten Effects have lower VIF & Ri^2 (the same as with “VP” in) :
  - Four clearly (A D E F)
  - One rather clearly (B)
  - Five less clearly (AC BC CD CE CF)
- The eleven remaining Effects present no change (C AB AD AE AF BD BE BF DE DF EF)

VIF don’t overpass 2,03 an Ri^2 0,53 which is acceptable.

This contrasted situation means that :

- Globally Effects would be correctly estimated
- “Main Effects” will be less precisely estimated than “2FIs”

Minimum Run Resolution V Characterization Design **corrected**

Design Evaluation of : **MinRun6F4VP_Cor_Norm** – "Verification points" excluded

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	31,70
Maximum Variance Mean	9,81
Average Variance Mean	0,3959
Minimum Variance Mean	0,0584
G Efficiency	10,20
Scaled D-optimality Criterion	1,18
Determinant of $(X'X)^{-1}$	1,08879E-28
Trace of $(X'X)^{-1}$	1,71
I (Cuboidal)	0,3956

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

All indicators have better values
(a little bit higher for **G Efficiency**
more or less lower for the other ones)
than before "R – Mw" Norm change
and than with "Verification points" in:
the "R – Mw" Norm modification
will improve the fitting

This corrected Norm-modified Design is a better solution.

$$\text{G Efficiency}(\%) \cong 100\left(\frac{\sqrt{p/N}}{Max.Var.Mean}\right)$$

P : number of coefficients ; N : number of runs

Beware :
The "R – Mw" Norm is different, so it's variation range is smaller and the global design space volume also. As the Maximum Variance Mean is usually observed in a corner of the design space it's value and thus the **G Efficiency** one can be fallacious.

Creating and correcting a

Rechtschaffner Matrix

Evaluating it

<u>after “R – Mw” correction</u>

including and excluding Verification Points

Rechtschaffner Matrix
Design Creation

The Rechtschaffner Matrices are 2 levels screening saturated Designs which allow to estimate all Main Effects and 2FIs (except for 3 Factors).

They contain ***N = 1+k+(k*(k-1))/2*** runs (k= number of Factors) i.e. exactly as much as the number of coefficients to be estimated.

They consist of:

- ***one*** line containing only: ***-1***
- ***k*** lines circular permutations of one line containing only: ***one -1*** among ***(k-1) 1***
- ***(k*(k-1))/2*** lines circular permutations of one line containing only: ***two -1*** among ***(k-2) 1***

They are not orthogonal (except for ***k=5***).
However their correlation coefficients are relatively weak and very symmetrical.

Rechtschaffner Matrix:

- does not exist for 2 Factors
- is Resolution III for 3 Factors (A=-BC ; B=-AC ; C=-AB)
- is equivalent to the Factorial Fractional Design 2^{5-1} for 5 Factors

The Rechtschaffner Matrices are not available in the Design Expert catalogue.
They have to be created outside it
and then recovered as “Historical Data”
or by another mean which will be exposed later.

Rechtschaffner Matrix
Design Creation in Excel

Code (-1 ; +1) Matrix

	X1	X2	X3	X4	X5	X6
1	-1	-1	-1	-1	-1	-1
2	-1	1	1	1	1	1
3	1	-1	1	1	1	1
4	1	1	-1	1	1	1
5	1	1	-1	-1	-1	-1
6	1	-1	1	-1	-1	-1
7	-1	1	1	-1	-1	-1
8	1	1	1	-1	1	1
9	1	-1	-1	1	-1	-1
10	-1	1	-1	1	-1	-1
11	-1	-1	1	1	-1	-1
12	1	1	1	1	-1	1
13	1	-1	-1	-1	1	-1
14	-1	1	-1	-1	1	-1
15	-1	-1	1	-1	1	-1
16	-1	-1	-1	1	1	-1
17	1	1	1	1	1	-1
18	1	-1	-1	-1	-1	1
19	-1	1	-1	-1	-1	1
20	-1	-1	1	-1	-1	1
21	-1	-1	-1	1	-1	1
22	-1	-1	-1	-1	1	1

Every Factor is defined with
10 +*1* levels & **12 -*1*** levels.
As a consequence
every 2 Factors combination
is defined with
7 -1 by -1
but only **5**
+1 by -1, -1 by +1 & +1 by +1.

That's good as we want
to make more runs at
minimum by minimum
for "R – Y ratio" by "R – Mw".

Note that
-1 must not necessarily
be smaller than ***+1***.
Extreme values can be reversed
to obtain any suitable imbalance.

Actual level Matrix

	X1	X2	X3	X4	X5	X6
Low	0,45	75,5	8821	300	650	3
High	0,65	76,0	9345	700	750	6
1	0,45	75,5	8821	300	650	3
2	0,45	76,0	9345	700	750	6
3	0,65	75,5	9345	700	750	6
4	0,65	76,0	8821	700	750	6
5	0,65	76,0	8821	300	650	3
6	0,65	75,5	9345	300	650	3
7	0,45	76,0	9345	300	650	3
8	0,65	76,0	9345	300	750	6
9	0,65	75,5	8821	700	650	3
10	0,45	76,0	8821	700	650	3
11	0,45	75,5	9345	700	650	3
12	0,65	76,0	9345	700	650	6
13	0,65	75,5	8821	300	750	3
14	0,45	76,0	8821	300	750	3
15	0,45	75,5	9345	300	750	3
16	0,45	75,5	8821	700	750	3
17	0,65	76,0	9345	700	750	3
18	0,65	75,5	8821	300	650	6
19	0,45	76,0	8821	300	650	6
20	0,45	75,5	9345	300	650	6
21	0,45	75,5	8821	700	650	6
22	0,45	75,5	8821	300	750	6

Rechtschaffner Matrix
Design Creation in Excel

Run	Type	X - G percent	R - Y ratio	R - Mw	Acid	Stirring speed	X - Add time
1	Factorial	0,45	76	8821	700	750	6
2	Factorial	0,65	76	9345	300	650	3
3	Factorial	0,65	75,5	9345	300	750	3
4	**Center**	**0,55**	**75,75**	**9083**	**500**	**700**	**4,5**
5	Factorial	0,65	76	8821	700	650	6
6	Factorial	0,45	75,5	8821	700	650	6
7	Factorial	0,65	75,5	8821	700	650	3
8	Factorial	0,45	76	9345	300	750	3
9	Factorial	0,45	75,5	9345	300	650	6
10	Factorial	0,65	75,5	8821	700	750	6
11	**Center**	**0,55**	**75,75**	**9083**	**500**	**700**	**4,5**
12	Factorial	0,45	75,5	8821	300	750	6
13	Factorial	0,65	76	9345	700	750	3
14	Factorial	0,45	75,5	9345	700	650	3
15	Factorial	0,65	76	9345	300	750	6
16	Factorial	0,45	75,5	8821	300	650	3
17	**Center**	**0,55**	**75,75**	**9083**	**500**	**700**	**4,5**
18	Factorial	0,45	76	8821	300	650	6
19	Factorial	0,45	75,5	9345	700	750	6
20	Factorial	0,65	75,5	8821	300	650	6
21	Factorial	0,45	76	8821	700	650	3
22	**Center**	**0,55**	**75,75**	**9083**	**500**	**700**	**4,5**
23	Factorial	0,45	75,5	8821	700	750	3
24	Factorial	0,65	75,5	9345	700	650	6
25	Factorial	0,65	76	8821	300	750	3
26	Factorial	0,45	76	9345	700	650	6

After having in Excel manually added “Centre points” and reordered runs the “initial” Rechschaffner Matrix appears as beside.

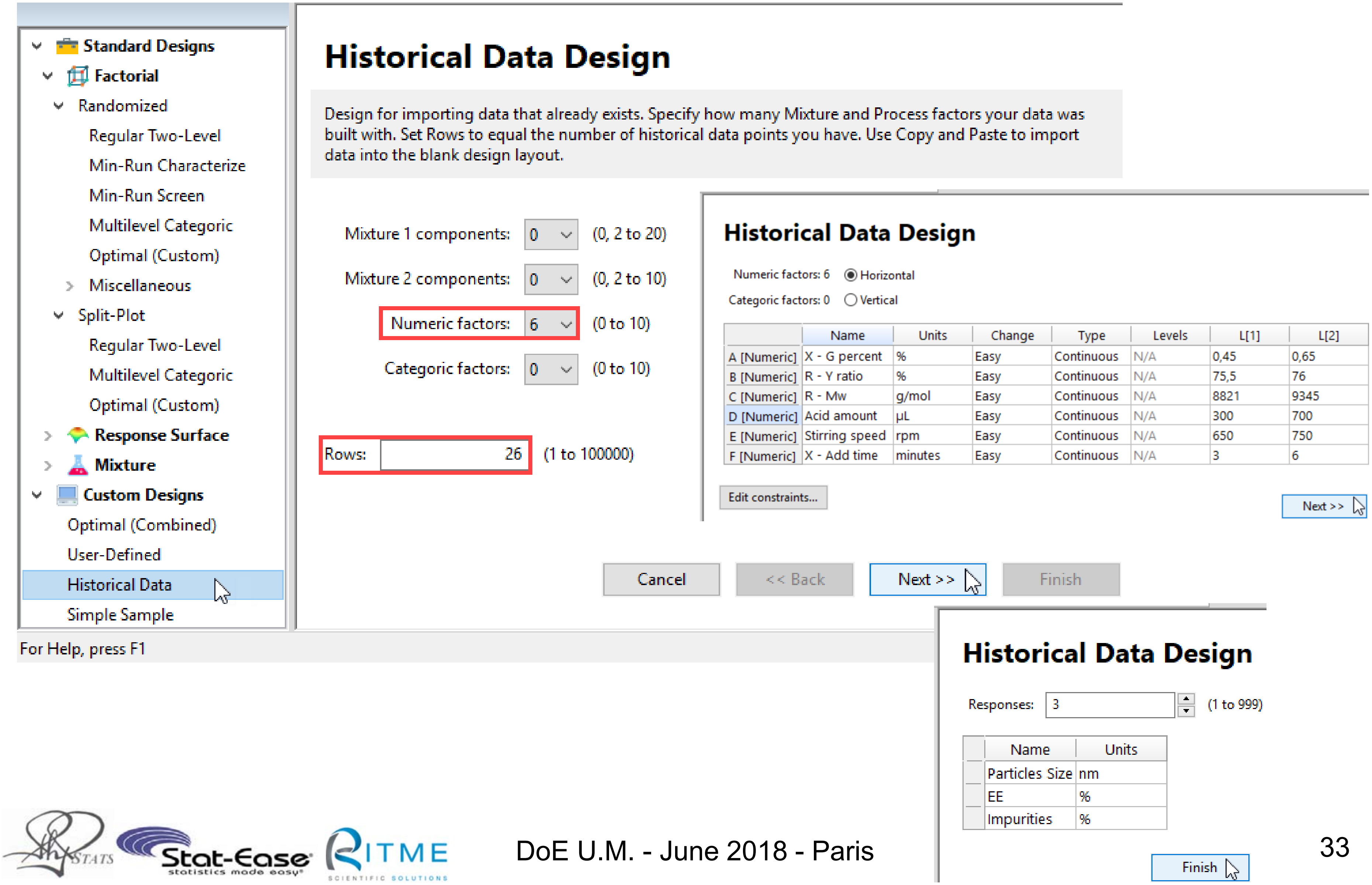
It now remains to introduce it in Design Expert.

It can be done by two different manners:

1. Creating in Design Expert a “Historical Data” “Custom design” with accurate Factors, levels, Responses and runs and paste the copied Excel cells in
2. Directly paste the copied Excel cells in place of the original “Min Run Characterize” Design Expert file cells

Rechtschaffner Matrix
Design Recovery in Design Expert

1. Creation of a "Historical Data" "Custom design":



Rechtschaffner Matrix
Design Recovery in Design Expert

1. Creation of a “Historical Data” “Custom design”:

Run	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio %	Factor 3 C:R - Mw g/mol	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
1									
2									
3									
4									
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									
21									
22									
23									
24									
25									
26									

Result :
an empty table …

Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
1	Unknown	0,45	76	8821	700	750	6			
2	Unknown	0,65	76	9345	300	650	3			
3	Unknown	0,65	75,5	9345	300	750	3			
4	Unknown	0,55	75,75	9083	500	700	4,5			
5	Unknown	0,65	76	8821	700	650	6			
6	Unknown	0,45	75,5	8821	700	650	6			
7	Unknown	0,65	75,5	8821	700	650	3			
8	Unknown	0,45	76	9345	300	750	3			
9	Unknown	0,45	75,5	9345	300	650	6			
10	Unknown	0,65	75,5	8821	700	750	6			
11	Unknown	0,55	75,75	9083	500	700	4,5			
12	Unknown	0,45	75,5	8821	300	750	6			
13	Unknown	0,65	76	9345	700	750	3			
14	Unknown	0,45	75,5	9345	700	650	3			
15	Unknown	0,65	76	9345	300	750	6			
16	Unknown	0,45	75,5	8821	300	650	3			
17	Unknown	0,55	75,75	9083	500	700	4,5			
18	Unknown	0,45	76	8821	300	650	6			
19	Unknown	0,45	75,5	9345	700	750	6			
20	Unknown	0,65	75,5	8821	300	650				
21	Unknown	0,45	76	8821	700	650	3			
22	Unknown	0,55	75,75	9083	500	700	4,5			
23	Unknown	0,45	75,5	8821	700	750	3			
24	Unknown	0,65	75,5	9345	700	650	6			
25	Unknown	0,65	76	8821	300	750	3			
26	Unknown	0,45	76	9345	700	650	6			

… to be filled in
by pasting

Disadvantages:

- “Space Type” is “unknown”
- **Evaluation** & **Analysis** will be performed under the assumption of “Polynomial” Model type instead of “Factorial”

Rechtschaffner Matrix
Design Recovery in Design Expert

2. Direct pasting onto the original “Min. Run Characterization” :

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Factorial	0,45	76	8821	700	750	6			
6	2	Factorial	0,65	76	9345	300	650	3			
4	3	Factorial	0,65	75,5	9345	300	750	3			
23	4	Center	0,55	75,75	9083	500	700	4,5			
10	5	Factorial	0,65	76	8821	700	650	6			
24	6	Factorial	0,45	75,5	8821	700	650	6			
22	7	Factorial	0,65	75,5	8821	700	650	3			
14	8	Factorial	0,45	76	9345	300	750	3			
12	9	Factorial	0,45	75,5	9345	300	650	6			
13	10	Factorial	0,65	75,5	8821	700	750	6			
1	11	Center	0,55	75,75	9083	500	700	4,5			
5	12	Factorial	0,45	75,5	8821	300	750	6			
18	13	Factorial	0,65	76	9345	700	750	3			
19	14	Factorial	0,45	75,5	9345	700	650	3			
16	15	Factorial	0,65	76	9345	300	750	6			
15	16	Factorial	0,45	75,5	8821	300	650	3			
25	17	Center	0,55	75,75	9083	500	700	4,5			
9	18	Factorial	0,45	76	8821	300	650	6			
17	19	Factorial	0,45	75,5	9345	700	750	6			
26	20	Factorial	0,65	75,5	8821	300	650	6			
11	21	Factorial	0,45	76	8821	700	650	3			
21	22	Center	0,55	75,75	9083	500	700	4,5			
2	23	Factorial	0,45	75,5	8821	700	750	3			
8	24	Factorial	0,65	75,5	9345	700	650	6			
20	25	Factorial	0,65	76	8821	300	750	3			
3	26	Factorial	0,45	76	9345	700	650	6			

Result :
the beside table

Advantages:
- “Space Type” is correctly defined
- **Evaluation** & **Analysis** will be performed under the assumption of “Factorial” Model type

This method was preferred.

File saved as : ***RS6F4CP_Initial.dxpx***

Rechtschaffner Matrix
Design Creation – Corrected Design

Std	Run	Space Type	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
7	1	Unknown	0,45	76	8983	700	750	6			
6	2	Factorial	0,65	76	9345	300	650	3			
4	3	Unknown	0,65	75,5	9321	300	750	3			
23	4	Unknown	0,55	75,5	8821	500	700	4,5			
10	5	Unknown	0,65	76	8983	700	650	6			
24	6	Factorial	0,45	75,5	8821	700	650	6			
22	7	Factorial	0,65	75,5	8821	700	650	3			
14	8	Factorial	0,45	76	9345	300	750	3			
12	9	Unknown	0,45	75,5	9321	300	650	6			
13	10	Factorial	0,65	75,5	8821	700	750	6			
1	11	Unknown	0,55	76	9345	500	700	4,5			
5	12	Factorial	0,45	75,5	8821	300	750	6			
18	13	Factorial	0,65	76	9345	700	750	3			
19	14	Unknown	0,45	75,5	9321	700	650	3			
16	15	Factorial	0,65	76	9345	300	750	6			
15	16	Factorial	0,45	75,5	8821	300	650	3			
25	17	Unknown	0,55	75,5	9321	500	700	4,5			
9	18	Unknown	0,45	76	8983	300	650	6			
17	19	Unknown	0,45	75,5	9321	700	750	6			
26	20	Factorial	0,65	75,5	8821	300	650	6			
11	21	Unknown	0,45	76	8983	700	650	3			
21	22	Unknown	0,55	76	8983	500	700	4,5			
2	23	Factorial	0,45	75,5	8821	700	750	3			
8	24	Unknown	0,65	75,5	9321	700	650	6			
20	25	Unknown	0,65	76	8983	300	750	3			
3	26	Factorial	0,45	76	9345	700	650	6			

When "R – Y ratio" = 75,5 maximum for "R – Mw" must be changed from 9345 to 9321.

When "R – Y ratio" = 76,0 minimum for "R – Mw" must be changed from 8821 to 8983.

The unique combination of "R – Y ratio" & "R – Mw" of the four "Centre points" are changed to the four combinations of their possible extreme values.

Those modifications have to be made by typing new values in the appropriate cells.
Beware : mistakes not allowed!

The "Space Type" of the modified runs becomes "Unknown".

File saved as : ***RS6F4VP_Cor.dxpx***

Rechtschaffner Matrix **corrected**

Design Evaluation of : **RS6F4VP_Cor** – “Verification points” included

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2292	1,14766	0,1287	89,6 %
B	0,2177	1,2251	0,1837	92,2 %
C	0,2661	1,4	0,2857	79,9 %
D	0,2292	1,14766	0,1287	89,6 %
E	0,2292	1,14766	0,1287	89,6 %
F	0,2292	1,14766	0,1287	89,6 %
AB	0,2389	1,24701	0,1981	87,2 %
AC	0,2680	1,2046	0,1699	79,4 %
AD	0,2265	1,12105	0,1080	90,2 %
AE	0,2265	1,12105	0,1080	90,2 %
AF	0,2265	1,12105	0,1080	90,2 %
BC	0,2661	1,29697	0,2290	79,9 %
BD	0,2389	1,24701	0,1981	87,2 %
BE	0,2389	1,24701	0,1981	87,2 %
BF	0,2389	1,24701	0,1981	87,2 %
CD	0,2680	1,2046	0,1699	79,4 %
CE	0,2680	1,2046	0,1699	79,4 %
CF	0,2680	1,2046	0,1699	79,4 %
DE	0,2265	1,12105	0,1080	90,2 %
DF	0,2265	1,12105	0,1080	90,2 %
EF	0,2265	1,12105	0,1080	90,2 %

Compared to **RS6F4VP_Initial** for which all VIFs are worth 1,139 all Ri² 0,1221 & all Power 89,8% :

- Sixteen Effects present higher VIF & Ri² :
  - One strongly (C “R – Mw” : the corrected Factor)
  - One rather strongly (BC)
  - Four very clearly (AB BD BE BF)
  - One clearly (B)
  - Four rather clearly (AC CD CE CF)
- Four Effects present almost unchanged VIF & Ri² : (A D E F)
- Six Effects have slightly lower VIF & Ri² : (AD AE AF DE DF EF)

VIF don’t overpass 1,4 an Ri² 0,29 which is very acceptable.

This contrasted situation means that:

- the “Main Effects” of “R - Mw” & “R – Y ratio”, their common “2FI” and their “2FIs” with the four other Factors

will be less precisely estimated than:

- the “Main Effects” of the four other Factors and their “2FIs”

Compared to **MinRun6F4VP_Cor** “CP included”:

- all VIF, Ri² and Standard Errors are more or less lower
- all Power are more or less higher

Thus for six Factors the ***corrected* Rechtschaffner Matrix** is a better Design than the ***corrected* Min Run Characterization**.

Rechtschaffner Matrix **corrected**

Design Evaluation of : **RS6F4VP_Cor** – “Verification points” included

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	4,16
Maximum Variance Mean	1,81
Average Variance Mean	0,2599
Minimum Variance Mean	0,0486
G Efficiency	46,67
Scaled D-optimality Criterion	1,36
Determinant of $(X'X)^{-1}$	6,3479E-29
Trace of $(X'X)^{-1}$	1,27
I (Cuboidal)	0,2579

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

Compared to **RS6F4VP_Initial** “CP included”:
all indicators are worse.

Compared to **MinRun6F4VP_Cor** “VP included”
all indicators are better:

- **Condition Number** is much lower (4,16 vs 27,23)
- **Variance Means** are more or less lower or equivalent (1,81 vs 8,73 ; 0,259 vs 0,361 ; 0,0486 vs 0,0481)
- as a consequence **G Efficiency** is much higher (46,67% vs 9,69%)
- **Scaled D-Opt. Crit.** Is lower (1,36 vs 1,48)
- **Det.** $\mathbf{(X'X)^{-1}}$ is lower (6,3E^{-29} vs 3,9E^{-28})
- **Trace** $\mathbf{(X'X)^{-1}}$ is lower (1,27 vs 1,71)
- **I (Cuboidal)** is lower (0,258 vs 0,361)

Thus for six Factors
the ***corrected*** **Rechtschaffner Matrix**
is a better Design than
the ***corrected*** **Min Run Characterization**.

Moreover it contains more runs to be realized with the “R” batch “Y ratio= 75,5 by Mw = 8821” than for the three other ones.

Rechtschaffner Matrix **corrected**

Design Evaluation of : **RS6F4VP_Cor** – "Verification points" excluded

Model Terms | Factorial Effects Aliases

Warning: Power not defined when the residual degrees of freedom are 0.

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2297	1,15101	0,1312	
B	0,2395	1,25191	0,2012	
C	0,2936	1,45164	0,3111	
D	0,2297	1,15101	0,1312	
E	0,2297	1,15101	0,1312	
F	0,2297	1,15101	0,1312	
AB	0,2393	1,24958	0,1997	
AC	0,2686	1,20905	0,1729	
AD	0,2270	1,12436	0,1106	
AE	0,2270	1,12436	0,1106	
AF	0,2270	1,12436	0,1106	
BC	0,2936	1,33251	0,2495	
BD	0,2393	1,24958	0,1997	
BE	0,2393	1,24958	0,1997	
BF	0,2393	1,24958	0,1997	
CD	0,2686	1,20905	0,1729	
CE	0,2686	1,20905	0,1729	
CF	0,2686	1,20905	0,1729	
DE	0,2270	1,12436	0,1106	
DF	0,2270	1,12436	0,1106	
EF	0,2270	1,12436	0,1106	

Compared to **RS6F4VP_Initial** for which all VIFs are worth 1,139 & all Ri² 0,1221 :
same situation as for "VF" included except that (B) comes just between (BC) & (AB BD BE BF) and would be less well estimated,

VIF don't overpass 1,46 an Ri² 0,32 which is very acceptable.

This contrasted situation means that:

- the "Main Effects" of "R - Mw" & "R – Y ratio", their common "2FI" and their "2FIs" with the four other Factors

will be less precisely estimated than:

- the "Main Effects" of the four other Factors and their "2FIs"

Compared to **MinRun6F4VP_Cor** "VP excluded":

- all VIF, Ri² and Standard Errors are more or less lower
- Power cannot be calculated as the Design is saturated

Thus for six Factors the ***corrected* Rechtschaffner Matrix** is a better Design than the ***corrected* Min Run Characterization**.

Rechtschaffner Matrix **corrected**
Design Evaluation of : **RS6F4VP_Cor** – "Verification points" excluded

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	4,39
Maximum Variance Mean	1,91
Average Variance Mean	0,2802
Minimum Variance Mean	0,0555
G Efficiency	52,27
Scaled D-optimality Criterion	1,19
Determinant of $(X'X)^{-1}$	1,36785E-28
Trace of $(X'X)^{-1}$	1,33
I (Cuboidal)	0,2796

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

Compared to **RS6F4VP_Initial** "CP excluded": all indicators are worse.

Compared to **MinRun6F4VP_Cor** "VP excluded" all indicators are better:

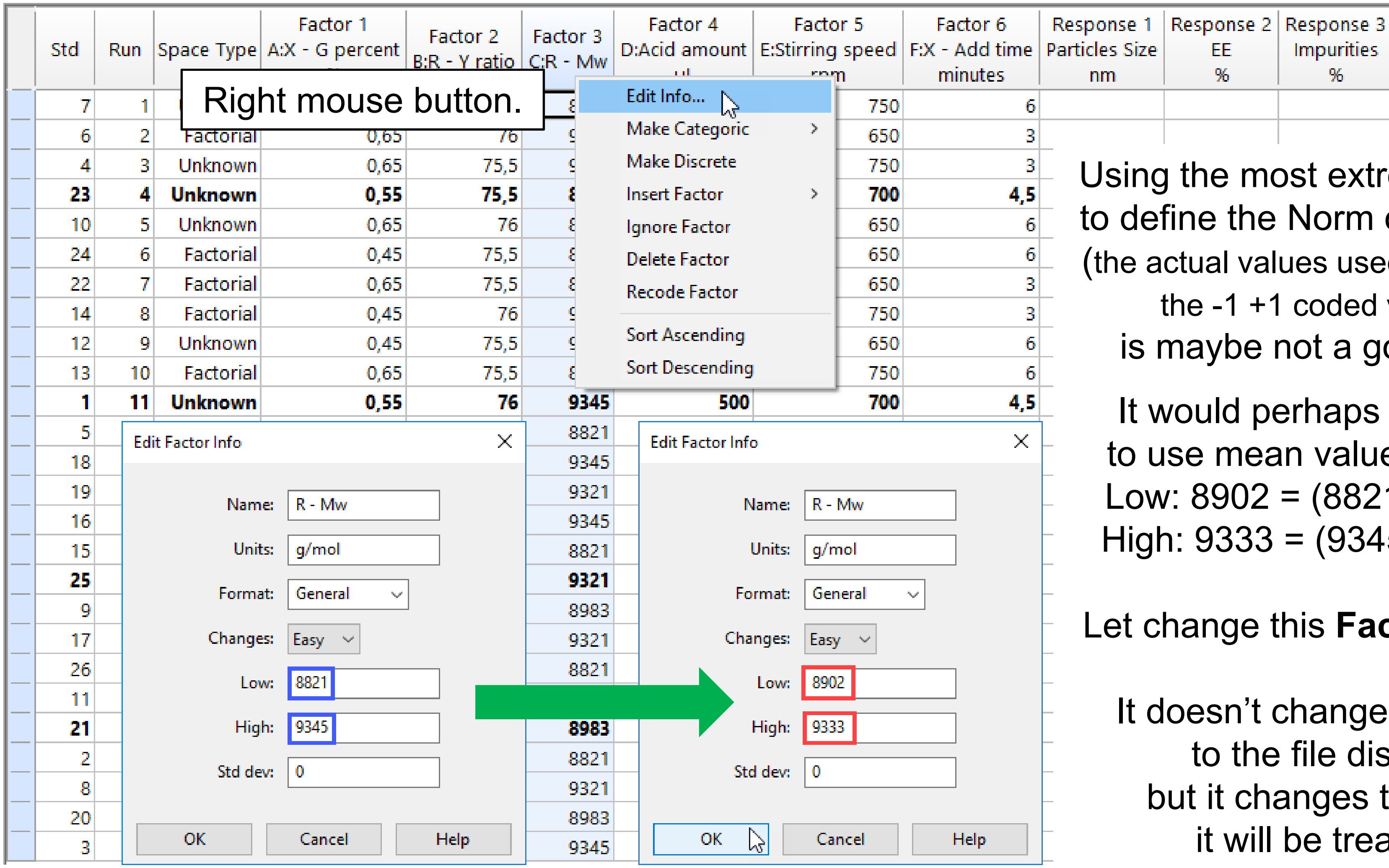
- **Condition Number** is much lower (4,39 vs 37,94)
- **Variance Means** are more or less lower (1,91 vs 12,22 ; 0,280 vs 0,438 ; 0,0555 vs 0,0567)
- as a consequence **G Efficiency** is much higher (52,27% vs 8,18%)
- **Scaled D-Opt. Crit.** is lower (1,19 vs 1,31) The only indicator which allows to validly compare Designs with different numbers of runs
- **Det. $(X'X)^{-1}$** is lower ($1{,}367E^{-28}$ vs $1{,}355E^{-27}$)
- **Trace $(X'X)^{-1}$** is lower (1,38 vs 1,98)
- **I (Cuboidal)** is lower (0,279 vs 0,439)

Thus for six Factors the ***corrected* Rechtschaffner Matrix** is a better Design than the ***corrected* Min Run Characterization**.

Moreover it contains more runs to be realized with the "R" batch "Y ratio= 75,5 by Mw = 8821" than for the three other ones.

Rechtschaffner Matrix **corrected**

Design Creation – Corrected Design – Modification of “R – Mw” Norm



Using the most extreme values to define the Norm of “R – Mw” (the actual values used to compute the -1 +1 coded values) is maybe not a good idea.

It would perhaps be better to use mean values instead
Low: 8902 = (8821+8983)/2
High: 9333 = (9345+9321)/2

Let change this **Factor Info** …

It doesn’t change anything to the file display but it changes the way it will be treated.

File saved as : ***RS6F4VP_Cor_Norm.dxpx***

Rechtschaffner Matrix **corrected & Norm changed**
Design Evaluation of : **RS6F4VP_Cor_Norm** – “Verification points” included

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2298	1,1533	0,1329	89,5 %
B	0,2137	1,17984	0,1524	93,0 %
C	0,2189	1,4	0,2857	91,9 %
D	0,2298	1,1533	0,1329	89,5 %
E	0,2298	1,1533	0,1329	89,5 %
F	0,2298	1,1533	0,1329	89,5 %
AB	0,2389	1,24701	0,1981	87,2 %
AC	0,2204	1,21768	0,1788	91,6 %
AD	0,2265	1,12105	0,1080	90,2 %
AE	0,2265	1,12105	0,1080	90,2 %
AF	0,2265	1,12105	0,1080	90,2 %
BC	0,2189	1,29809	0,2296	91,9 %
BD	0,2389	1,24701	0,1981	87,2 %
BE	0,2389	1,24701	0,1981	87,2 %
BF	0,2389	1,24701	0,1981	87,2 %
CD	0,2204	1,21768	0,1788	91,6 %
CE	0,2204	1,21768	0,1788	91,6 %
CF	0,2204	1,21768	0,1788	91,6 %
DE	0,2265	1,12105	0,1080	90,2 %
DF	0,2265	1,12105	0,1080	90,2 %
EF	0,2265	1,12105	0,1080	90,2 %

Compared to the corrected situation before Norm change:

- VIF & Ri^2 are not or little modified except for B for which they are lower
- Standard Error & Power are not or little modified except for C and all its “2FIs” with all other Factors for which they are enhanced

VIF don’t overpass 1,4 an Ri^2 0,29 which is very acceptable.

The Norm change will improve estimation of B,C and its “2FIs”.

$$VIF = \frac{1}{1 - Ri^2}$$

Rechtschaffner Matrix **corrected & Norm changed**
Design Evaluation of : **RS6F4VP_Cor_Norm** – "Verification points" included

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	3,79
Maximum Variance Mean	1,51
Average Variance Mean	0,2357
Minimum Variance Mean	0,0459
G Efficiency	56,08
Scaled D-optimality Criterion	1,22
Determinant of $(X'X)^{-1}$	6,0867E-30
Trace of $(X'X)^{-1}$	1,13
I (Cuboidal)	0,2357

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

Compared to the corrected situation **before Norm change** all indicators are better.

- **Condition Number** is lower (3,79 vs 4,16)
- **Variance Means** are more or less lower (1,51 vs 1,81 ; 0,236 vs 0,259 ; 0,0459 vs 0,0486)
- as a consequence **G Efficiency** is higher (56,08% vs 46,67%)
- **Scaled D-Opt. Crit.** is lower (1,22 vs 1,36)
- **Det. $(X'X)^{-1}$** is lower ($6{,}09E^{-30}$ vs $6{,}35E^{-29}$)
- **Trace $(X'X)^{-1}$** is lower (1,13 vs 1,27)
- **I (Cuboidal)** is lower (0,236 vs 0,258)

Thus for six Factors ***changing the Norm*** of the ***corrected*** **Rechtschaffner Matrix** results in a better Design.

Beware :
The "R – Mw" Norm is different, so it's variation range is smaller and the global design space volume also.
As the Maximum Variance Mean is usually observed in a corner of the design space it's value and thus the **G Efficiency** one can be fallacious.

It is the solution which was implemented.

Rechtschaffner Matrix **corrected & Norm changed**

Design Evaluation of : **RS6F4VP_Cor_Norm** – “Verification points” excluded

Model Terms | Factorial Effects Aliases

Warning: Power not defined when the residual degrees of freedom are 0.

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2302	1,1562	0,1351	
B	0,2353	1,20769	0,1720	
C	0,2415	1,45164	0,3111	
D	0,2302	1,1562	0,1351	
E	0,2302	1,1562	0,1351	
F	0,2302	1,1562	0,1351	
AB	0,2393	1,24958	0,1997	
AC	0,2209	1,22176	0,1815	
AD	0,2270	1,12436	0,1106	
AE	0,2270	1,12436	0,1106	
AF	0,2270	1,12436	0,1106	
BC	0,2415	1,33928	0,2533	
BD	0,2393	1,24958	0,1997	
BE	0,2393	1,24958	0,1997	
BF	0,2393	1,24958	0,1997	
CD	0,2209	1,22176	0,1815	
CE	0,2209	1,22176	0,1815	
CF	0,2209	1,22176	0,1815	
DE	0,2270	1,12436	0,1106	
DF	0,2270	1,12436	0,1106	
EF	0,2270	1,12436	0,1106	

Compared to the corrected situation before Norm change:

- VIF & Ri² are not or little modified except for B for which they are lower
- Standard Error & Power are not or little modified except for C and all its “2FIs” with all other Factors for which they are enhanced

VIF don’t overpass 1,46 an Ri² 0,32 which is very acceptable.

The Norm change will improve estimation of B,C and its “2FIs”.

$$VIF = \frac{1}{1 - Ri^2}$$

Rechtschaffner Matrix **corrected & Norm changed**

Design Evaluation of : **RS6F4VP_Cor_Norm** – “Verification points” excluded

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

	Description	Value
	Condition Number of Coefficient Matrix	4,09
	Maximum Variance Mean	1,58
	Average Variance Mean	0,2560
	Minimum Variance Mean	0,0541
	G Efficiency	63,42
	Scaled D-optimality Criterion	1,07
	Determinant of $(X'X)^{-1}$	1,31157E-29
	Trace of $(X'X)^{-1}$	1,18
	I (Cuboidal)	0,2550

If the condition number is 100-1000, there is moderate to strong multicollinearity. Values above 1000 indicate severe multicollinearity.

When comparing designs, a smaller Scaled D-optimality Criterion is better.

The determinant, trace, and 'I' values can only be used when comparing designs with the same number of runs. A smaller value is better.

Compared to the corrected situation **before Norm change** all indicators are better.

- **Condition Number** is lower (4,09 vs 4,39)
- **Variance Means** are more or less lower (1,58 vs 1,91 ; 0,256 vs 0,280 ; 0,054 vs 0,055)
- as a consequence **G Efficiency** is higher (63,42% vs 52,27%)
- **Scaled D-Opt. Crit.** is lower (1,07 vs 1,19)
- **Det.** $\mathbf{(X'X)^{-1}}$ is lower ($1,31E^{-29}$ vs $1,37E^{-28}$)
- **Trace** $\mathbf{(X'X)^{-1}}$ is lower (1,18 vs 1,33)
- **I (Cuboidal)** is lower (0,255 vs 0,279)

Thus for six Factors ***changing the Norm*** of the ***corrected*** **Rechtschaffner Matrix** results in a better Design.

According to **Scaled D-Opt. Crit.** the Design “VP” excluded is better than “VP” included.

It is the solution which was implemented.

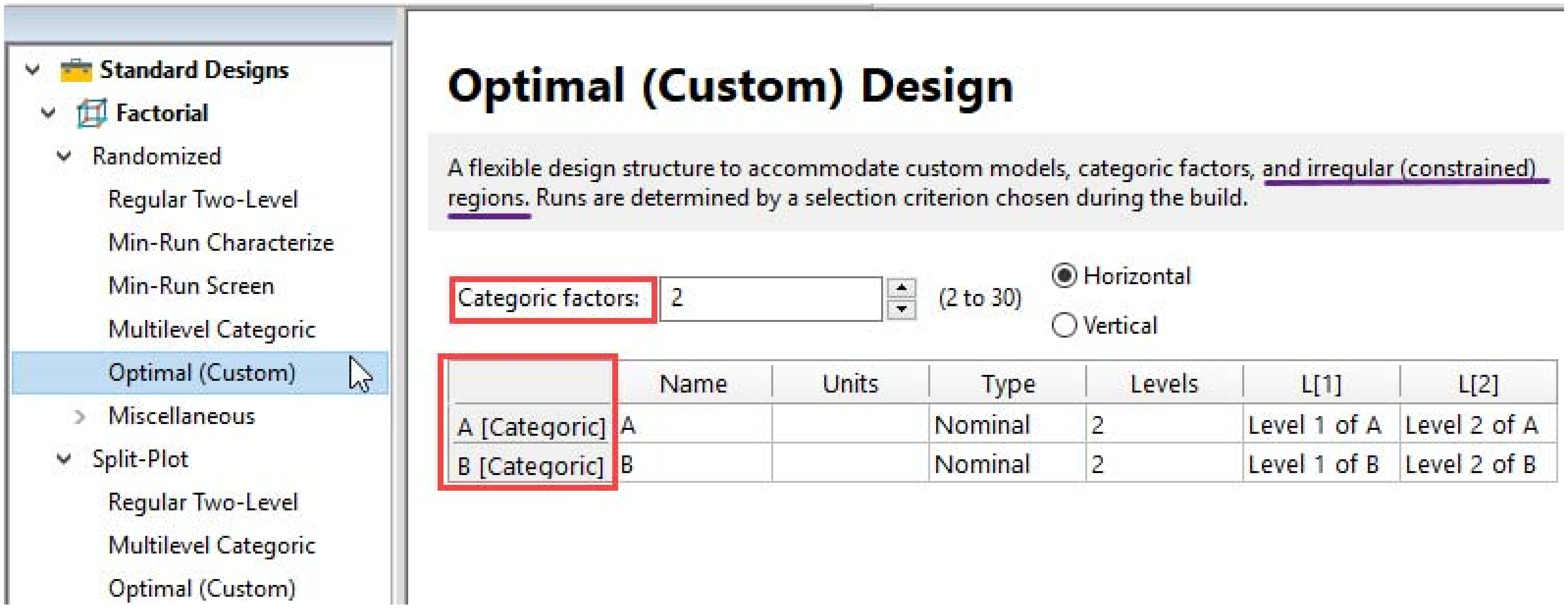
Creating a

Constrained Optimal (Custom) Design

Evaluating it

including and excluding Verification Points

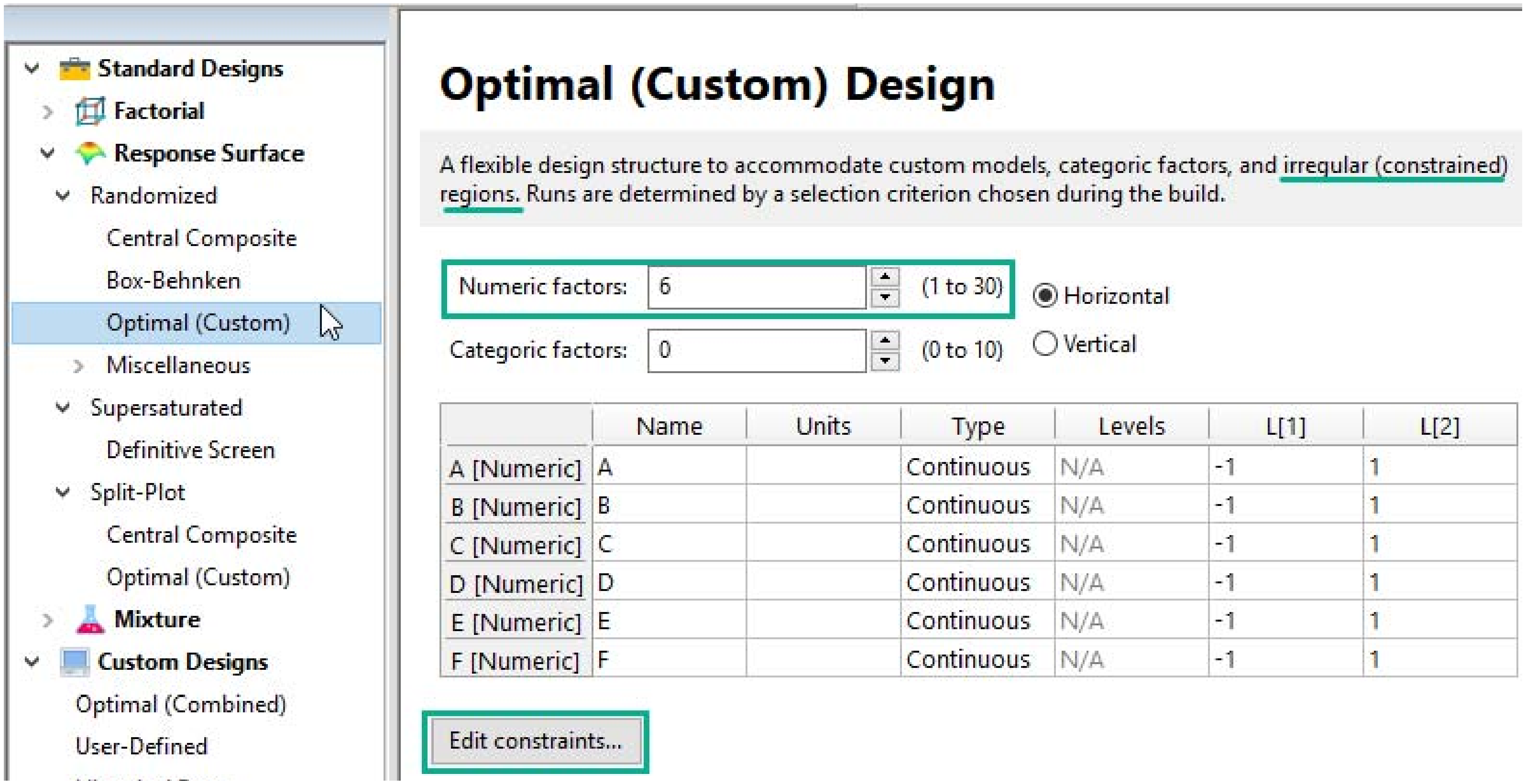
Constrained Optimal (Custom) Design
Design Creation



The Design Expert “Factorial” entry proposes to built “Optimal (Custom)” designs but it allows to take into account only “Categoric factors” although the definition talks about “irregular (constrained) regions” which apply only to “Numeric factors”.

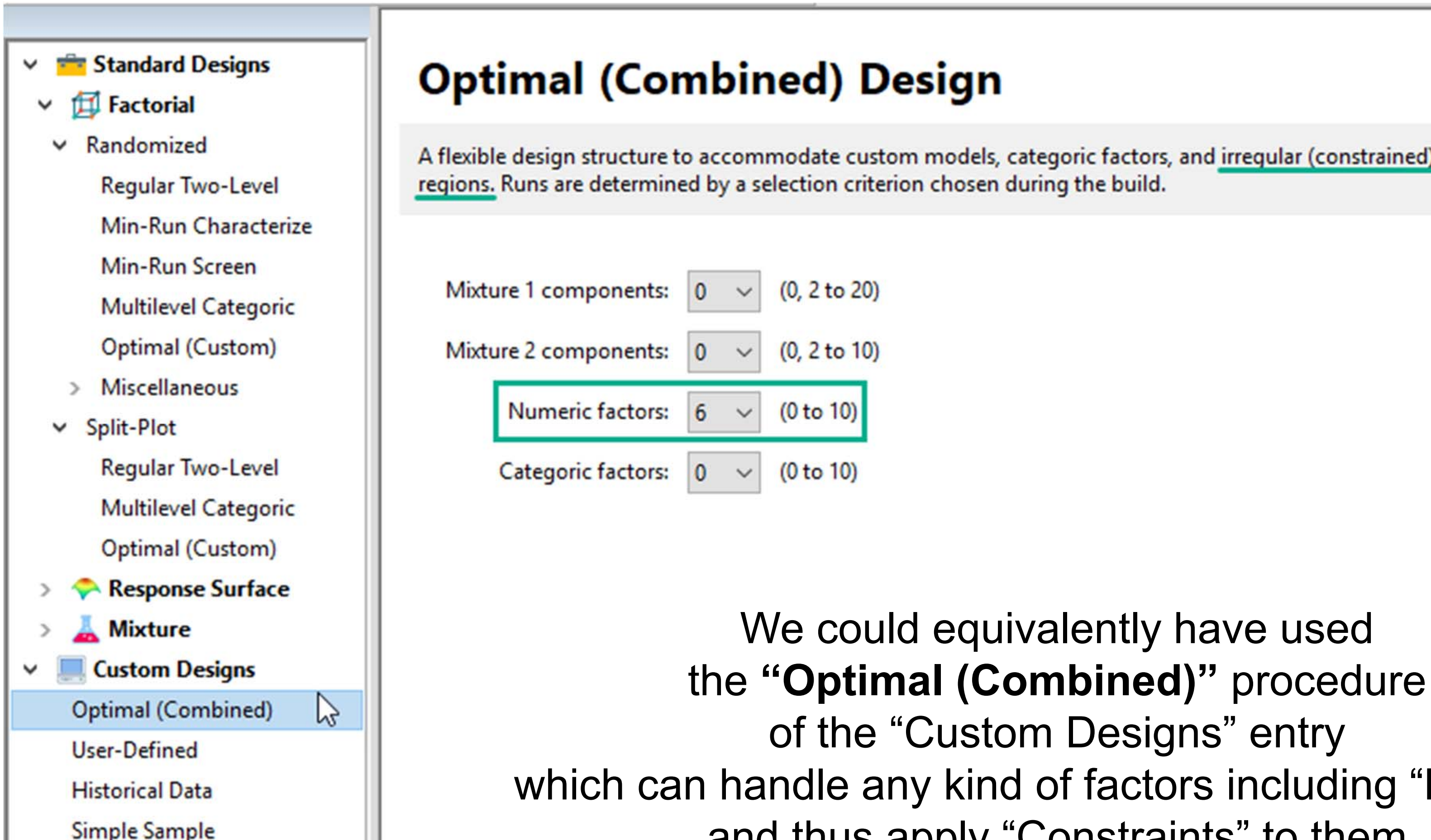
So this procedure isn’t appropriate.

Constrained Optimal (Custom) Design
Design Creation



We **will use instead** the “Optimal (Custom)” procedure
of the “Response Surface” entry
which is intended to handle “Numeric factors”
and thus apply “Constraints” to them
optionally in association with “Categoric factors.

Constrained Optimal (Custom) Design
Design Creation



We could equivalently have used
the **"Optimal (Combined)"** procedure
of the "Custom Designs" entry
which can handle any kind of factors including "Numeric"
and thus apply "Constraints" to them
(and/or to "Mixture … components").

Constrained Optimal (Custom) Design
Design Creation – Defining “Factors” and Editing “Constraints”

- Standard Designs
  - Factorial
  - Response Surface
    - Randomized
      - Central Composite
      - Box-Behnken
      - Optimal (Custom)
    - Miscellaneous
    - Supersaturated
      - Definitive Screen
    - Split-Plot
      - Central Composite
      - Optimal (Custom)
  - Mixture
- Custom Designs
  - Optimal (Combined)
  - User-Defined

Optimal (Custom) Design

A flexible design structure to accommodate custom models, categoric factors, and irregular (constrained) regions. Runs are determined by a selection criterion chosen during the build.

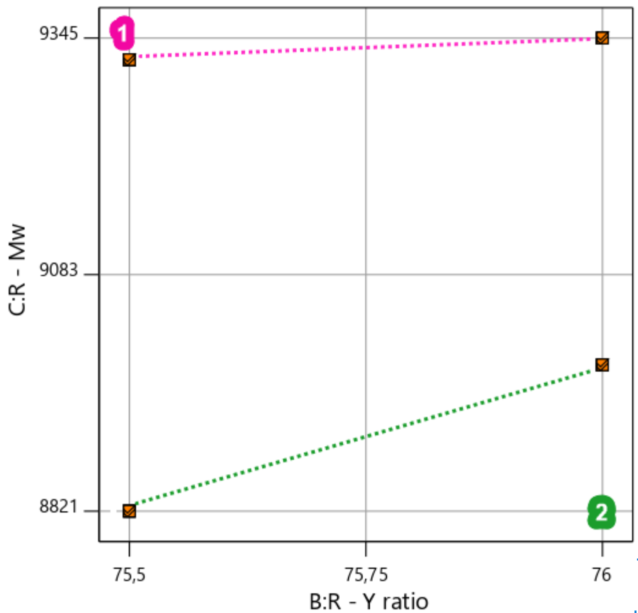
Numeric factors: 6 (1 to 30) ◉ Horizontal

Categoric factors: 0 (0 to 10) ○ Vertical

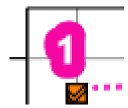
	Name	Units	Type	Levels	L[1]	L[2]
A [Numeric]	X - G percent	%	Continuous	N/A	0,45	0,65
B [Numeric]	R - Y ratio	%	Continuous	N/A	75,5	76
C [Numeric]	R - Mw	g/mol	Continuous	N/A	8821	9345
D [Numeric]	Acid amount	µL	Continuous	N/A	300	700
E [Numeric]	Stirring spee	rpm	Continuous	N/A	650	750
F [Numeric]	X - Add time	minutes	Continuous	N/A	3	6

Edit constraints...

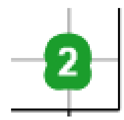
Constrained Optimal (Custom) Design
Design Creation – Defining “Constraints”



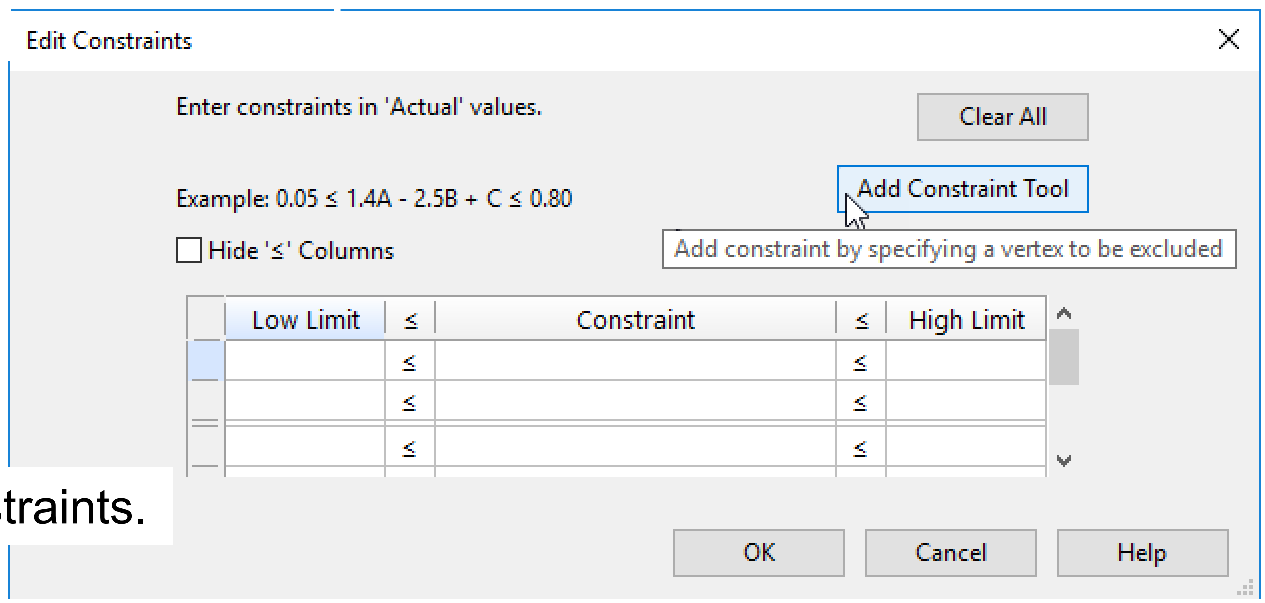
We want to exclude vertices according to the dotted lines:



75,5 vs **9321** instead of 75,5 vs 9345



76,0 vs **8983** instead of 76,0 vs 8821



We have to define two constraints.

Constrained Optimal (Custom) Design

Design Creation – Defining "Constraint "

Edit Constraints

In the Vertex field enter the coordinates in actual values for the combination you want to exclude.

Then enter in the Constraint Point field the level for each factor where it becomes feasible to run.

Finally, click the '<> skip' field to designate for each factor whether it must exceed (>) the Constraint Point or fall below it (<). If a factor is not involved, leave it as is or set it to 'skip'.

When done, click the OK button. Press Help for further guidance and examples.

	Name	Low Actual	High Actual	Vertex	< > skip	Constraint Point
A:	X - G	0,45	0,65	0,65	skip	0,65
B:	R - Y r	75,5	76	75,5	B >	76
C:	R - M	8821	9345	9345	C <	9321
D:	Acid a	300	700	700	skip	700
E:	Stirrin	650	750	750	skip	750
F:	X - Ad	3	6	6	skip	6

OK Cancel Help

Vertex to be excluded

B can vary up to 76

C must be less than 9321

Not concerned "Factors" A, D, E & F set to "skip"

The first constraint is expressed as the beside linear combination

	Low Limit	≤	Constraint	≤	High Limit
		≤	-24 B +0,5 C	≤	2848,5
		≤		≤	

Constrained Optimal (Custom) Design

Design Creation – Defining "Constraint 2"

Edit Constraints

In the Vertex field enter the coordinates in actual values for the combination you want to exclude.

Then enter in the Constraint Point field the level for each factor where it becomes feasible to run.

Finally, click the '<> skip' field to designate for each factor whether it must exceed (>) the Constraint Point or fall below it (<). If a factor is not involved, leave it as is or set it to 'skip'.

When done, click the OK button. Press Help for further guidance and examples.

	Name	Low Actual	High Actual	Vertex	< > skip	Constraint Point
A:	X - G	0,45	0,65	0,65	skip	0,65
B:	R - Y r	75,5	76	76	B <	75,5
C:	R - Mv	8821	9345	8821	C >	8983
D:	Acid a	300	700	700	skip	700
E:	Stirrin	650	750	750	skip	750
F:	X - Ad	3	6	6	skip	6

OK | Cancel | Help

Vertex to be excluded

B can vary down to 75,5

C must be greater than 8983

Not concerned "Factors" A, D, E & F set to "skip"

The second constraint is expressed as the beside linear combination

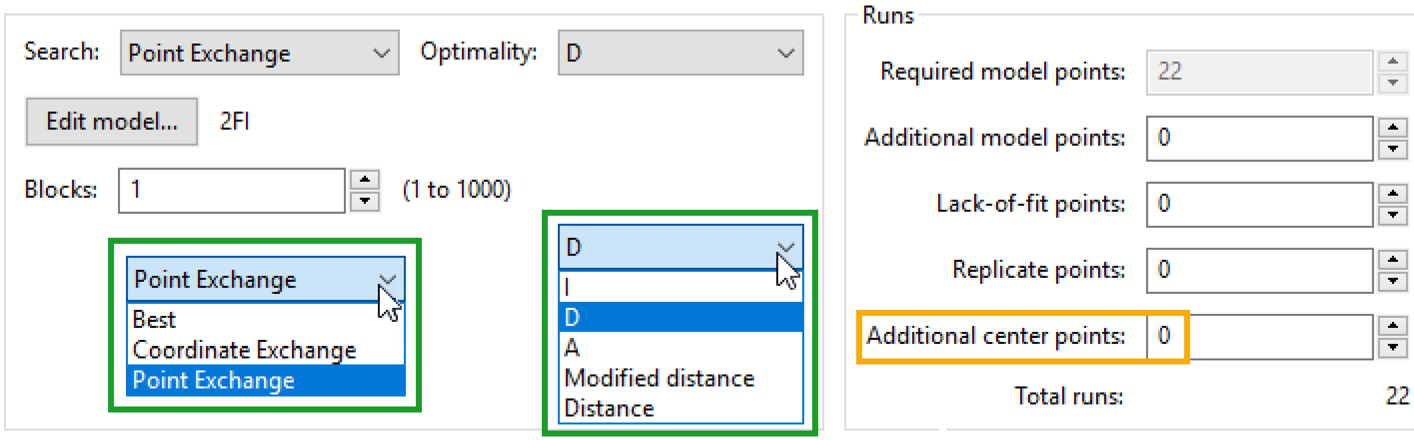
Low Limit	≤	Constraint	≤	High Limit
	≤	-24 B +0,5 C	≤	2848,5
	≤	+162 B -0,5 C	≤	7820,5

Next >>

Constrained Optimal (Custom) Design

Design Creation – Defining “Search” method / “Optimality” criterion / “Model” / “Run” numbers

Optimal (Custom) Design



We want a saturated Design. So no more runs than the number required to estimate the 22 “Model” coefficients.

Point Exchange searches a set of candidates for the best design points. The candidates can be generated by the program, or read in from a file.

D-optimality produces a design that best estimates the effects of the factors, which is particularly suited for screening studies. The algorithm picks points that minimize the volume of the confidence ellipsoid for the coefficients (i.e. it minimizes the determinant of the X'X inverse matrix).

We could have added 4 “Centre points” and then correct them as “Verifi. points”. We prefer to directly add 4 “Verif. points” after having created the saturated Design.

Edit candidate points... Options...

“Point Exchange” to be sure that only the vertices will be selected

“D Optimality” because we want to create a “Screening Design”…

… and the goal of “Screening Designs” is to estimate Effects as precisely as possible.

Optimal (Custom) Design

Responses: 3 (1 to 999)

Name	Units
Particles Size	nm
EE	%
Impurities	%

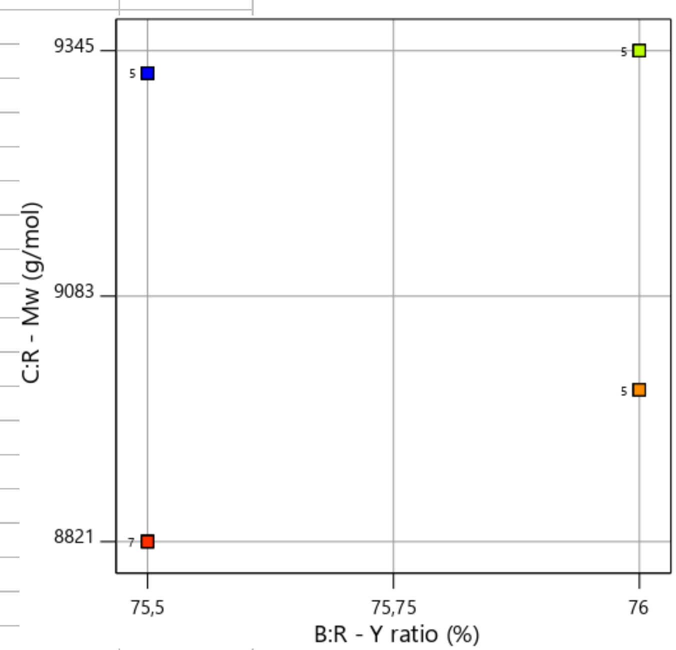
Finish

Constrained Optimal (Custom) Design

Design Creation – Defining "Responses" / Resulting Design

After several sequences of Design Creation the following Design is generated in which there are more runs for "R" batch [75,5 / 8821] as for the three other batches

Run	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio %	Factor 3 C:R - Mw g/mol	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
1	0,45	75,5	9321	700	750	6			
2	0,65	75,5	8821	700	750	3			
3	0,65	75,5	9321	300	650	6			
4	0,65	76	8983	300	750	3			
5	0,65	75,5	8821	300	650	3			
6	0,45	76	8983	300	650	3			
7	0,65	75,5	9321	700	650	3			
8	0,45	76	9345	700	650	6			
9	0,65	75,5	8821	700	650	6			
10	0,45	76	9345	700	750	3			
11	0,45	75,5	8821	300	650	6			
12	0,45	75,5	9321	300	650	3			
13	0,65	75,5	9321	300	750	3			
14	0,45	75,5	8821	700	650	3			
15	0,65	76	8983	700	650	3			
16	0,65	76	9345	700	750	6			
17	0,65	76	8983	300	650	6			
18	0,45	76	9345	300	750	6			
19	0,45	75,5	8821	300	750	3			
20	0,45	76	8983	700	750	6			
21	0,65	76	9345	300	650	3			
22	0,65	75,5	8821	300	750	6			



File saved as : ***DOpt6F_Cnstrnt.dxpx***

Constrained Optimal (Custom) Design

Design Creation – Adding “Verification points”

18	0,45	76	9345	300	750	6
19	0,45	75,5	8821	300	750	3
20	0,45	76	8983	700	750	6
21	0,65	76	9345	300	650	3
22	0,65	75,5	8821	300	750	6

- Insert Row(s) >
  - Before This Row
  - After This Row
- Set Row Status >
- Delete Row(s)
- Duplicate
- Edit Comment

Right Mouse Button

18	0,45	76	9345	300	750	6
19	0,45	75,5	8821	300	750	3
20	0,45	76	8983	700	750	6
21	0,65	76	9345	300	650	3
22	0,65	75,5	8821	300	750	6
~~23~~						
~~24~~						
~~25~~						
~~26~~						

Cells to be filled in by hand.

18	0,45	76	9345	300	750	6
19	0,45	75,5	8821	300	750	3
20	0,45	76	8983	700	750	6
21	0,65	76	9345	300	650	3
22	0,65	75,5	8821	300	750	6
23	0,55	75,5	9321	500	700	4,5
24	0,55	76	8983	500	700	4,5
25	0,55	75,5	8821	500	700	4,5
26	0,55	76	9345	500	700	4,5

Run	Factor 1 A:X - G percent	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw

- Randomize...
- Re-Order as Currently Displayed
- Hide Run Order
- Sort Ascending
- Sort Descending

At the end it’s cautious to “Randomize” all the runs

Constrained Optimal (Custom) Design

Design Creation – Resulting reordered Design

Run	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio %	Factor 3 C:R - Mw g/mol	Factor 4 D:Acid amount µL	Factor 5 E:Stirring speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE %	Response 3 Impurities %
1	0,65	76	8983	700	650	3			
2	0,65	76	8983	300	750	3			
3	0,55	75,5	9321	500	700	4,5			
4	0,65	76	9345	300	650	3			
5	0,45	76	8983	300	650	3			
6	0,45	75,5	8821	700	650	3			
7	0,65	75,5	9321	300	650	6			
8	0,65	75,5	8821	300	650	3			
9	0,45	75,5	8821	300	650	6			
10	0,45	76	9345	300	750	6			
11	0,65	76	8983	300	650	6			
12	0,55	76	9345	500	700	4,5			
13	0,65	75,5	8821	700	650	6			
14	0,45	75,5	9321	700	750	6			
15	0,45	76	9345	700	750	3			
16	0,45	75,5	8821	300	750	3			
17	0,55	76	8983	500	700	4,5			
18	0,45	75,5	9321	300	650	3			
19	0,45	76	9345	700	650	6			
20	0,65	76	9345	700	750	6			
21	0,65	75,5	8821	700	750	3			
22	0,55	75,5	8821	500	700	4,5			
23	0,65	75,5	9321	300	750	3			
24	0,45	76	8983	700	750	6			
25	0,65	75,5	9321	700	650	3			
26	0,65	75,5	8821	300	750	6			

Table after Randomization

File saved as : ***DOpt6F4VP_Cnstrnt.dxpx***

Constrained Optimal (Custom) Design

Design Evaluation of : **DOpt6F4VP_Cnstrnt** – "Verification points" included

Model Terms | Alias Matrix

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2292	1,14766	0,1287	89,6 %
B	0,2177	1,2251	0,1837	92,2 %
C	0,2661	1,4	0,2857	79,9 %
D	0,2292	1,14766	0,1287	89,6 %
E	0,2292	1,14766	0,1287	89,6 %
F	0,2292	1,14766	0,1287	89,6 %
AB	0,2389	1,24701	0,1981	87,2 %
AC	0,2680	1,2046	0,1699	79,4 %
AD	0,2265	1,12105	0,1080	90,2 %
AE	0,2265	1,12105	0,1080	90,2 %
AF	0,2265	1,12105	0,1080	90,2 %
BC	0,2661	1,29697	0,2290	79,9 %
BD	0,2389	1,24701	0,1981	87,2 %
BE	0,2389	1,24701	0,1981	87,2 %
BF	0,2389	1,24701	0,1981	87,2 %
CD	0,2680	1,2046	0,1699	79,4 %
CE	0,2680	1,2046	0,1699	79,4 %
CF	0,2680	1,2046	0,1699	79,4 %
DE	0,2265	1,12105	0,1080	90,2 %
DF	0,2265	1,12105	0,1080	90,2 %
EF	0,2265	1,12105	0,1080	90,2 %

The **Model Terms** table is perfectly identical to that of Rechtschaffner Matrix corrected **…**

… in the **Matrix Measures** table:

- **Condition Number**, **Scaled D-Optimality Crit.**, **Det. (X'X)$^{-1}$** & **Trace (X'X)$^{-1}$** are perfectly identical to that of Rechtschaffner Matrix corrected
- **Variance(s)** & **I** are lower and, as a consequence, **G Efficiency** is higher.
  This is due to the fact that the Constraint Domain volume is smaller than the Unconstraint one

Those two Designs do not consist of exactly the same runs but are perfectly symmetric.

We could have obtained the same result by the use of a Rechtschaffner Matrix with reversed extreme -1/+1 values for some Factors.

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	4,16
Maximum Variance Mean	1,22
Average Variance Mean	0,2305
Minimum Variance Mean	0,0447
G Efficiency	69,39
Scaled D-optimality Criterion	1,36
Determinant of $(X'X)^{-1}$	6,3479E-29
Trace of $(X'X)^{-1}$	1,27
I	0,2300

Constrained Optimal (Custom) Design
Design Evaluation of : **HD_DOpt6F4VP_Cnstrnt** – "Verification points" included

Model Terms | Alias Matrix

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2292	1,14766	0,1287	89,6 %
B	0,2177	1,2251	0,1837	92,2 %
C	0,2661	1,4	0,2857	79,9 %
D	0,2292	1,14766	0,1287	89,6 %
E	0,2292	1,14766	0,1287	89,6 %
F	0,2292	1,14766	0,1287	89,6 %
AB	0,2389	1,24701	0,1981	87,2 %
AC	0,2680	1,2046	0,1699	79,4 %
AD	0,2265	1,12105	0,1080	90,2 %
AE	0,2265	1,12105	0,1080	90,2 %
AF	0,2265	1,12105	0,1080	90,2 %
BC	0,2661	1,29697	0,2290	79,9 %
BD	0,2389	1,24701	0,1981	87,2 %
BE	0,2389	1,24701	0,1981	87,2 %
BF	0,2389	1,24701	0,1981	87,2 %
CD	0,2680	1,2046	0,1699	79,4 %
CE	0,2680	1,2046	0,1699	79,4 %
CF	0,2680	1,2046	0,1699	79,4 %
DE	0,2265	1,12105	0,1080	90,2 %
DF	0,2265	1,12105	0,1080	90,2 %
EF	0,2265	1,12105	0,1080	90,2 %

If we paste the **DOpt6F4VP_Cnstrnt** runs into a "Historical Data" file with same Factors & Response definition but <u>without Constraints</u> and Evaluate it relatively to the same "Model" (<u>2FI</u>) …
(File : ***HD_DOpt6F4VP_NC***)

… the **Model Terms** table <u>remains identical</u>…

… in the **Matrix Measures** table:

- **Condition Number**, **Scaled D-Optimality Crit.** **Det. $(X'X)^{-1}$** & **Trace $(X'X)^{-1}$** <u>remain identical</u>
- …

- **…**
- **Max.Var.Mean & I** <u>become identical</u> and **G Efficiency** <u>also</u>
- Avg & Min. Var.Mean become almost identical

This **D Optimal Design** is <u>perfectly equivalent</u> to the **Corrected Rechtschaffner Matrix**

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	4,16
Maximum Variance Mean	1,81
Average Variance Mean	0,2581
Minimum Variance Mean	0,0487
G Efficiency	46,67
Scaled D-optimality Criterion	1,36
Determinant of $(X'X)^{-1}$	6,3479E-29
Trace of $(X'X)^{-1}$	1,27
I (Cuboidal)	0,2579

Constrained Optimal (Custom) Design
Design Evaluation of : **HD_DOpt6F4VP_Cnstrnt** – “Verification points” included

Of course evaluating this D Optimal Design in all the other ways
(“Verification points” excluded & “R – Mw” Norm change)
gives equivalent results.

[Note that Design Expert doesn’t allow to change a Norm for a Constrained Design without either changing the Constraint(s) or the run levels]

We can so conclude that correcting the runs
of a perfectly orthogonal or close to orthogonality Design
is equivalent or almost equivalent
to create a D Optimal Constrained Design
at least when the Constraint(s) result in an Experimental Domain with the same number of vertices as the original one.

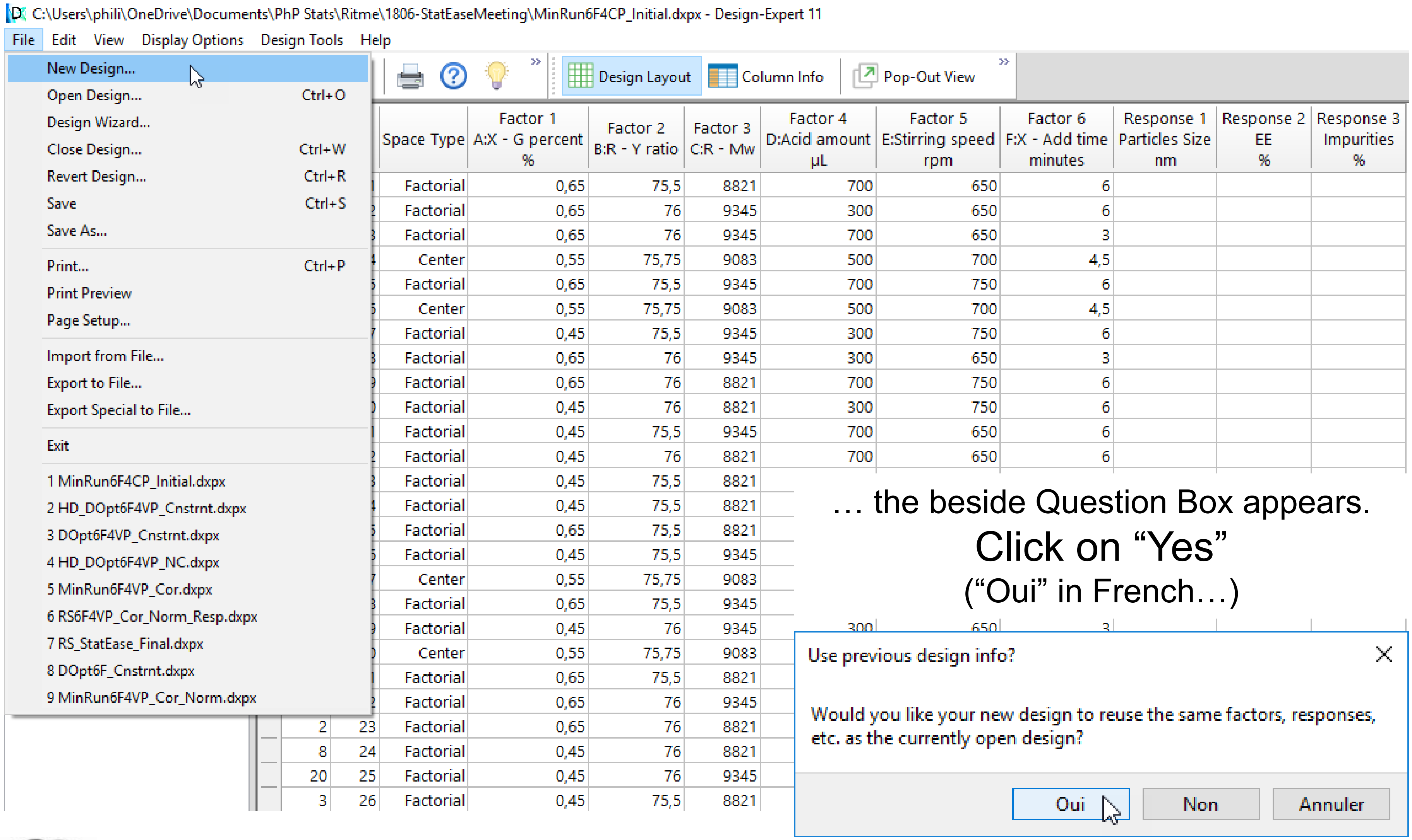
Trick

to quickly create a New Design with same Factor & Response Definition as an existing one.

Design Expert Trick

An existing Design being displayed (here : ***MinRun6F4CP_Initial.dxpx***)

click on File / New Design…



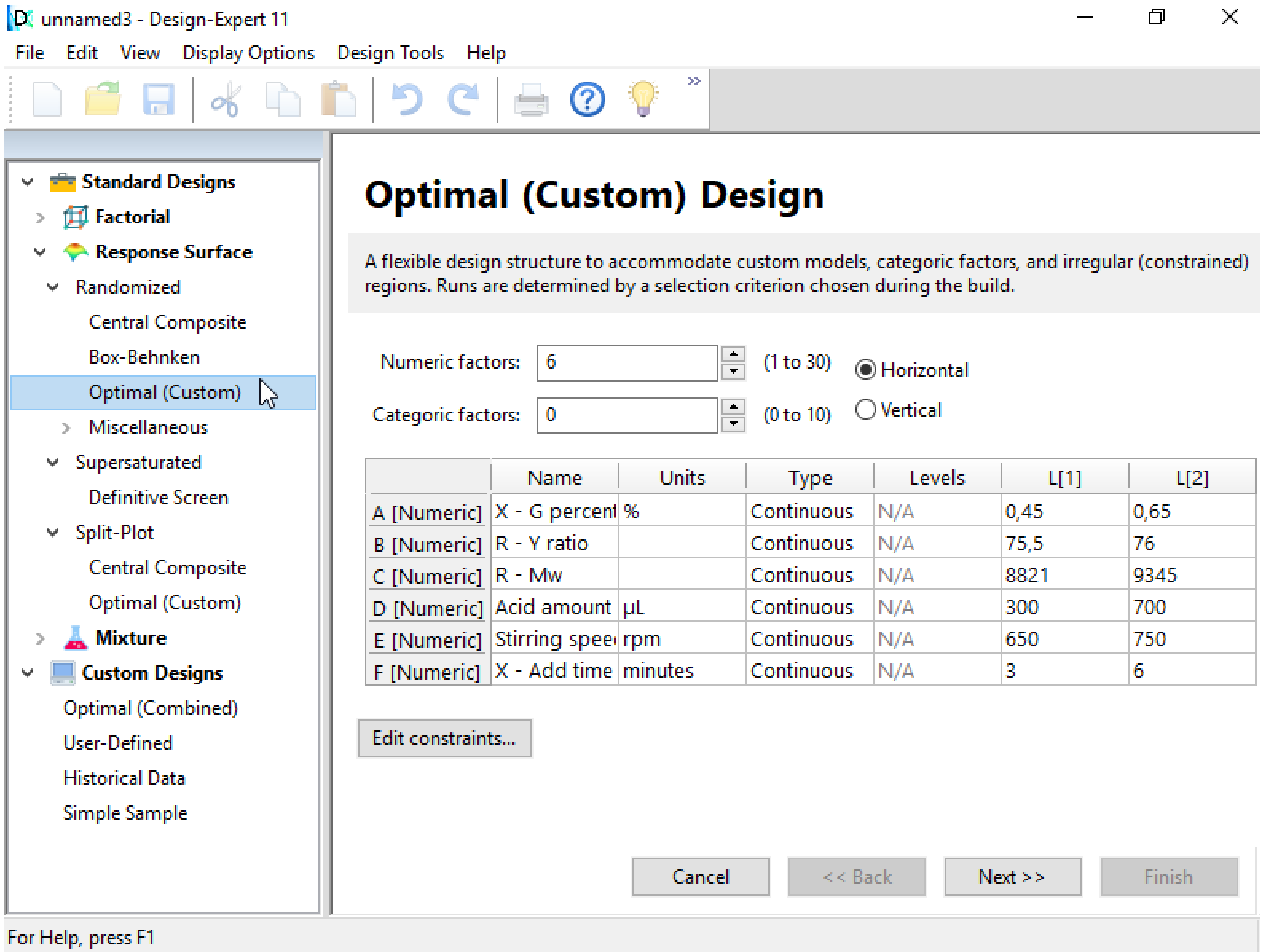
… the beside Question Box appears.

Click on "Yes"

("Oui" in French…)

Design Expert Trick

… and one will get the opportunity of creating a new design of the same type or a different one based on the same Factors & Responses which can be eventually completed or modified:



What to do ex-post when some levels do not meet the initial values?

Evaluation is still useful.

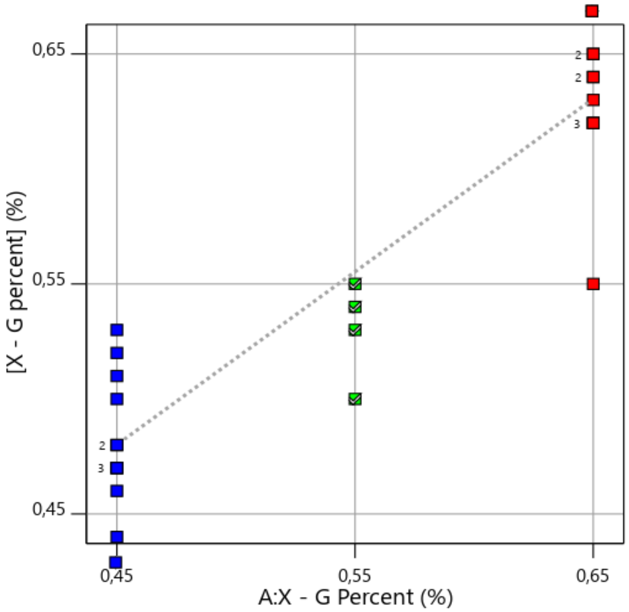
What to do ex-post?

The table below displays the final results including Responses.
As feared from the beginning actual values for Factors
“X – G percent” “Stirring speed” & “X – Add time”
are more or less different from the initial ones.

Std	Run	Factor 1 A:X - G percent %	Factor 2 B:R - Y ratio	Factor 3 C:R - Mw	Factor 4 D:Acid amount µL	Factor 5 E:Stirring Speed rpm	Factor 6 F:X - Add time minutes	Response 1 Particles Size nm	Response 2 EE	Response 3 Impurities %
12	1	0,53	76	8983	700	750	6,25	239	98,2	0,62
4	2	0,64	76	9345	300	650	3,23	400	98,5	0,68
3	3	0,67	75,5	9321	300	748	3,27	236	98,3	0,51
23	**4**	**0,55**	**75,5**	**8821**	**500**	**702**	**3,45**	**252**	**98,6**	**1,18**
1	5	0,65	76	8983	700	650	6,13	382	99	0,91
8	6	0,52	75,5	8821	700	648	5,2	235	98,3	1,16
19	7	0,63	75,5	8821	700	649	3,23	349	98,5	0,48
15	8	0,47	76	9345	300	751	3,33	230	97,8	0,91
22	9	0,42	75,5	9321	300	647	5,58	202	97,5	1,01
16	10	0,62	75,5	8821	700	751	5,85	222	98,4	0,77
24	**11**	**0,53**	**76**	**9345**	**500**	**699**	**4,5**	**282**	**98,2**	**0,8**
7	12	0,47	75,5	8821	300	751	5,83	178	97,7	0,99
18	13	0,62	76	9345	700	749	3,4	280	98,2	0,42
21	14	0,48	75,5	9321	700	649	3,18	243	98,3	0,55
14	15	0,55	76	9345	300	751	6	274	98,4	0,74
20	16	0,48	75,5	8821	300	649	3,23	217	97,7	0,92
25	**17**	**0,54**	**75,5**	**9321**	**500**	**700**	**4,43**	**230**	**98,1**	**0,64**
13	18	0,46	76	8983	300	650	5,7	250	98	1,35
11	19	0,47	75,5	9321	700	751	5,73	193	97,8	0,6
2	20	0,62	75,5	8821	300	651	5,82	254	97,8	0,65
9	21	0,5	76	8983	700	650	3,05	307	97,7	1,11
26	**22**	**0,5**	**76**	**8983**	**500**	**701**	**4,23**	**280**	**98,2**	**1,18**
17	23	0,44	75,5	8821	700	751	3,25	230	98,3	0,93
6	24	0,64	75,5	9321	700	651	5,93	290	98,8	0,82
5	25	0,65	76	8983	300	749	3,25	255	98,2	0,95

File saved as : ***RS6F4VP_Cor_Norm_Resp.dxpx***

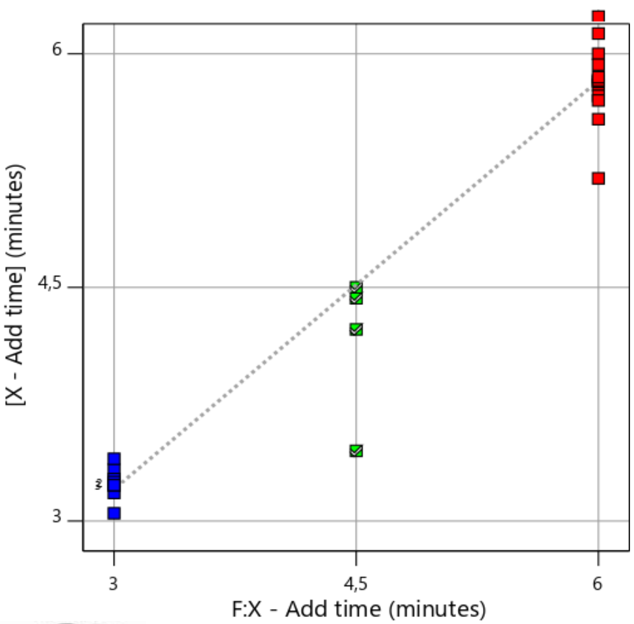
What to do ex-post?



For “X – G percent” we have the beside and following situation:

Initial Values	Observed Values	
	Mean	*Std Dev.*
0,45	0,48	*0,032*
0,55	0,53	*0,022*
0,65	0,63	*0,032*

- Low values are higher
- High and intermediate values are lower
- Dispersion is wide compared to initial range but relatively homogeneous

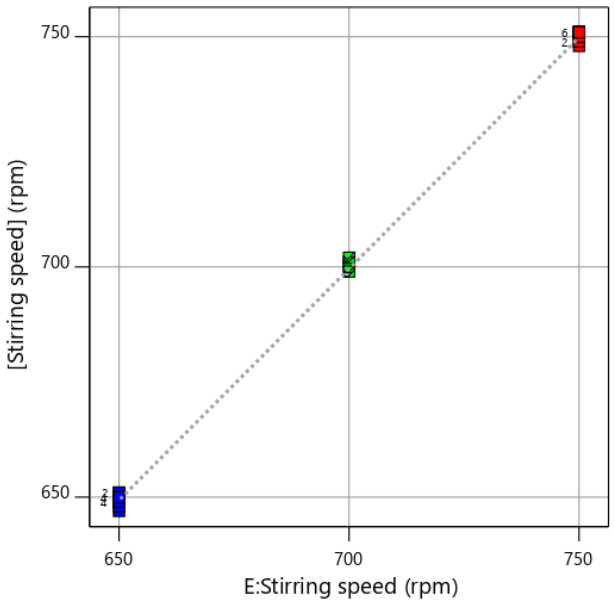


For “X – Add time” we have the beside and following situation:

Initial Values	Observed Values	
	Mean	*Std Dev.*
3	3,24	*0,09*
4,5	4,15	*0,48*
6	5,82	*0,27*

- Low values are higher
- High and intermediate values are lower
- Dispersion is wide compared to initial range and strongly heterogeneous

What to do ex-post?



For “Stirring speed” we have the beside and following situation:

Initial Values	Observed Values	
	Mean	*Std Dev.*
650	649,5	*1,16*
700	700,5	*1,29*
750	750,2	*1,13*

- Mean values are equivalent to initial
- Dispersion is small compared to initial range and relatively homogeneous

Two questions arise :

How much do those variations perturbate the Design Quality?

Is it interesting to correct the Norm for “X – G percent” & “X – Add time” the ranges of Means of which are smaller than the initial ranges?

(It’s obviously not necessary to ask the second question for “Stirring speed” the observed values of which are almost identical in mean to initial ones with small dispersion)

Constrained Optimal (Custom) Design

Design Evaluation of : **RS6F4VP_Cor_Norm_Resp** – "Verification points" included

Original Norm for "X – G percent" & "X – Add time"

Compared to the situation before correcting values of "X – G percent", "X – Add time" & "Stirring speed" (**RS6F4VP_Cor_Norm**)…

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,3165	1,45684	0,3136	66,2 %
B	0,2129	1,17182	0,1466	93,2 %
C	0,2198	1,41147	0,2915	91,7 %
D	0,2462	1,32452	0,2450	85,3 %
E	0,2315	1,19057	0,1601	89,0 %
F	0,2976	1,5195	0,3419	71,2 %
AB	0,2996	1,30371	0,2330	70,7 %
AC	0,2862	1,30021	0,2309	74,4 %
AD	0,3062	1,34012	0,2538	68,9 %
AE	0,3238	1,52314	0,3435	64,3 %
AF	0,3818	1,50831	0,3370	51,2 %
BC	0,2271	1,39722	0,2843	90,1 %
BD	0,2471	1,33395	0,2503	85,1 %
BE	0,2559	1,45546	0,3129	82,7 %
BF	0,2685	1,24063	0,1940	79,3 %
CD	0,2238	1,25505	0,2032	90,8 %
CE	0,2301	1,36039	0,2649	89,4 %
CF	0,2613	1,29298	0,2266	81,3 %
DE	0,2314	1,18973	0,1595	89,1 %
DF	0,2781	1,28098	0,2193	76,6 %
EF	0,2596	1,13887	0,1219	81,7 %

…**Std Errors**, **VIF** & **Ri²** are globally higher and **Power** globally lower, mainly for "X – G percent" & "X – Add time" and their interactions with all other Factors because those two Factors are the most perturbated…

…and all **Matrix Measures** are worse…

… thus,
as we could be afraid of,
this perturbated Design is worse…

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	6,85
Maximum Variance Mean	2,73
Average Variance Mean	0,3070
Minimum Variance Mean	0,0477
G Efficiency	30,98
Scaled D-optimality Criterion	1,54
Determinant of $(X'X)^{-1}$	9,89525E-28
Trace of $(X'X)^{-1}$	1,58
I (Cuboidal)	0,3079

… but it is largely better than
the Corrected Min. Run Characterization Design
and remains acceptable

Constrained Optimal (Custom) Design

Design Evaluation of : **RS6F4VP_Cor_Norm_Resp** – "Verification points" excluded

Original Norm for "X – G percent" & "X – Add time"

Compared to the situation before correcting values of "X – G percent", "X – Add time" & "Stirring speed" (**RS6F4VP_Cor_Norm**)…

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,3225	1,48726	0,3276	
B	0,2367	1,22238	0,1819	
C	0,2439	1,48078	0,3247	
D	0,2473	1,33413	0,2504	
E	0,2332	1,20566	0,1706	
F	0,3089	1,57212	0,3639	
AB	0,3119	1,37209	0,2712	
AC	0,2922	1,3422	0,2550	
AD	0,3076	1,35238	0,2606	
AE	0,3276	1,55899	0,3586	
AF	0,3840	1,52162	0,3428	
BC	0,2538	1,47911	0,3239	
BD	0,2482	1,34384	0,2559	
BE	0,2590	1,48814	0,3280	
BF	0,2754	1,26438	0,2091	
CD	0,2255	1,27274	0,2143	
CE	0,2335	1,39894	0,2852	
CF	0,2679	1,28474	0,2216	
DE	0,2327	1,20132	0,1676	
DF	0,2792	1,2888	0,2241	
EF	0,2606	1,14711	0,1282	

…**Std Errors**, **VIF** & **Ri²** are globally higher, mainly for "X – G percent" & "X – Add time" and their interactions with all other Factors because those two Factors are the most perturbated…

…and all **Matrix Measures** are worse…

… thus, as we could be afraid of, this perturbated Design is worse..

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	7,34
Maximum Variance Mean	2,82
Average Variance Mean	0,3358
Minimum Variance Mean	0,0570
G Efficiency	35,52
Scaled D-optimality Criterion	1,37
Determinant of $(X'X)^{-1}$	2,89406E-27
Trace of $(X'X)^{-1}$	1,67
I (Cuboidal)	0,3375

… but it is largely better than the Corrected Min. Run Characterization Design and remains acceptable

Constrained Optimal (Custom) Design

Design Evaluation of : **RS6F4VP_Cor_NrmNrm_Resp** – "Verification points" included

Norm for "X – G percent" & "X – Add time" set to extreme Means

Compared to the situation before correcting values of "X – G percent", "X – Add time" & "Stirring speed" (**RS6F4VP_Cor_Norm**)…

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2385	1,47047	0,3199	87,3 %
B	0,2131	1,17384	0,1481	93,1 %
C	0,2209	1,42659	0,2990	91,5 %
D	0,2474	1,33713	0,2521	85,0 %
E	0,2326	1,20149	0,1677	88,8 %
F	0,2587	1,55219	0,3558	82,0 %
AB	0,2247	1,32097	0,2430	90,6 %
AC	0,2146	1,32096	0,2430	92,8 %
AD	0,2296	1,35144	0,2600	89,5 %
AE	0,2429	1,54084	0,3510	86,2 %
AF	0,2463	1,51126	0,3383	85,3 %
BC	0,2271	1,39722	0,2843	90,1 %
BD	0,2471	1,33395	0,2503	85,1 %
BE	0,2559	1,45546	0,3129	82,7 %
BF	0,2309	1,23783	0,1921	89,2 %
CD	0,2238	1,25505	0,2032	90,8 %
CE	0,2301	1,36039	0,2649	89,4 %
CF	0,2248	1,29291	0,2265	90,6 %
DE	0,2314	1,18973	0,1595	89,1 %
DF	0,2392	1,27541	0,2159	87,1 %
EF	0,2233	1,13324	0,1176	91,0 %

… **VIF** & **Ri²** are globally higher (and very close to with the original Norms) and **Std Errors** are less higher and **Power** less lower, mainly for "X – G percent" & "X – Add time" and their interactions with all other Factors …

…and among **Matrix Measures**
G Efficiency, **Scaled D-opt.Crit.**, **Det.(X'X)-1** & **Trace(X'X)-1**
are not very different

thus,
correcting the Norm for
"X – G percent" & "X – Add time"
improves the Design Quality a bit.

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	7,29
Maximum Variance Mean	2,12
Average Variance Mean	0,2520
Minimum Variance Mean	0,0463
G Efficiency	39,88
Scaled D-optimality Criterion	1,21
Determinant of $(X'X)^{-1}$	5,1303E-30
Trace of $(X'X)^{-1}$	1,20
I (Cuboidal)	0,2522

… and this perturbated Design is largely better than the Corrected Min. Run Characterization Design and remains acceptable

Constrained Optimal (Custom) Design

Design Evaluation of : **RS6F4VP_Cor_NrmNrm_Resp** – “Verification points” excluded

Norm for “X – G percent” & “X – Add time” set to extreme Means

Compared to the situation before correcting values of “X – G percent”, “X – Add time” & “Stirring speed” (**RS6F4VP_Cor_Norm**)…

Model Terms | Factorial Effects Aliases

Model Terms

Term	Standard Error*	VIF	R_i^2	Power
A	0,2429	1,50058	0,3336	
B	0,2354	1,20857	0,1726	
C	0,2445	1,48718	0,3276	
D	0,2483	1,3455	0,2568	
E	0,2340	1,21443	0,1766	
F	0,2684	1,60478	0,3769	
AB	0,2340	1,38129	0,2760	
AC	0,2191	1,35851	0,2639	
AD	0,2307	1,36391	0,2668	
AE	0,2457	1,57701	0,3659	
AF	0,2477	1,52277	0,3433	
BC	0,2538	1,47911	0,3239	
BD	0,2482	1,34384	0,2559	
BE	0,2590	1,48814	0,3280	
BF	0,2369	1,25867	0,2055	
CD	0,2255	1,27274	0,2143	
CE	0,2335	1,39894	0,2852	
CF	0,2304	1,2808	0,2192	
DE	0,2327	1,20132	0,1676	
DF	0,2401	1,28327	0,2207	
EF	0,2241	1,14145	0,1239	

… **VIF** & **Ri²** are globally higher (and very close to with the original Norms) and **Std Errors** are less higher, mainly for “X – G percent” & “X – Add time” and their interactions with all other Factors …

…and among **Matrix Measures G Efficiency**, **Scaled D-opt.Crit.**, **Det.(X’X)-1** & **Trace(X’X)-1** are not very different

thus,
correcting the Norm for “X – G percent” & “X – Add time” improves the Design Quality a bit.

Correlation Matrix | Pearson's r | Matrix Measures

Matrix Measures

Description	Value
Condition Number of Coefficient Matrix	7,70
Maximum Variance Mean	2,20
Average Variance Mean	0,2776
Minimum Variance Mean	0,0573
G Efficiency	45,44
Scaled D-optimality Criterion	1,08
Determinant of $(X'X)^{-1}$	1,50046E-29
Trace of $(X'X)^{-1}$	1,27
I (Cuboidal)	0,2786

… and this perturbated Design is largely better than the Corrected Min. Run Characterization Design and remains acceptable

Conclusion

When classical Designs which are orthogonal (or almost) by construction

Factorials: Regular 2 levels, Plackett-Burman

Response Surface : Central Composite, Box-Behnken

cannot be used

always evaluate the alternate possibilities to compare their quality before running an experiment.

Having a good quality Design from the beginning provides

better Effect estimation

better guaranty against Factor bad control.

In this case we spent a lot of time in preparing the Design and ran the Analysis on the base of the Norm corrected Factors "R – Mw" (from the beginning) and "X – G percent" & "X – Add time" (at the end) "Verification points" excluded.

For Responses where "Verification points" were well fitted we also ran the Analysis by including them and we got very accurate conclusions.