DoE for Scale-Up

… using MODDE® and DoE-DiVa®

Session 3: Use of dependent Factors: Spray Drying -- 01.02. 2023

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umesoft

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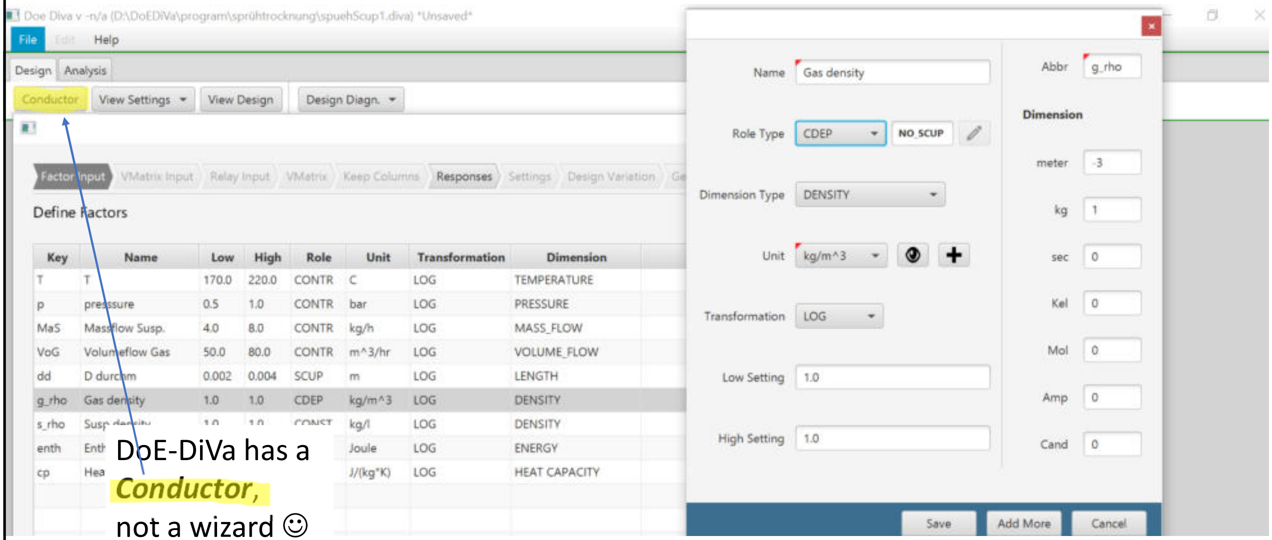
For those who don‘t yet know *DoE-DiVa*

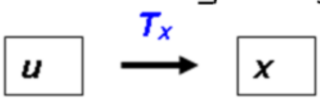
- ***DoE-DiVa*** is a user-friendly Software for Engineers and Scientists in R&D, developed in JAVA by umesoft
- ***DoE-DiVa*** *enhances* ***D****esign* ***of E****xperiments and makes it more intelligent , with* ***U****ser-factors* ***and*** *e****X****plaining-factors*
- ***DoE-DiVa*** *enhances Similarity Theory for* ***Di****mensionless* ***Va****riables by integrating DoE for* ***Scale-Up*** *and* ***Scale-Down***

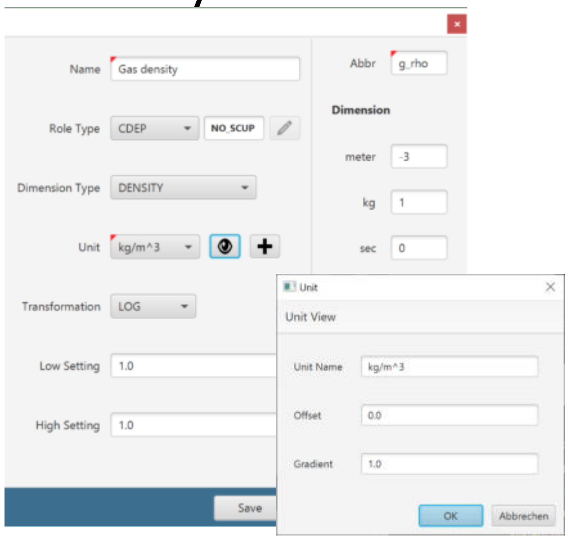
This is how the ***DoE-DiVa*** looks.



DoE-DiVa's conductor is friendly

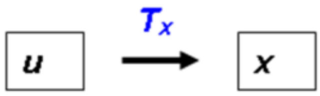
- ***DoE-DiVa*** let's the user choose his ***Dimensions, Units, Transforms*** *and* ***Scaling*** and carries them through all the User-Software work session
- ***DoE-DiVa*** differentiates between ***User-factors and eXplaining-factors***



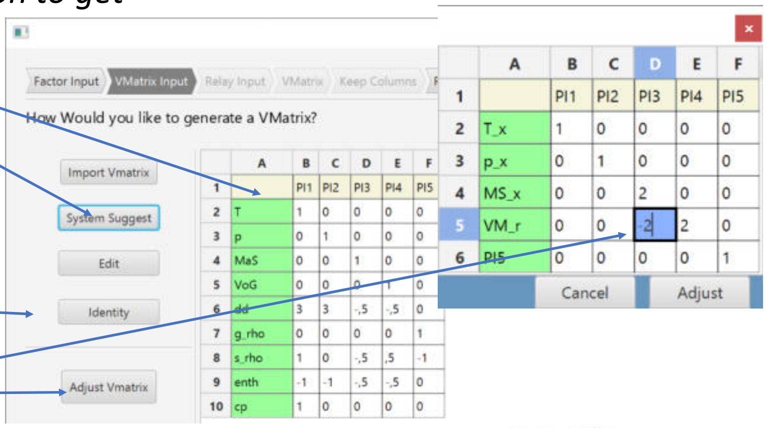


DoE-DiVa's conductor is helpful

- Based on factor dimensions ***DoE-DiVa*** *suggests* the ***Tr****ansformation to get dimensionless* ***x****-factors,*



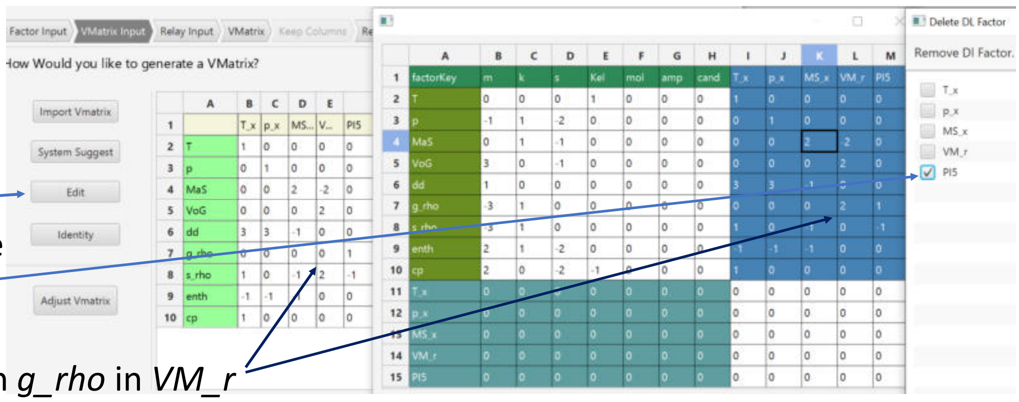
- Sometimes, dependencies are already taken up as *cdep* ***u****-factors*, then it may be opportune to just use an *identity*-matrix
- *Or just adjust …* .



DoE-DiVa's conductor is flexible

- ***DoE-DiVa*** allows ***overriding the suggestions*** for the ***Tr****ansformation* to get dimensionless ***x****-factors,*

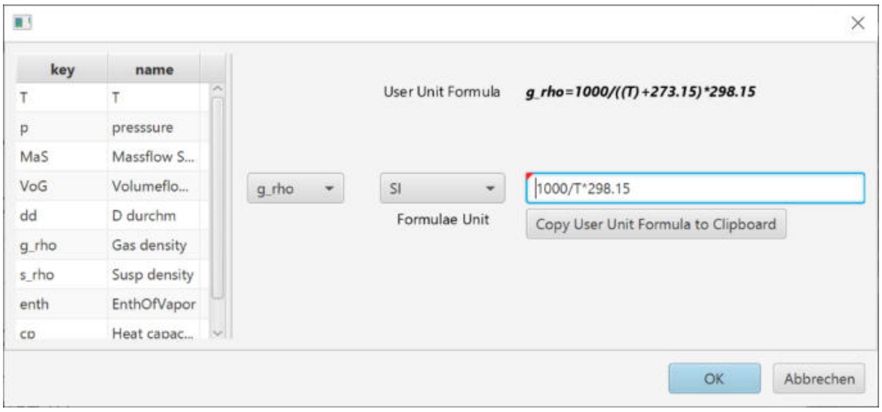
and even helps you do this: Edit to remove *PI5*, and switch *s_rho* with *g_rho* in *VM_r*



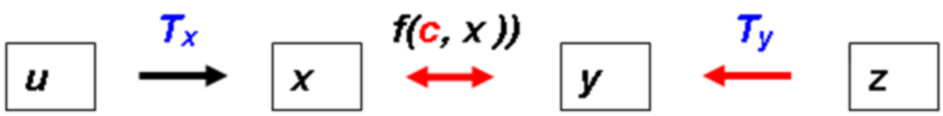
DoE-DiVa's conductor is virtuoso

- ***DoE-DiVa*** accepts dependency formulae in ***user units*** or ***SI-units***, converts them for you.

- ***DoE-DiVa*** can generate formulae to export to MODDE® for ***optimization***



The ***DoE-DiVa***-approach

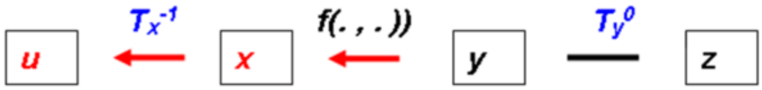


u: *User-factor,* to be set in the experiment, e.g. *Temp, pressure etc.*
x: *eXplaining-factor,* to be used in the model, e.g. *a force-ratio*
T_x: *transformation* to get from ***u*** to ***x***, e.g. *ratio, dimensionless variable*
c: *coefficients or parameters in the model,* ***f***, *to be determined by model FIT*
z: *measured response value*
y: *transformed response value, e.g. ratio or product of a* ***z*** *and some* ***u***
T_y: *transformation* to get from ***z*** to ***y***, *may also just be log or neg-log*

The role of the ***Transformations***

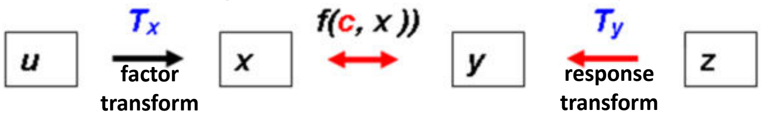
Design: How to get ***u*** from ***f*** and the ***tr*****ansformation**

DoE-DiVa



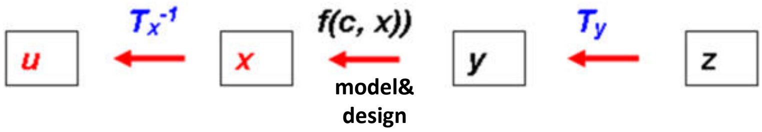
Model Fit: how to get coefficients, ***c***, from ***x*** and ***y***

DoE-DiVa/ MODDE®



Optimization: how to get the ***u*** from the specification for ***z***

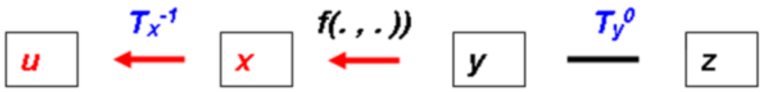
MODDE®



TODAY:

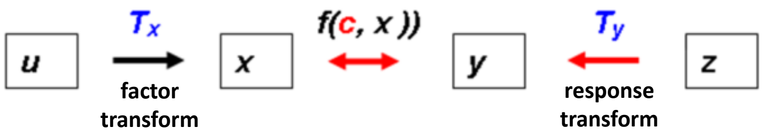
The ***Approximation*** Trick to get T_x^{-1}

Design: To get **u** from ***x***, T_x has to be inverted



Inverting a non-linear T_x may be difficult or impossible, so T_x is approximated by a linear T_{approx} and *<u>when we write T_x^{-1} we mean T_{approx}^{-1}</u>*

Model Fit: To get ***x*** from ***u*** for Fit, T_x need <u>not</u> be inverted, T_{approx} is <u>not</u> needed.



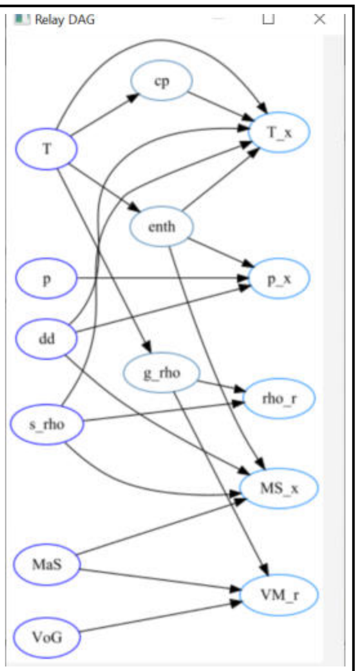
1. **TODAY: The concept of dependent u-factors**
2. Example: Spray drying, *x_design* and *u_design*
3. Optimization and Scale-Up considerations

Types of *factor dependencies*

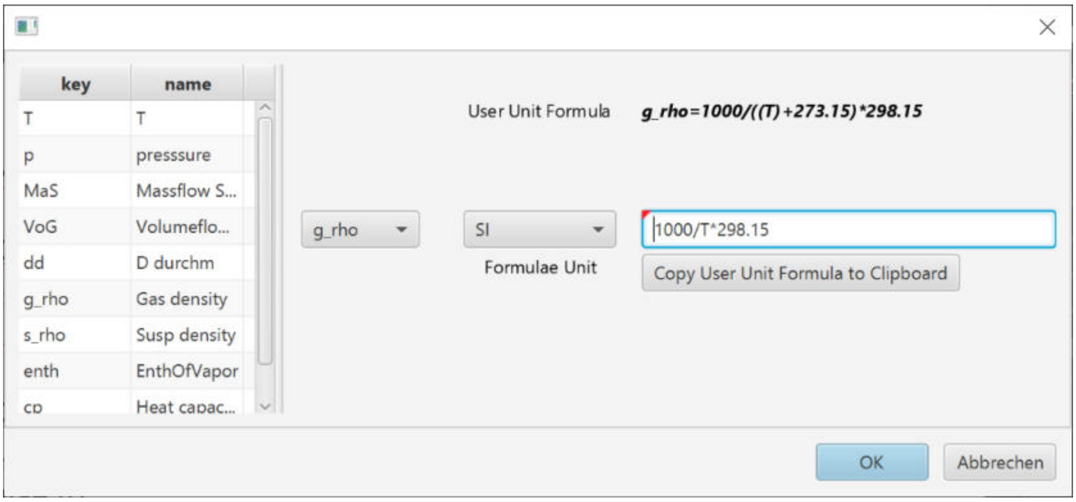
- ***Quotients** and **Products*** of controlled (or constant) ***u**-factors* can be directly used as ***x**-factor **T_x**ransforms* by placing *correct exponents* into the *V-matrix.*

BUT this is not always possible for**:**

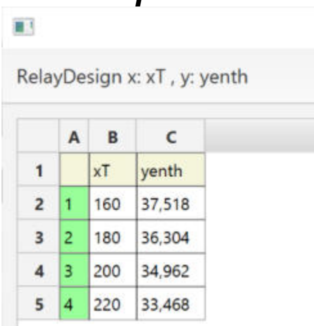
- ***Nested formulae***: „Vol-Mass-ratio, *VM_r* depends on *gas-density*, *g_rho*, *g_rho* depends on *temperature*",
- ***Non-linear formulae,***
- ***Prior experimental* or *simulation results***, available only as ***data tables***.



Factor dependencies as formulae (possibly non-linear)



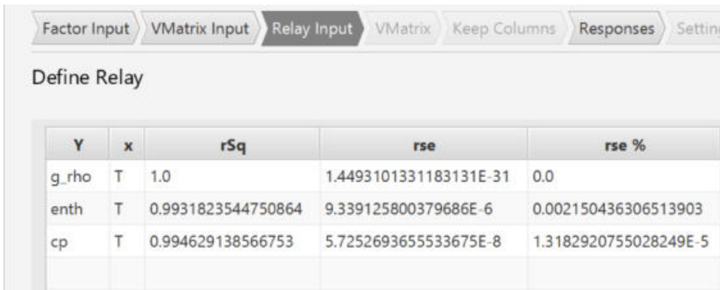
Factor dependencies as data tables (from *experimentation*, *simulation* or *experience*)



RelayDesign x: xT , y: yenth

	A	B	C
1		xT	yenth
2	1	160	37,518
3	2	180	36,304
4	3	200	34,962
5	4	220	33,468

Data table with the *enthalpy* dependency



Y	x	rSq	rse	rse %
g_rho	T	1.0	1.4493101331183131E-31	0.0
enth	T	0.9931823544750864	9.339125800379686E-6	0.002150436306513903
cp	T	0.994629138566753	5.7252693655533675E-8	1.3182920755028249E-5

Quality of the ***approximation*** is given as R^2 and rse, and relative rse in %
(rse = residual standard error)

Relaying Factor dependencies to ***x**-factors*

How Would you like to generate a VMatrix?

Import Vmatrix

System Suggest

Edit

Identity

Adjust Vmatrix

	A	B	C	D	E	F
1		T_x	p_x	MS_x	VM_r	rho_r
2	T	1	0	0	0	0
3	p	0	1	0	0	0
4	MaS	0	0	2	-1	0
5	VoG	0	0	0	1	0
6	dd	3	3	-1	0	0
7	g_rho	0	0	0	1	1
8	s_rho	1	0	-1	0	-1
9	enth	-1	-1	-1	0	0
10	cp	1	0	0	0	0

Relayed VMatrix

	A	B	C	D	E	F
1		T_x	p_x	MS_x	VM_r	rho_r
2	T	1,9558226	,8782884	,8782884	-1	-1
3	T__N	-,9558226	-,8782884	-,8782884	1	1
4	p	0	1	0	0	0
5	MaS	0	0	2	-1	0
6	VoG	0	0	0	1	0
7	dd	3	3	-1	0	0
8	g_rho__D	0	0	0	1	1
9	s_rho	1	0	-1	0	-1
10	enth__D	-1	-1	-1	0	0

Temperature, T, dependency is ***relayed on to*** *Vol-Mass-ratio, VM_r* via ***g_rho***.

1. TODAY: The concept of dependent u-factors
2. ***Example: Spray drying, x_design and u_design***
3. Optimization and Scale-Up considerations

Spray-Drying

u → (T_x) → **x** … **z**

From a common project with Fraunhofer IKTS, Institut für Keramische Technologien und Systeme in Dresden

***u:** User-factors,*
***T**=GasTemp,*
***VoG**=gasflow,*
***MaS**=suspension,*
***p**=pressure,*
dd ← *scale up factor nozzle diameter*

***z:** measured responses*
***d50** of granulate,*
***grad** of distribution,*
***GranF F** = hardness,*
***Grrho** density of gran,*
***Gfes** hardness of a pressed preform*

https://www.ikts.fraunhofer.de/de/abteilungen/strukturkeramik/verfahren_und_bauteile/pulvertechnologie/spruehtrocknung_wirbelschicht.html

Todays ***Spray-Drying***-example (Sprühtrocknung)

u → (T_x) → **x** ↔ (f(**c**, x)) ↔ **y** ← (T_y) ← **z**

scale up factor nozzle diameter → ***dd***

u:** User-factors, **T**=GasTemp, **P**=pressure, **MaS**=suspension, **VoG**=gasflow, **dd
***x: dimensionless** e**X**plaining-factor: **T_x, p_x, MS_x, MG/MS*rho**$_G$ (T)*
*T_x: transformation: **T_x**=T, **p_x**=p*d³/enth(T), **MS_x**=MS²/dd/ rho$_S$ / **c**$_p$ (T)*
***c: c**oefficients or parameters in the model, **f**, to be determined by model FIT*
z:** measured response value; **d50, grad, GranF, Grrho, Gfes
***y: dimless** responses, PI6__d50, grad__y, PI8__GranF, PI9__Grrho, Gfes__y*
T_y: transformation to get from ***z*** to ***y**, solutions from Buckingham's theorem*

Step 1: ***u-factors***

Key	Name	Low	High	Role	Unit	Transformation	Dimension
T	T	170.0	220.0	CONTR	C	LOG	TEMPERATURE
p	presssure	0.5	1.0	CONTR	bar	LOG	PRESSURE
MaS	Massflow Susp.	4.0	8.0	CONTR	kg/h	LOG	MASS_FLOW
VoG	Volumeflow Gas	50.0	80.0	CONTR	m^3/hr	LOG	VOLUME_FLOW
dd	D durchm	0.002	0.004	SCUP	m	LOG	LENGTH
g_rho	Gas density	1.0	1.0	CDEP	kg/m^3	LOG	DENSITY
s_rho	Susp density	1.0	1.0	CONST	kg/l	LOG	DENSITY
enth	EnthOfVapor	1.0	1.0	CDEP	Joule	LOG	ENERGY
cp	Heat capacity	1.0	1.0	CDEP	J/(kg*K)	LOG	HEAT CAPACITY

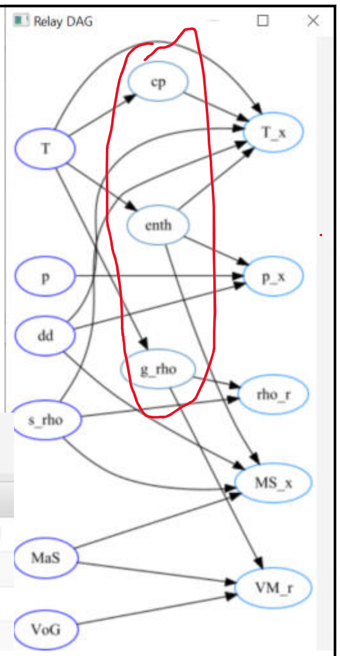
Step 2: ***x-factors***

	A	B	C	D	E	F
1		T_x	p_x	MS_x	VM_r	rho_r
2	T	1	0	0	0	0
3	p	0	1	0	0	0
4	MaS	0	0	2	-1	0
5	VoG	0	0	0	1	0
6	dd	3	3	-1	0	0
7	g_rho	0	0	0	1	1
8	s_rho	1	0	-1	0	-1
9	enth	-1	-1	-1	0	0
10	cp	1	0	0	0	0

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	factorKey	m	k	s	Kel	mol	amp	cand	T_x	p_x	MS_x	VM_r	rho_r
2	T	0	0	0	1	0	0	0	1	0	0	0	0
3	p	-1	1	-2	0	0	0	0	0	1	0	0	0
4	MaS	0	1	-1	0	0	0	0	0	0	2	-1	0
5	VoG	3	0	-1	0	0	0	0	0	0	0	1	0
6	dd	1	0	0	0	0	0	0	3	3	-1	0	0
7	g_rho	-3	1	0	0	0	0	0	0	0	0	1	1
8	s_rho	-3	1	0	0	0	0	0	1	0	-1	0	-1
9	enth	2	1	-2	0	0	0	0	-1	-1	-1	0	0
10	cp	2	0	-2	-1	0	0	0	1	0	0	0	0
11	T_x	0	0	0	0	0	0	0	0	0	0	0	0
12	p_x	0	0	0	0	0	0	0	0	0	0	0	0
13	MS_x	0	0	0	0	0	0	0	0	0	0	0	0
14	VM_r	0	0	0	0	0	0	0	0	0	0	0	0
15	rho_r	0	0	0	0	0	0	0	0	0	0	0	0

Step 3: ***u-factor dependencies***

Key	Name	Low	High	Role	
T	T	170.0	220.0	CONTR	C
dd	D durchm	0.002	0.004	SCUP	m
g_rho	Gas density	1.0	1.0	CDEP	kg
s_rho	Susp density	1.0	1.0	CONST	kg
enth	EnthOfVapor	1.0	1.0	CDEP	Jo
cp	Heat capacity	1.0	1.0	CDEP	J/



Define Relay

Y	x	rSq	rse
g_rho	T	1.0	1.4493101331183131E-31
enth	T	0.9931823544750864	9.339125800379686E-6
cp	T	0.9946291385566753	5.7252693655533675E-8

CDEP is short for: *continuous dependency*

Step 3f: ***u-factor dependencies***

Define Relay

Y	x	rSq	rse	rse %
g_rho	T	1.0	1.4493101331183131E-31	0.0
enth	T	0.9931823544750864	9.339125800379686E-6	0.002150436306513903
cp	T	0.9946291385566753	5.7252693655533675E-8	1.3182920755028249E-5

RelayDesign x: xT , y: yenth

	A	B	C
1		xT	yenth
2	1	160	37,518
3	2	180	36,304
4	3	200	34,962
5	4	220	33,468

as data table

RelayDesign x: xT , y: ycp

	A	B	C
1		xT	ycp
2	1	160	1,0196
3	2	180	1,0228
4	3	200	1,026
5	4	220	1,03

User Unit Formula ***g_rho=1000/((T)+273.15)*298.15***

as formulae

g_rho | SI | 1000/T*298.15

Formulae Unit | Copy User Unit Formula to Clipboard

4: Info, T_{approx} – *transformation as a matrix*

Factor Input | VMatrix Input | Relay Input | VMatrix | Keep Columns | Responses | Set

How Would you like to generate a VMatrix?

Import Vmatrix

System Suggest

Edit

Identity

Adjust Vmatrix

Before …

	A	B	C	D	E	F
1		T_x	p_x	MS_x	VM_r	rho_r
2	T	1	0	0	0	0
3	p	0	1	0	0	0
4	MaS	0	0	2	-1	0
5	VoG	0	0	0	1	0
6	dd	3	3	-1	0	0
7	g_rho	0	0	0	1	1
8	s_rho	1	0	-1	0	-1
9	enth	-1	-1	-1	0	0
10	cp	1	0	0	0	0

Previous | Next | Abbrechen

Factor Input | VMatrix Input | Relay Input | VMatrix | Keep Columns

Relayed VMatrix

… and after Relaying…

	A	B	C	D	E	F
1		T_x	p_x	MS_x	VM_r	rho_r
2	T	1,9558226	,8782884	,8782884	-1	-1
3	T_N	-,9558226	-,8782884	-,8782884	1	1
4	p	0	1	0	0	0
5	MaS	0	0	2	-1	0
6	VoG	0	0	0	1	0
7	dd	3	3	-1	0	0
8	g_rho_D	0	0	0	1	1
9	s_rho	1	0	-1	0	-1
10	enth_D	-1	-1	-1	0	0

Step 5: *choose x-factors to use*

Factor Input | VMatrix Input | Relay Input | VMatrix | Keep Columns | Responses | Settings | Design Variation | Generate Design

Select Dimension-less factor(s) to Keep

- [x] T_x
- [x] p_x
- [x] MS_x
- [x] VM_r
- [ ] rho_r

Max 4 x-factors is possible.

VMatrix : Correlation

	A	B	C	D	E	F
1	#	T_x	p_x	MS_x	VM_r	rho_r
2	T	1,9558226	,8782884	,8782884	-1	-1
3	p	0	1	0	0	0
4	MaS	0	0	2	-1	0
5	VoG	0	0	0	1	0

Previous | Next | Abbrechen

Step 6: ***define z-response(s)***

Factor Input | VMatrix Input | Relay Input | VMatrix | Keep Columns | Responses | Settings | Design Variation | Generate Design

Define Z-Response(s)

Key	Name	Low	High	Unit	Transformation	Dimension
d50	d50	45.0	55.0	µm	LOG	LENGTH
grad	grad	0.5	2.0	SI	LOG	DIMENSION_LESS
GranF	GranF	0.5	1.0	kN	LOG	FORCE
Gfes	Gfes	0.8	1.0	SI	LOG	DIMENSION_LESS
Grrho	Grrho	1.0	2.0	kg/l	LOG	DENSITY

d50, grad, GranF, Grrho, Gfes

Previous | Next | Abbrechen

Step 6ff: ***define y-response(s)***

(Uses *Buckingham's PI-theorem* intro-duced in session 2)

Vmatrix | x-Settings | u-Settings | VRes | Wres | y-response(s)

	A	B	C	D	E	F
1		PI6_d50	grad_y	PI8_GranF	Gfes_y	Grrho_y
2	T	0	0	0	0	0
3	p	,25	0	-,5	0	0
4	MaS	-,25	0	-,5	0	-1
5	VoG	-,25	0	-,5	0	1
11	d50	1	0	0	0	0
12	grad	0	1	0	0	0
13	GranF	0	0	1	0	0
14	Gfes	0	0	0	1	0
15	Grrho	0	0	0	0	1

… to find useful exponents for the factors …

Suggest

Import

… to make the responses dimensionless

Adjust

Step 7: *view T_{approx} and its inverse T_{approx}^{-1}*

Vmatrix | x-Settings | u-Settings | VRes | Wres | y-response(s)

	A	B	C
1		T_x	p_
2	T	1,9558226	,8
3	T_N	-,9558226	-,
4	p	0	1
5	MaS	0	0
6	VoG	0	0
7	dd	3	3
8	g_rho_D	0	0
9	s_rho	1	0
10	enth_D	-1	-1
11	cp_D	1	0

Vmatrix | x-Settings | u-Settings | VRes | Wres | y-response(s)

	A	B	C	D	E	F	G	H	I	J	K
1		T	T_N	p	MaS	VoG	dd	g_rho_D	s_rho	enth_D	cp_D
2	T_x	,4286821	0	-,5380803	-,1613243	,2673578	,0538579	0	0	0	0
3	p_x	-,3339453	0	,6401625	,2555065	-,0784389	,2177126	0	0	0	0
4	MS_x	,0821633	0	,0885338	,4371356	,519299	-,0535656	0	0	0	0
5	VM_r	-,0727948	0	-,0784389	,0556964	,9829016	,0474579	0	0	0	0
6	T_N	,2614016	1	,204135	,3984457	-,3401526	,1481891	0	0	0	0
7	g_rho_D	,0727948	0	,0784389	-,0556964	-,9829016	-,0474579	1	0	0	0
8	s_rho	-,3465188	0	,6266141	,5984599	,2519411	-,1074236	0	1	0	0
9	enth_D	,1769001	0	,1906159	,5313178	,7082179	,2180049	0	0	1	0
10	cp_D	-,4286821	0	,5380803	,1613243	-,2673578	-,0538579	0	0	0	1
11	dd_su	-1,5338814	0	-1,6528097	1,1735951	-,3602863	1	0	0	0	0

Step 7ff: *view and edit x-settings*

Vmatrix | x-Settings | u-Settings | VRes | Wres | y-response(s)

#	Weight	Outer Low	User Low	Inner Low	Mean	Inner High	User High	Outer High
T_x	1.0	-3.10516	-3.10516	-3.10516	-3.059...	-3.01436	-3.01436	-3.01436
p_x	1.0	-4.06185	-4.02107	-4.02107	-3.890...	-3.76082	-3.76082	-3.72004
MS_x	1.0	-8.07754	-7.84516	-7.84516	-7.756...	-7.66708	-7.66708	7.43471
VM_r	1.0	3.87837	3.80861	3.80861	3.85312	3.89764	3.89764	3.82788
T_N	0.0	2.66976	2.66976	2.66976	2.66976	2.66976	2.66976	2.66976
g_rho_D	0.0	2.80467	2.80467	2.80467	2.80467	2.80467	2.80467	2.80467
s_rho	0.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0
enth_D	0.0	1.54661	1.54661	1.54661	1.54661	1.54661	1.54661	1.54661

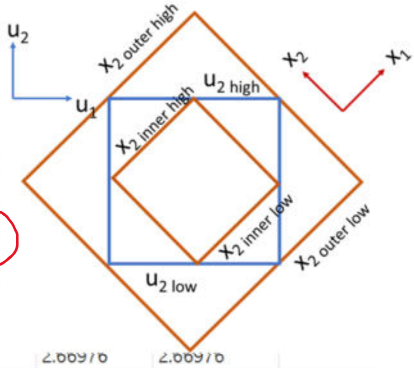
x-settings have been generated for Scale Up

Transformation: (•) LOG

Use: ( ) Inner ( ) Outer

[Setting] [**Generate x-Settings**]

Step 7ff: ***x-settings***

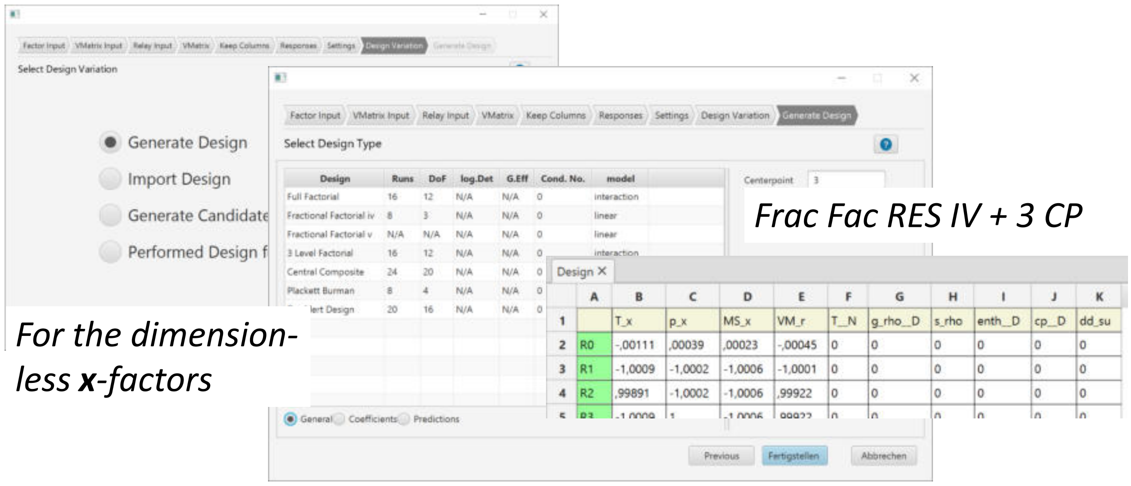


#	Weight	Outer Low	User Low	Inner Low	Mean	Inner H		
T_x	1.0	-3.10516	-3.10516	-3.10516	-3.059...	-3.01436		
p_x	1.0	-4.06185	-4.02107	-4.02107	-3.890...	-3.76082		
MS_x	1.0	-8.07754	-7.84516	-7.84516	-7.756...	-7.66708		
VM_r	1.0	3.87837	3.80861	3.80861	3.85312	3.89764		
T_N	0.0	2.66976	2.66976	2.66976	2.66976	2.66976	2.66976	2.66976
g_rho__D	0.0	2.80467	2.80467	2.80467	2.80467	2.80467	2.80467	2.80467
s_rho	0.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0
enth__D	0.0	1.54661	1.54661	1.54661	1.54661	1.54661	1.54661	1.54661

For ***VM_r inner limits*** and ***outer limits*** are ***different***

User limits can always be chosen inbetween the two.

Step 8: ***Select the design variation- Generate***



Frac Fac RES IV + 3 CP

*For the dimension-less **x**-factors*

Step 8f: ***Look at the design (uu-design)***

Design | Analysis

Conductor | View Settings | View Design | Design Diagn.

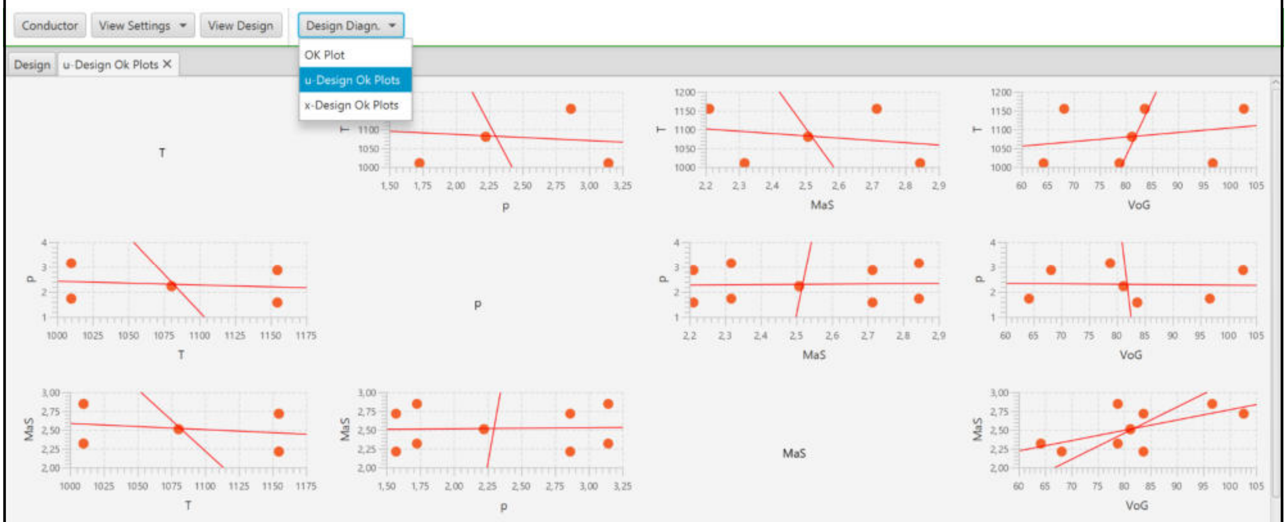
Design ×

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1		T	p	MaS	VoG	dd	g_rho	s_rho	enth	cp	d50	grad	GranF	Gfes	Grrho
2	R0	1.080,428352	2,223804	2,5079028	81,1819354	,002	220,2679957	1	13,8384198	1,113533	0	0	0	0	0
3	R1	1.009,9951891	1,726949	2,3171129	64,1797766	,002	232,3587332	1	14,5033892	1,1089289	0	0	0	0	0
4	R2	1.154,7447605	1,5722044	2,2108639	83,6437318	,002	208,8038971	1	13,2038019	1,1181573	0	0	0	0	0
5	R3	1.009,9951891	3,1446296	2,3171129	78,7767756	,002	232,3587332	1	14,5033892	1,1089289	0	0	0	0	0
6	R4	1.080,428352	2,223804	2,5079028	81,1819354	,002	220,2679957	1	13,8384198	1,113533	0	0	0	0	0
7	R5	1.154,7447605	2,8628527	2,2108639	68,1449066	,002	208,8038971	1	13,2038019	1,1181573	0	0	0	0	0
8	R6	1.009,9951891	1,726949	2,8444755	96,7059511	,002	232,3587332	1	14,5033892	1,1089289	0	0	0	0	0
9	R7	1.154,7447605	1,5722044	2,7140447	83,6543253	,002	208,8038971	1	13,2038019	1,1181573	0	0	0	0	0
10	R8	1.080,428352	2,223804	2,5079028	81,1819354	,002	220,2679957	1	13,8384198	1,113533	0	0	0	0	0
11	R9	1.009,9951891	3,1446296	2,8444755	78,7867527	,002	232,3587332	1	14,5033892	1,1089289	0	0	0	0	0
12	R10	1.154,7447605	2,8628527	2,7140447	102,6806007	,002	208,8038971	1	13,2038019	1,1181573	0	0	0	0	0

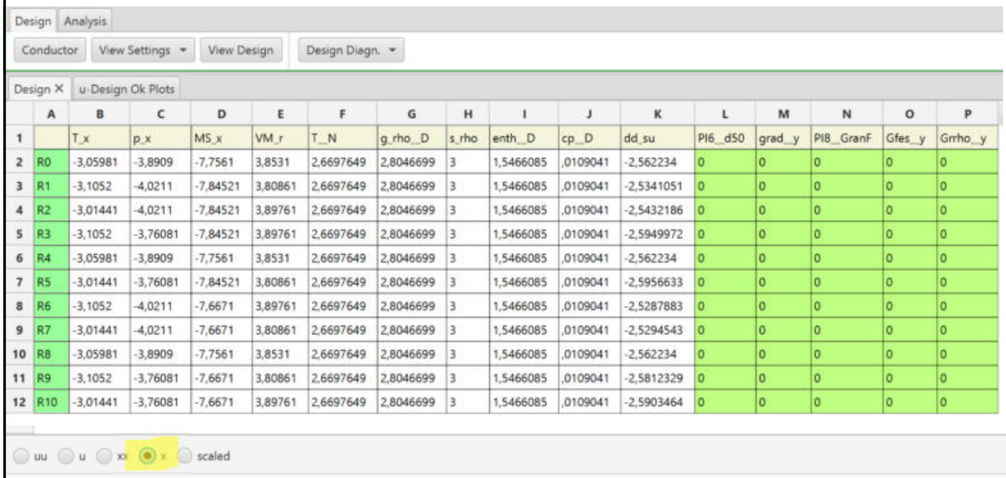
uu | u | xx | x | scaled

…. unfortunately ***z****-response* data are not available

Step 8ff: ***ok-plot for u-design*** ***(collinear!!)***



Step 8fff: *Look at the design (x-design)*

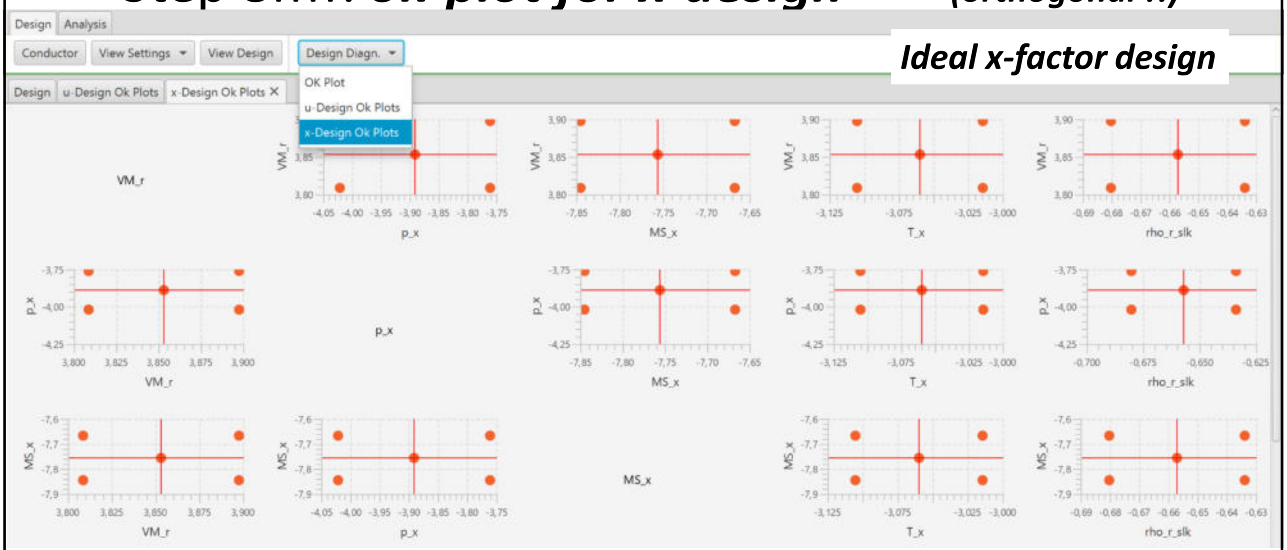


	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1		T_x	p_x	MS_x	VM_r	T__N	g_rho__D	s_rho	enth__D	cp__D	dd_su	PI6__d50	grad__y	PI8__GranF	Gfes__y	Grrho__y
2	R0	-3,05981	-3,8909	-7,7561	3,8531	2,6697649	2,8046699	3	1,5466085	,0109041	-2,562234	0	0	0	0	0
3	R1	-3,1052	-4,0211	-7,84521	3,80861	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5341051	0	0	0	0	0
4	R2	-3,01441	-4,0211	-7,84521	3,89761	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5432186	0	0	0	0	0
5	R3	-3,1052	-3,76081	-7,84521	3,89761	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5949972	0	0	0	0	0
6	R4	-3,05981	-3,8909	-7,7561	3,8531	2,6697649	2,8046699	3	1,5466085	,0109041	-2,562234	0	0	0	0	0
7	R5	-3,01441	-3,76081	-7,84521	3,80861	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5956633	0	0	0	0	0
8	R6	-3,1052	-4,0211	-7,6671	3,89761	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5287883	0	0	0	0	0
9	R7	-3,01441	-4,0211	-7,6671	3,80861	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5294543	0	0	0	0	0
10	R8	-3,05981	-3,8909	-7,7561	3,8531	2,6697649	2,8046699	3	1,5466085	,0109041	-2,562234	0	0	0	0	0
11	R9	-3,1052	-3,76081	-7,6671	3,80861	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5812329	0	0	0	0	0
12	R10	-3,01441	-3,76081	-7,6671	3,89761	2,6697649	2,8046699	3	1,5466085	,0109041	-2,5903464	0	0	0	0	0

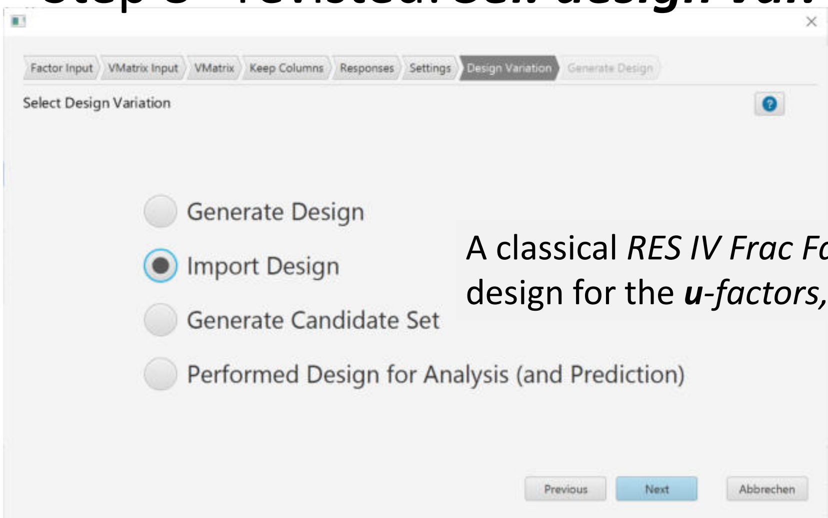
.... consequently ***y****-response* data are not available either

Step 8ffff: *ok-plot for x-design* *(orthogonal !!)*

Ideal x-factor design



Step 8 - revisted: ***Sel. design var. - Import***



A classical *RES IV Frac Fac* design for the ***u**-factors,* for which response data are available

Step 8f - revisited: ***Look at the design (uu-design)***

for which response data are available

Conductor | View Settings | View Design | Design Diagn.

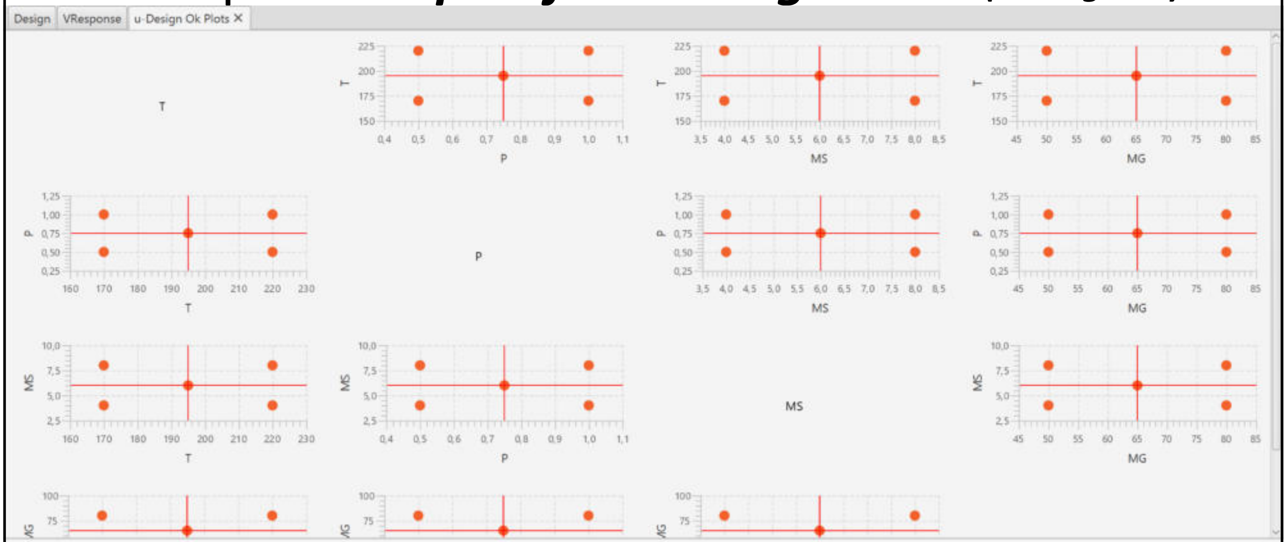
Design

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1		T	p	MaS	VoG	dd	g_rho	s_rho	enth	cp	d50	grad	GranF	Gfes	Grrho
2	R0	170,0000473	,5	4,0000001	80,0000025	,002	672,7969283	1	36,897522	1,0211845	85	1,9294	,7	,551	2,38
3	R1	219,9999575	,5	4,0000001	49,9999996	,002	604,5828172	1	33,5907577	1,0296841	33	1,7717	,65	,593	2,348
4	R2	170,0000473	1	4,0000001	49,9999996	,002	672,7969283	1	36,897522	1,0211845	25	,461	,67	,756	2,347
5	R3	219,9999575	1	4,0000001	80,0000025	,002	604,5828172	1	33,5907577	1,0296841	40	1,625	,78	,633	2,367
6	R4	170,0000473	,5	8,0000003	49,9999996	,002	672,7969283	1	36,897522	1,0211845	54	1,7407	,81	,598	2,353
7	R5	219,9999575	,5	8,0000003	80,0000025	,002	604,5828172	1	33,5907577	1,0296841	97	1,6049	,72	,545	2,379
8	R6	170,0000473	1	8,0000003	80,0000025	,002	672,7969283	1	36,897522	1,0211845	73	2,2489	,55	,483	2,378
9	R7	219,9999575	1	8,0000003	49,9999996	,002	604,5828172	1	33,5907577	1,0296841	26	1,3846	,69	,72	2,348
10	R8	194,9999701	,7500001	5,9999993	65,0000066	,002	636,8685456	1	35,1612171	1,025539	42	1,7143	,74	,617	2,368
11	R9	194,9999701	,7500001	5,9999993	65,0000066	,002	636,8685456	1	35,1612171	1,025539	42	1,5714	,65	,61	2,361

uu | u | xx | x | scaled

Experimental results for the 5 ***z**-responses* have been copied into the columns here

Step 8ff: ***ok-plot for u-design*** ***(orthogonal)***



Step 8fff: ***Look at the design (x-design)***

Design | Analysis

Conductor | View Settings | View Design | Design Diagn.

***y**-response* data calculated

Design | u-Design Ok Plots | x-Design Ok Plots

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1		T_x	p_x	MS_x	VM_r	T__N	g_rho__D	s_rho	enth__D	cp__D	dd_su	PI6__d50	grad__y	PI8__GranF	Gfes__y	Grrho__y
2	R0	-4,0082523	-4,9649372	-7,7765122	4,128914	2,6697649	2,8046699	3	1,5466085	,0109041	-2,2915044	-1,74397482...	,28542227...	2,79934054...	-,258848401...	4,67760695...
3	R1	-3,9174468	-4,9241598	-7,7357348	3,8783658	2,6697649	2,8046699	3	1,5466085	,0109041	-2,291198	-2,10384981...	,24839018...	2,86921585...	-,226945306...	4,46760809...
4	R2	-4,0082523	-4,6639072	-7,7765122	3,9247941	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3473553	-2,14916624...	-,3362990...	2,73186230...	-,121478204...	4,46742308...
5	R3	-3,9174468	-4,6231298	-7,7357348	4,0824858	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3664231	-1,99607625...	,21085336...	2,69582210...	-,198596289...	4,67522825...
6	R4	-4,0082523	-4,9649372	-7,1744522	3,6237641	2,6697649	2,8046699	3	1,5466085	,0109041	-2,2352813	-1,96522749...	,24072392...	2,81427251...	-,223298816...	4,16750192...
7	R5	-3,9174468	-4,9241598	-7,1336748	3,7814558	2,6697649	2,8046699	3	1,5466085	,0109041	-2,2543491	-1,76187951...	,20544797...	2,66105999...	-,263603497...	4,37639444...
8	R6	-4,0082523	-4,6639072	-7,1744522	3,827884	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3105065	-1,81007088...	,35197014...	2,39357518...	-,316052869...	4,37621185...
9	R7	-3,9174468	-4,6231298	-7,1336748	3,5773358	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3102	-2,20739040...	,14132432...	2,59412159...	-,142667503...	4,16657809...
10	R8	-3,9616366	-4,7679126	-7,4033963	3,8388119	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3031559	-2,02760028...	,23408682...	2,69247126...	-,209714835...	4,40914389...
11	R9	-3,9616366	-4,7679126	-7,4033963	3,8388119	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3031559	-2,02760028...	,19628674...	2,63615290...	-,214670164...	4,40785818...
12	R10	-3,9616366	-4,7679126	-7,4033963	3,8388119	2,6697649	2,8046699	3	1,5466085	,0109041	-2,3031559	-2,04878958...	,20411998...	2,68057204...	-,218963061...	4,40822592...

uu u xx x scaled

Step 8ffff: ***ok-plot for x-design*** ***(not orthogonal)***

*This is **not** ideal for fitting the **y ~ f(c,x)** -model*

Step 9: ***Analyse – Summary of Fit***

File Edit Help

Design | Analysis

Fit a Model | Coefficients | Edit Model | Model Diagn.

Design | x-Design Ok Plots | summary-of-fit

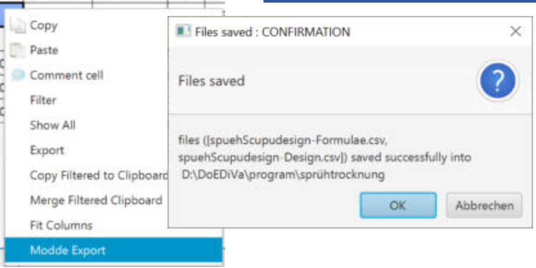
Response	RSquared	qSquared	rsd	rsdPercentage	no of runs	degreeOfFr
PI6__d50	0.9436561539534315	0.9136960999469821	0.013365759080477555	3.125426829947764	11	6
Gfes__y	0.7275512183804331	0.3455181527236393	0.00787879070530632	1.8307144248187912	11	6
Grrho__y	0.9999945109793064	0.9999909637830152	1.472055541240581E-6	3.3895388897864365E-4	11	6
grad__y	0.5106394607587582	-0.18543218795211658	0.15781103983514863	43.81726976832723	11	6
PI8__GranF	0.8933356158084262	0.7564903091396313	0.017296045364006567	4.0629289502801536	11	6

1. TODAY: The concept of dependent u-factors
2. Example: Spray drying, x_design and u_design
3. ***Optimization and Scale-Up considerations***

Step 10: ***Export of x-Design and u-formulae***

Design × | summary-of-fit

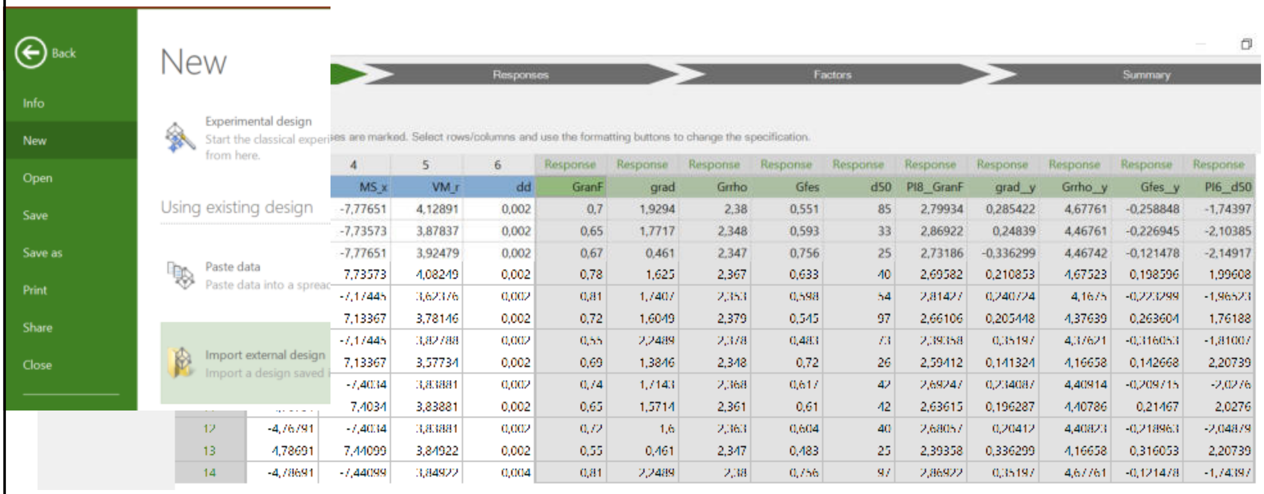
	A	B	C	D	E	F	G
1		T	p	MaS	VoG	dd	g_r
2	R0	170,0000473	,5	4,0000001	80,0000025	,002	672
3	R1	219,9999575	,5	4,0000001	49,9999996	,002	604
4	R2	170,0000473	1	4,0000001	49,9999996	,002	672
5	R3	219,9999575	1	4,0000001	80,0000025	,002	604
6	R4	170,0000473	,5	8,0000003	49,9999996	,002	672
7	R5	219,9999575	,5	8,0000003	80,0000025	,002	604
8	R6	170,0000473	1				
9	R7	219,9999575	1				
10	R8	194,9999701	,750000				
11	R9	194,9999701	,750000				
12	R10	194,9999701	,750000				



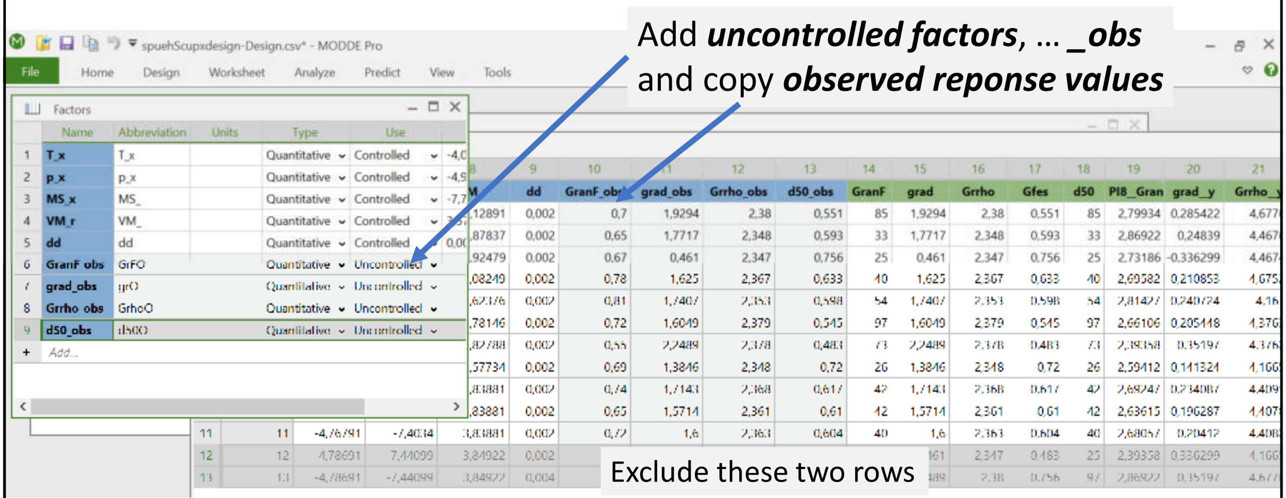
	T_x	p_x	MS_x	VM_r	dd	GranF	grad	Grrho	Gfes	d50	PI8__GranF	grad__y	Grrho__y	Gfes__y	PI6__d50
R0	-4,0083	-4,9649	-7,7765	4,1289	0,002	0,7	1,9294	2,38	0,551	85	2,79934	0,28542	4,67761	-0,2588	-1,744
R1	-3,9174	-4,9242	-7,7357	3,8784	0,002	0,65	1,7717	2,348	0,593	33	2,86922	0,24839	4,46761	-0,2269	-2,1038
R2	-4,0083	-4,6639	-7,7765	3,9248	0,002	0,67	0,461	2,347	0,756	25	2,73186	-0,3363	4,46742	-0,1215	-2,1492
R3	-3,9174	-4,6231	-7,7357	4,0825	0,002	0,78	1,625	2,367	0,633	40	2,69582	0,21085	4,67523	-0,1986	-1,9961
R4	-4,0083	-4,9649	-7,1745	3,6238	0,002	0,81	1,7407	2,353	0,598	54	2,81427	0,24072	4,1675	-0,2233	-1,9652
R5	-3,9174	-4,9242	-7,1337	3,7815	0,002	0,72	1,6049	2,379	0,545	97	2,66106	0,20545	4,37639	-0,2636	-1,7619
R6	-4,0083	-4,6639	-7,1745	3,8279	0,002	0,55	2,2489	2,378	0,483	73	2,39358	0,35197	4,37621	-0,3161	-1,8101
R7	-3,9174	-4,6231	-7,1337	3,5773	0,002	0,69	1,3846	2,348	0,72	26	2,59412	0,14132	4,16658	-0,1427	-2,2074
R8	-3,9616	-4,7679	-7,4034	3,8388	0,002	0,74	1,7143	2,368	0,617	42	2,69247	0,23409	4,40914	-0,2097	-2,0276
R9	-3,9616	-4,7679	-7,4034	3,8388	0,002	0,65	1,5714	2,361	0,61	42	2,63615	0,19629	4,40786	-0,2147	-2,0276
R10	-3,9616	-4,7679	-7,4034	3,8388	0,002	0,72	1,6	2,363	0,604	40	2,68057	0,20412	4,40823	-0,219	-2,0488

T_C	(10^(0.428682*v1 - 0.333945*v2+0.0821633*v3 - 0.036
p_C	(10^(- 0.53808*v1+0.640162*v2+0.0885338*v3 - 0.039
MaS_C	(10^(- 0.161324*v1+0.255506*v2+0.437136*v3+0.0278
VoG_C	(10^(0.267358*v1 - 0.0784389*v2+0.519299*v3+0.4914
dd_C	(10^(0.0538579*v1+0.217713*v2 - 0.0535656*v3+0.023
Grrho_C	(10^(v20+(- 0.161324*v1+0.255506*v2+0.437136*v3+(
GranF_C	(10^(v18+(- 0.53808*v1+0.640162*v2+0.0885338*v3 -
Gfes_C	(10^(v19))
d50_C	(10^(v16+(- 0.53808*v1+0.640162*v2+0.0885338*v3 -
grad_C	(10^(v17))
PI6__d50_C	Log10(v6*1.0E-6)+(- 0.53808*v1+0.640162*v2+0.0885
grad__y_C	Log10(v7)
PI8__GranF_	Log10(v8*1000.0)+(- 0.53808*v1+0.640162*v2+0.0885
Gfes__y_C	Log10(v9)
Grrho__y_C	Log10(v10*1000.0) - (- 0.161324*v1+0.255506*v2+0.43

Step 10: *Use MODDE® to Analyse and Optimize*



Step 9f: *Prepare the worksheet (... obs-columns)*



Step 10: ***Use MODDE® to Analyse and Optimize***

Step 9ff: ***Check the worksheet (u-T[-1]ransforms)***

spuehScup1-Design.csv.mip* - MODDE Pro - [Worksheet]

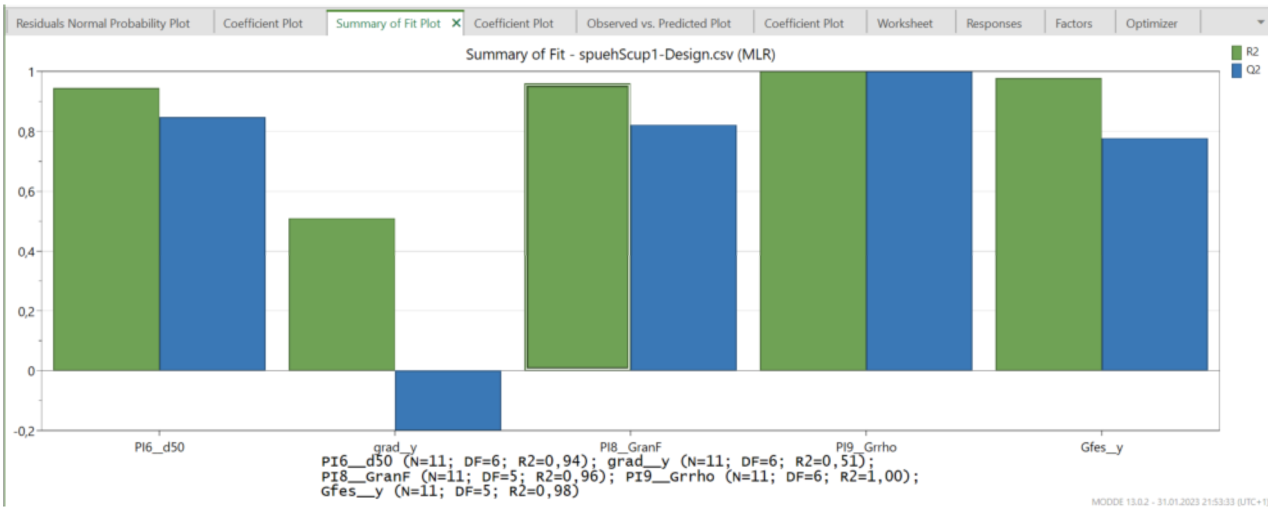
File | Home | Design | Worksheet | Analyze | Predict | View | Tools

Worksheet | Responses | Factors | Summary of Fit Plot

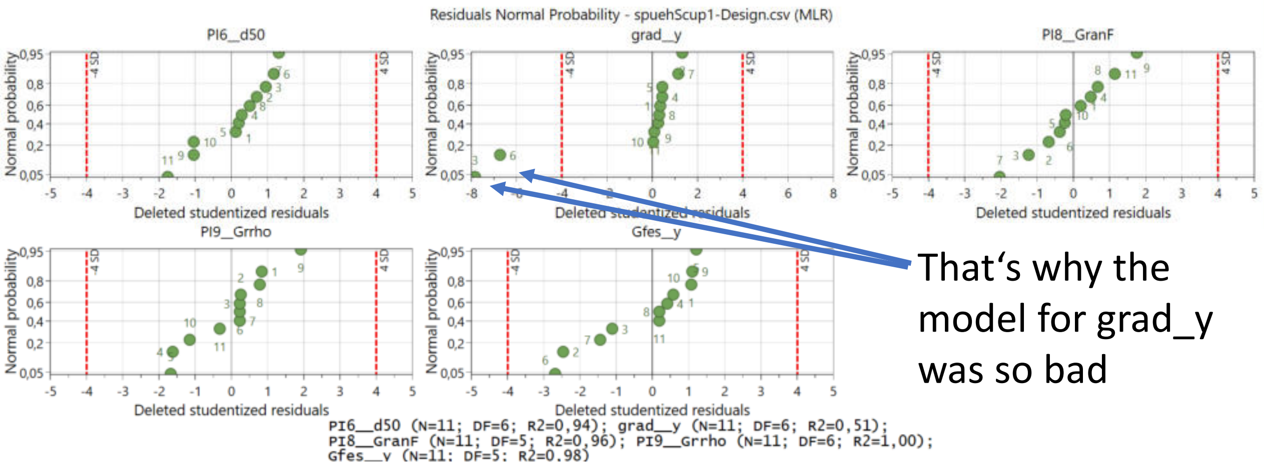
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
	No	Exp	Ru	Incl/E	p_x	MS_x	StrVh	T_x	dd	d50_o	grad_o	GrF_o	Grho	Gfeso	d50	grad	GranF	Grrho	Gfes	PI6_d50	grad_y	PI8_Gr	PI9_Grr	Gfes_y	T_C	P_C	MS_C
1	1	R0	6	Incl	-4,96494	-9,21862	4,12891	2,64655	0,002	85	1,9294	0,7	2,38	0,551	85	1,9294	0,7	2,38	0,551	-1,74397	0,285422	2,79934	0,677607	-0,258848	169,999	0,500004	4,00002
2	2	R1	9	Incl	-4,92416	-9,22222	3,87837	2,69298	0,002	33	1,7717	0,65	2,348	0,593	33	1,7717	0,65	2,348	0,593	-2,10385	0,24839	2,86922	0,671728	-0,226945	220,001	0,500004	4,00003
3	3	R2	12	Incl	-4,66391	-9,21862	3,92479	2,64655	0,002	25	0,461	0,67	2,347	0,756	25	0,461	0,67	2,347	0,756	-2,14917	-0,336299	2,73186	0,370513	-0,121478	169,999	1,00001	4,00003
4	4	R3	5	Incl	-4,62313	-9,22222	4,08249	2,69298	0,002	40	1,625	0,78	2,367	0,633	40	1,625	0,78	2,367	0,633	-1,99608	0,210853	2,69582	0,374198	-0,198596	220,001	1,00001	4,00002
5	5	R4	7	Incl	-4,96494	-8,61656	3,62376	2,64655	0,002	54	1,7407	0,81	2,353	0,598	54	1,7407	0,81	2,353	0,598	-1,96523	0,240724	2,81427	0,672652	-0,223299	169,999	0,500004	8,00006
6	6	R5	13	Incl	4,92416	8,62016	3,78146	2,69298	0,002	97	1,6049	0,72	2,379	0,545	97	1,6049	0,72	2,379	0,545	1,76188	0,205448	2,66106	0,677424	0,263604	220,001	0,500004	8,00005
7	7	R6	8	Incl	-4,66391	-8,61656	3,82788	2,64655	0,002	73	2,2489	0,55	2,378	0,483	73	2,2489	0,55	2,378	0,483	-1,81007	0,35197	2,39358	0,376212	-0,316053	169,999	1,00001	8,00005
8	8	R7	10	Incl	4,62313	8,62016	3,57734	2,69298	0,002	26	1,3846	0,69	2,348	0,72	26	1,3846	0,69	2,348	0,72	2,20739	0,141324	2,59412	0,370698	0,142668	220,001	1,00001	8,00005
9	9	R8	1	Incl	-4,76791	-8,86828	3,83881	2,67038	0,002	42	1,7143	0,74	2,368	0,617	42	1,7143	0,74	2,368	0,617	-2,0276	0,234087	2,69247	0,49932	-0,209715	194,995	0,750021	6,00007
10	10	R9	11	Incl	4,76791	8,86828	3,83881	2,67038	0,002	42	1,5714	0,65	2,361	0,61	42	1,5714	0,65	2,361	0,61	2,0276	0,196287	2,63615	0,498035	0,21467	194,995	0,750021	6,00007
11	11	R10	4	Incl	-4,76791	-8,86828	3,83881	2,67038	0,002	40	1,6	0,72	2,363	0,604	40	1,6	0,72	2,363	0,604	-2,04879	0,20412	2,68057	0,498402	-0,218963	194,995	0,750021	6,00007
12	12	R11	2	Excl	4,78691	8,90545	3,84922	2,66993	0,002						25	0,461	0,55	2,347	0,483	2,20739	0,336299	2,39358	0,370513	0,316053			
13	13	R12	3	Excl	-4,78691	-8,90545	3,84922	2,66993	0,004						97	2,2489	0,81	2,38	0,756	-1,74397	0,35197	2,86922	0,677607	-0,121478			

all experiments done at ***dd = 2mm*** *(nozzle diameter)*

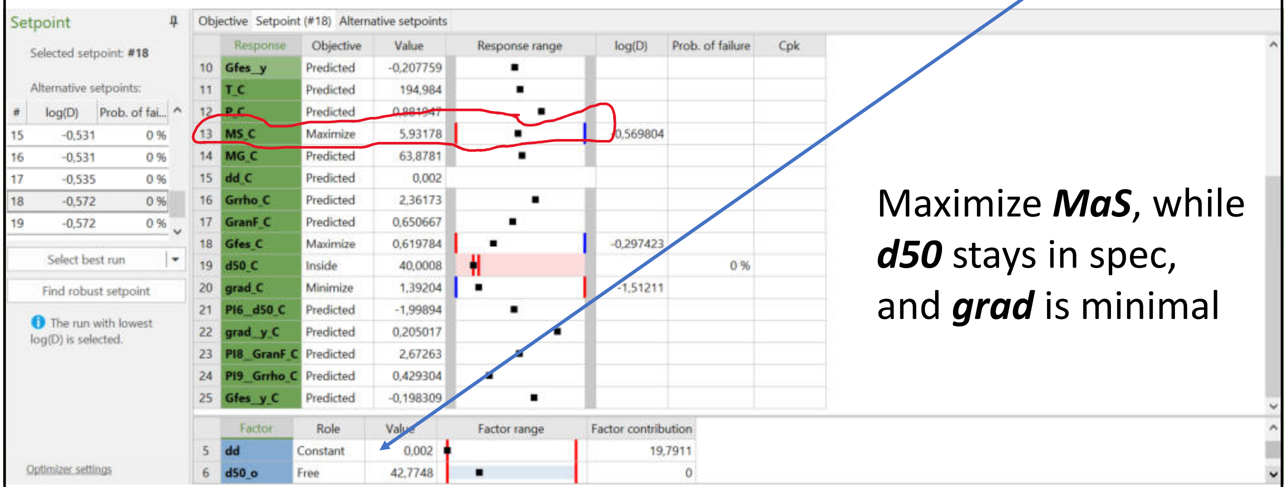
Step 9ff: ***FIT the model – y-response to x-design***



Step 9ff: ***Diagnose the model for the y-responses***



Step 10: *Optimize for the low Scale, dd = 2 mm*



Maximize ***MaS***, while ***d50*** stays in spec, and ***grad*** is minimal

Step 10ff: *Optimize for the high Scale, dd = 4 mm*

MaS, 2 times higher ***d50*** better in spec, and ***grad*** is smaller

Vielen Dank!

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ganz besonders an:

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