OMARS Designs: Factor Screening and Response Surface Optimization in a Single Step

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Joint work with José Núñez Ares

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Initial OMARS designs ?

- Experimental designs for quantitative factors
- Every factor is studied at three levels
- Therefore, they are called **response surface** designs
- All main effects are orthogonal to each other
- Therefore, they are called **orthogonal** designs
- All main effects are orthogonal
  - to all two-factor interactions
  - to all quadratic effects
- Therefore, they are called **minimally aliased**

<u>O</u>rthogonal

<u>M</u>inimally

<u>A</u>liased

<u>R</u>esponse

<u>S</u>urface

designs

Well-known OMARS designs

- Traditional response surface designs
  - **Central composite designs**
  - **Box-Behnken designs**
- These designs are “strong” OMARS designs
  - Interaction effects are orthogonal to each other
  - Interaction effects are orthogonal to quadratic effects
  - Can be viewed as resolution V designs
- **Definitive screening designs**
  - Substantial aliasing among interactions
  - Substantial aliasing between interactions and quadratics
  - A bit better than resolution IV designs

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  - **Box-Behnken designs**
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- **Definitive screening designs** (SMALL)
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  - Substantial aliasing between interactions and quadratics
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Catalog of OMARS designs

- There is a large variety of OMARS designs (using ILP)
- Bridges the gap between the small definitive screening designs and traditional response surface designs
- Major selling points of OMARS designs:
  - Flexibility in terms of number of runs
  - Better power for quadratic effects
  - Screening and response surface experiment in one
    - Good projection properties
    - OMARS designs rely less on factor sparsity assumption than definitive screening designs
    - Ideal when budget does not allow optimal design of experiments
  - Better looking color maps

Color map of an OMARS design

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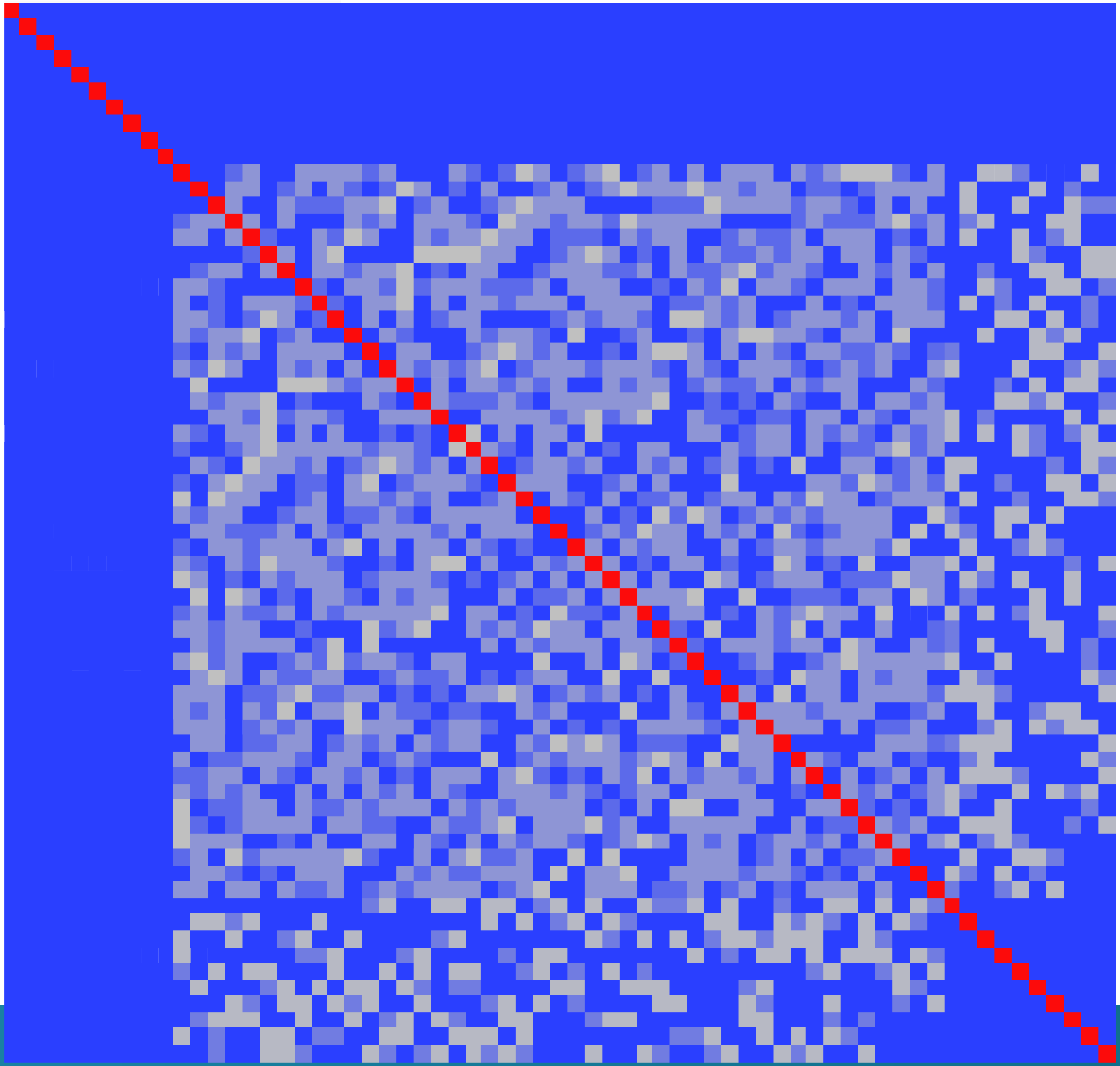


Original OMARS designs

- Our original designs are **uniform-precision** OMARS designs
- Every column in the design matrix has the same number of zeros
- Every main effect can be estimated equally precisely
- The power for detecting an existing main effect is the same for every factor
- The power for detecting a quadratic effect is also the same for every factor
- DSDs belong to the family of uniform-precision OMARS designs

Uniform-precision OMARS design

X1	X2	X3	X4	X5
-1	-1	-1	-1	-1
-1	-1	1	0	-1
-1	-1	1	1	1
-1	0	-1	0	0
-1	0	0	-1	1
-1	1	-1	1	1
-1	1	0	-1	0
-1	1	1	1	-1
0	-1	-1	1	0
0	-1	0	0	1
0	0	-1	1	-1
0	0	1	-1	1
0	1	0	0	-1
0	1	1	-1	0
1	-1	-1	-1	1
1	-1	0	1	0
1	-1	1	-1	-1
1	0	0	1	-1
1	0	1	0	0
1	1	-1	-1	-1
1	1	-1	0	1
1	1	1	1	1

Numbers of uniform-precision OMARS designs

		nruns								
		14	16	20	22	24	26	27	28	30
$m = 6$	#sol	1	1	2	4	25	519	7	485	8,864
	#nodes	82	250	502	2,532	16,252	718,458	704,220	1,173,594	39,415,295
	time	6s	13s	20s	69s	457s	7.7h	6.9h	12h	15.9d
$m = 7$	#sol	1	1	1	1	5	549	0	106	20,019
	#nodes	60	262	634	832	13,726	2,053,001	372,331	4,263,183	555,221,657
	time	25s	100s	158s	128	1702s	5.4d	21.1h	8.9d	4.4y
$m = 8$	#sol	-	1	1	0	3	853	-	9	11
	#nodes	-	110	646	236	11,985	6,807,971	-	9,497,041	11,900,209
	time	-	113s	572s	99s	3.1h	3m	-	6.2m	5.6m

Numbers of uniform-precision OMARS designs

		nruns					
		31	32	34	35	36	40
$m = 6$	#sol	37	69,677	227,902	258	65,836	-
	#nodes	50,649,649	358,608,938	976,161,360	1,644,770,934	226,213,340	-
	time	16.5d	5m	1.9y	4.4m	2.8m	-
$m = 7$	#sol	9	49,269	16,952	3	57,727	1,656
	#nodes	712,279,617	280,674,367	430,079,736	3,140,152,715	3,366,592,634	72,419,243,247
	time	4.7y	19.7y	3.5y	20.2y	22.2y	2.3y
$m = 8$	#sol	-	31	0	-	0	284
	#nodes	-	981,101,888	86,365	-	269,792,124	23,824,792,213
	time	-	106.5y	16.4h	-	25.3y	28.8y

What if …

- … you have prior knowledge concerning factor effects?
- … you have specific desires for certain factors?

- … you may know certain factors are unlikely to have quadratic effects?
- … you may care more about certain main effects than others?
- … you may wish to study certain quadratic effects in more detail than others?

- … certain factors are categorical and have only two levels?

Then …

- … you do not want the same precision and the same power for every main effect
- … you do not want the same power for every quadratic effect
- … you do not want the same number of zeros in every column of your OMARS design
- … you need a **non-uniform precision OMARS design**
- … you need to make a small modification to our construction method (integer programming) to broaden the spectrum of OMARS designs

Then …

- … you do not want the same precision and the same power for every main effect
- … you do not want the same power for every quadratic effect
- … you do not want the same number of zeros in every column of your OMARS design
- … you need a **non-uniform precision OMARS design**
- … you need to make a small modification to our construction method (integer programming) to broaden the spectrum of OMARS designs
- … and you will find many more OMARS designs

Total numbers of OMARS designs

#runs/#factors	3	4	5	6	7	8	9	10	11	12	13	14	15	16
14	46	128	11	4	2									
16	159	190	152	61	8	3								
18	198	359	552	171	30	11								
20	572	1,621	5,569	5,117	997	171	7	3						
22	1,438	5,788	42,262	97,792	37,941	3,021	145	6						
24	1,921	12,765	168,045	886,015	1,919,652	142,192	12,637	1,658	152	35				
26	2,235	21,482	807,530	9,611,789	5,086,943	1,815,173	898,596	287,208	298,799	1,426	7			
28	492	3,285	91,111	1,022,895	1,255,206	265,213	37,228	7,676	1,505	487	93			
30	1,263	18,761	1,822,824	27,311,163	55,340,120	26,620,971	3,231,476	60,050	560	31	8	1		
32	33	656	5,177	47,237	114,145	99,398	47,574	17,237	3,594	430				
34	38	651	8,564	139,985	171,785	15,654	878	177	27	15	4	4	1	1
36	64	2,157	38,368	1,926,480	4,971,761	1,646,150	53,536	669	11	1	1	1		
38	95	4,420	137,380	15,097,844	7,034,284	3,086,804	28,877	232	27	15	4	4	1	1
40	129	9,688	919,100	59,240,843	66,439,987	7,590,489	983,545	12,560	26	13	3	3	1	1
TOTAL	8,683	81,951	4,046,645	115,387,396	142,372,861	41,285,250	5,294,499	387,476	304,701	2,453	120	13	3	3
GRAND TOTAL	309,172,054													

Mixed-level OMARS design

- We were able to create OMARS designs where
  - Some quantitative factors have three levels
  - Other factors have two levels
- Special case where certain columns have no zeros
- Useful when you want to study certain factors at two levels
  - Two-level categorical factors
  - Quantitative factors without quadratic effects
- Mixed-level OMARS designs preserve the orthogonality and minimal aliasing property (unlike definitive screening designs)

Mixed-level OMARS design 1

1	0	-	+	+	+	+	+	-
2	0	+	-	-	-	-	-	+
3	-	0	+	+	+	-	-	-
4	+	0	-	-	-	+	+	+
5	-	-	0	-	+	-	+	+
6	+	+	0	+	-	+	-	-
7	-	-	-	0	-	-	+	-
8	+	+	+	0	+	+	-	+
9	-	+	-	+	+	-	-	+
10	+	-	+	-	-	+	+	-
11	-	+	+	-	+	+	+	+
12	+	-	-	+	-	-	-	-
13	0	-	+	-	-	-	-	+
14	0	+	-	+	+	+	+	-
15	-	0	-	+	-	+	+	+
16	+	0	+	-	+	-	-	-
17	-	+	0	-	-	+	-	-
18	+	-	0	+	+	-	+	+
19	-	+	+	0	-	-	+	-
20	+	-	-	0	+	+	-	+
21	-	-	-	-	+	+	-	-
22	+	+	+	+	-	-	+	+
23	-	-	+	+	-	+	-	+
24	+	+	-	-	+	-	+	-

Mixed-level OMARS design 2

1	0	-	+	0	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2	0	+	0	0	0	-	-	-	-	-	-	-	-	-	+	+	+	+	+
3	0	0	0	+	0	-	-	-	-	-	-	+	+	+	-	-	-	+	+
4	0	0	-	+	+	-	-	-	-	+	+	-	-	+	-	+	+	-	-
5	0	0	-	-	-	-	-	-	+	-	+	-	+	-	+	-	-	-	+
6	0	+	0	-	+	-	-	-	+	+	-	+	+	+	+	-	+	-	-
7	-	-	+	0	-	-	-	+	-	-	+	+	+	+	+	+	+	-	-
8	+	0	0	0	0	-	-	+	-	+	+	-	+	+	+	-	+	+	+
9	0	+	+	0	+	-	-	+	+	-	+	+	-	-	+	+	-	+	-
10	-	0	-	0	-	-	-	+	+	+	-	+	-	-	-	+	+	-	+
11	+	0	0	0	-	-	-	+	+	+	-	+	-	+	-	-	-	+	-
12	0	-	0	0	+	-	-	+	+	+	+	-	+	-	-	+	-	+	+
13	0	0	+	-	0	-	+	-	-	+	-	+	+	-	-	+	+	+	+
14	-	0	-	0	0	-	+	-	-	+	+	+	-	-	+	-	-	+	-
15	+	0	0	-	-	-	+	-	+	-	+	-	-	+	-	+	+	+	-
16	0	+	0	+	0	-	+	-	+	-	+	+	+	+	-	+	-	-	+
17	-	-	0	0	0	-	+	-	+	+	-	-	+	+	+	+	-	+	-
18	+	-	+	+	0	-	+	-	+	+	+	+	-	-	+	-	+	-	+
19	+	-	-	-	+	-	+	+	-	-	-	+	-	+	+	+	-	-	+
20	0	0	-	0	0	-	+	+	-	-	+	+	+	-	-	-	+	+	-
21	+	+	0	+	-	-	+	+	-	+	-	-	+	-	+	+	-	-	-
22	-	+	+	-	0	-	+	+	-	+	+	-	-	+	-	-	-	-	+
23	-	0	0	+	0	-	+	+	+	-	-	-	-	+	+	-	+	+	+
24	0	0	0	0	+	-	+	+	+	-	-	-	+	-	-	-	+	-	-
25	0	0	0	0	-	+	-	-	-	+	+	+	-	+	+	+	-	+	+
26	+	0	0	-	0	+	-	-	-	+	+	+	+	-	-	+	-	-	-
27	+	-	-	+	0	+	-	-	+	-	-	+	+	-	+	+	+	+	-
28	-	-	0	-	+	+	-	-	+	-	+	+	-	+	-	-	+	+	+
29	0	0	+	0	0	+	-	-	+	+	-	-	-	+	+	+	-	-	+
30	-	+	+	+	-	+	-	-	+	+	+	-	+	-	-	-	+	+	-
31	-	+	-	-	0	+	-	+	-	-	-	-	+	+	-	+	-	+	-
32	+	+	0	0	0	+	-	+	-	-	+	+	-	-	-	-	+	-	+
33	0	-	0	-	0	+	-	+	-	+	-	-	-	-	+	-	+	+	-
34	-	0	0	+	+	+	-	+	-	+	-	+	+	-	+	-	-	-	+
35	+	0	+	0	0	+	-	+	+	-	-	-	+	+	-	+	+	-	+
36	0	0	-	+	0	+	-	+	+	-	+	-	-	+	+	-	-	-	-
37	0	+	0	0	-	+	+	-	-	-	-	+	-	+	+	-	+	-	-
38	-	0	0	0	+	+	+	-	-	-	+	-	+	-	+	+	+	-	+
39	+	0	+	0	+	+	+	-	-	-	+	-	+	+	+	-	-	+	-
40	0	-	-	0	-	+	+	-	-	+	-	-	+	+	-	-	+	-	+
41	-	0	0	0	0	+	+	-	+	-	-	+	-	-	-	+	-	-	-
42	+	+	-	0	+	+	+	-	+	+	-	-	-	-	-	-	-	+	+
43	0	-	0	+	-	+	+	+	-	-	+	-	-	-	-	+	-	+	+
44	0	0	+	+	+	+	+	+	-	+	-	+	-	+	-	+	+	+	-
45	0	0	+	-	-	+	+	+	+	-	-	+	+	-	+	-	-	+	+
46	0	0	0	-	0	+	+	+	+	+	+	-	-	-	+	+	+	-	-
47	0	-	0	0	0	+	+	+	+	+	+	+	+	+	-	-	-	-	-
48	0	+	-	0	0	+	+	+	+	+	+	+	+	+	+	+	+	+	+

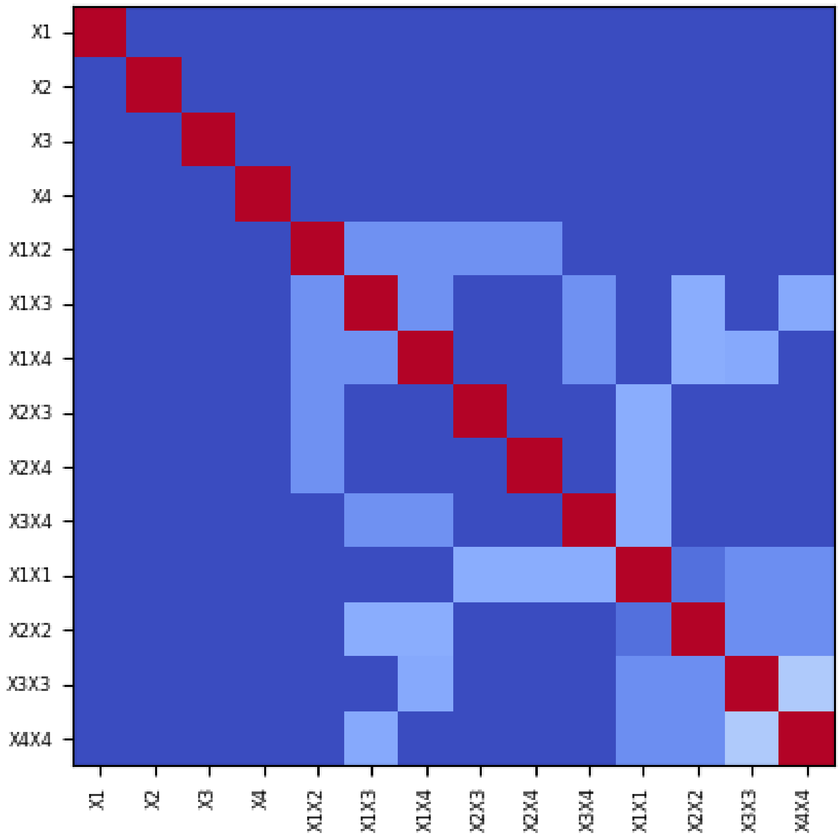
Mixed-level OMARS design 3

1	-	-	-	-	-	-	-	-	-	-
2	-	-	-	+	-	-	-	+	+	+
3	-	-	0	-	+	0	+	-	+	-
4	-	-	+	0	0	+	-	-	-	+
5	-	0	0	+	-	+	+	-	+	-
6	-	0	+	-	0	-	+	+	+	+
7	-	0	+	0	+	-	+	+	-	-
8	-	0	+	+	+	0	-	-	+	+
9	-	+	-	0	+	0	-	+	-	+
10	-	+	-	+	0	0	+	-	-	-
11	-	+	0	-	0	+	-	+	-	-
12	-	+	0	0	-	+	+	+	+	+
13	0	-	-	0	+	+	+	+	+	-
14	0	-	-	+	+	0	+	+	-	+
15	0	-	0	-	-	+	+	+	-	+
16	0	-	+	+	0	+	-	+	-	-
17	0	0	-	-	+	+	-	-	+	+
18	0	0	+	+	-	-	+	+	-	-
19	0	+	-	-	0	-	+	-	+	+
20	0	+	0	+	+	-	-	-	+	-
21	0	+	+	-	-	0	-	-	+	-
22	0	+	+	0	-	-	-	-	-	+
23	+	-	0	0	+	-	-	-	-	-
24	+	-	0	+	0	-	+	-	+	+
25	+	-	+	-	0	0	-	+	+	+
26	+	-	+	0	-	0	+	-	+	-
27	+	0	-	-	-	0	+	+	-	-
28	+	0	-	0	-	+	-	-	+	+
29	+	0	-	+	0	+	-	-	-	-
30	+	0	0	-	+	-	-	+	-	+
31	+	+	-	0	0	-	+	+	+	-
32	+	+	0	+	-	0	-	+	-	+
33	+	+	+	-	+	+	+	-	-	-
34	+	+	+	+	+	+	+	+	+	+
35	0	0	0	0	0	0	-	+	+	-
36	0	0	0	0	0	0	-	+	+	-
37	0	0	0	0	0	0	-	+	+	-
38	0	0	0	0	0	0	+	-	-	+
39	0	0	0	0	0	0	+	-	-	+
40	0	0	0	0	0	0	+	-	-	+

A non-uniform precision OMARS design

X1	X2	X3	X4		X1	X2	X3	X4
1	-1	-1	1		1	0	0	0
0	1	0	1		0	-1	-1	0
0	-1	1	0		0	-1	1	-1
-1	0	1	1		-1	0	1	-1
-1	1	-1	-1		1	1	-1	0
1	-1	1	1		0	1	-1	1
1	0	-1	-1		-1	1	1	0
-1	0	-1	1		1	0	0	0
-1	-1	-1	-1		-1	-1	0	1
-1	-1	0	0		1	1	1	1
1	1	1	-1		1	-1	0	-1
-1	1	0	0		0	1	0	-1

Color map



GSK’s first OMARS design application

The case study

- Goal: find relevant factors and optimal settings to increase biomass
- Factors:
  - Holding Time
  - Inoculum Dilution
  - Iron
  - pH
  - Temperature
  - Speed Pump
- The Ambr250 system automatically manages 24 bioreactors (250ml) at the same time

NOTE:

1 intercept

6 main effects

6 quadratic effects

6 × 5 / 2 = 15 interactions

So 28 parameters

Optimal design approach infeasible

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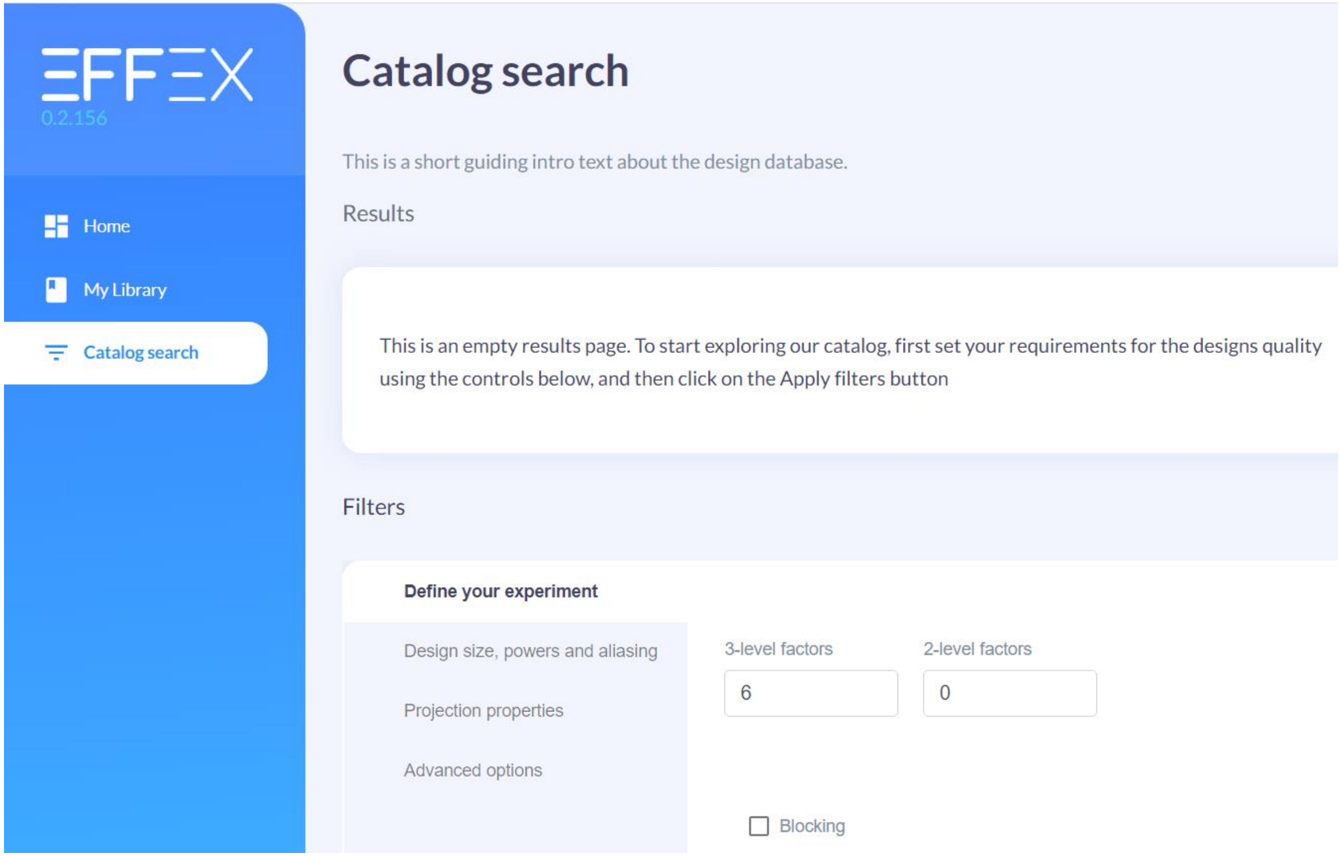
A powerful combo: OMARS designs and Ambr250 system

EFFEX™ software



The selected OMARS design

- 24 runs
- 3 duplicated test combinations (one of which is the center point)
- Fold-over design
- Non-uniform precision
  - X1-X4 have 6 zeros
  - X5 has 8 zeros
  - X6 has 10 zeros

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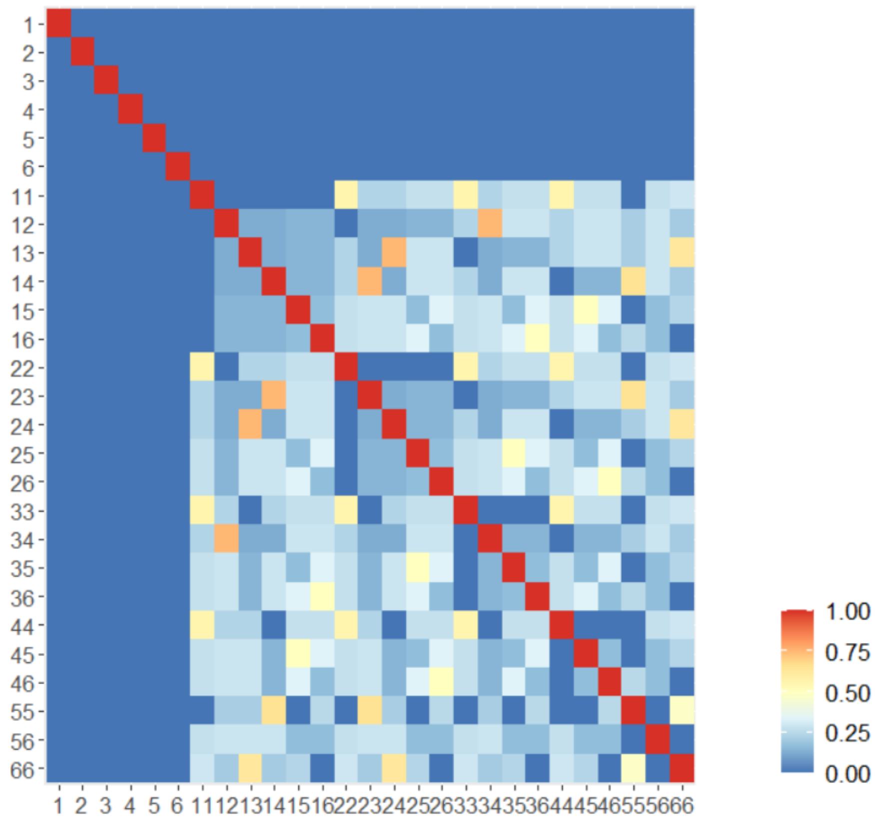
Color map on correlations



Projection estimation capacity

- There are 15 subsets of 4 out of 6 factors
- The OMARS design allows estimation of the main-effects-plus-interactions model in any of these subsets

X1 SP	X2 HT	X3 Dil	X4 Fe	X5 T	X6 pH
	✓	✓	✓		✓
✓		✓		✓	✓
✓		✓	✓	✓	
✓		✓	✓		✓
✓	✓	✓		✓	

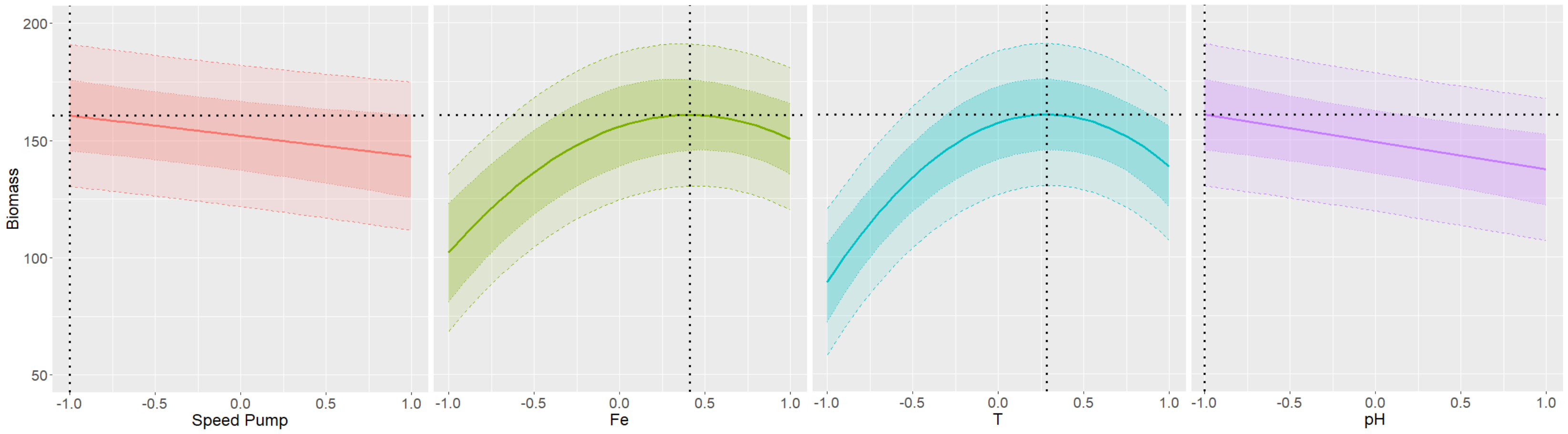
Projection estimation capacity

- There are 20 subsets of 3 out of 6 factors
- The OMARS design allows estimation of the full quadratic response surface model in any of these subsets

X1 SP	X2 HT	X3 Dil	X4 Fe	X5 T	X6 pH
✓				✓	✓
✓		✓			✓
	✓		✓	✓	
✓		✓	✓		
	✓	✓		✓	

Results

- Active factors: Speed Pump, Iron, Temperature, pH
- Inactive factors: Holding Time, Inoculum Dilution
- Optimal settings:



Bernard Francq
(Lead Statistician, GSK Biologicals)

Presentation at ENBIS conference

DOE in Pharma Industry

- Screening and optimization are 2 distinct phases
- You need a 1st DOE
- Time is needed in between
  - to get the data
  - to analyze the data
  - to select the impactful factors
- Then, a 2nd DOE has to be constructed
- Time goes by
  - to get the data
  - to analyze the data
  - to draw conclusions

DOE in Pharma Industry

- Screening and optimiza[illegible]re 2 distinct phases
- You need a 1st DOE
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    - to get the data
    - to analyze the data
    - to select the impactful factors
- Then, a 2nd DOE has to be constructed
- Time goes by
    - to get the data
    - to analyze the data
    - to draw conclusions

"Why not combine Screening & Optimization in only one step ??"

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Bernard’s conclusions

- The OMARS design allowed GSK to screen 6 fermentation factors and to optimize the productivity with just 24 tests
- With the Ambr system, it was possible to do so in one week
- The combination of the OMARS design and the Ambr system has saved time and resources
- The vast catalog of OMARS designs allows
  - Screening and optimization to be combined
  - Multi-criteria selection of OMARS designs
  - Can be done in the EFFEX™ software

EFFEX

A collaborative platform for your experimental plans

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EFFEX™

- Spin-off company to valorize the OMARS designs (see effex.app)
- 500,000 OMARS Pareto-optimal designs are available in the web-based EFFEX™ software
  - Three-level OMARS designs
  - Mixed-level OMARS designs
  - Orthogonally blocked OMARS designs
- Multi-criteria design selection
- If interested, visit the website or talk to me

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WLGore's Heart Valve Experiment

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Application at WLGore

Step	Factor	Unit	Low	High	No. Levels	Symbol
Polymerization					3	X1
Polymerization	CONFIDENTIAL				3	X2
Coagulation					2	X3
Coagulation					2	X4
Coagulation	Coag Temp	°C	40	65	3	X5
Coagulation	Wash Temp	°C	50	85	3	X6
Coagulation	No. Cycles		6	12	2	X7
Drying	Drying Temperature	°C	130	150	3	X8

Application at WLGore

Factors	X1	X2	X3	X4	X5	X6	X7	X8
X1	H	NO	L	L	NO	NO	NO	NO
X2		H	M	L	NO	NO	L	NO
X3			NO	H	H	L	M	L
X4				NO	H	L	M	L
X5					H	L	L	NO
X6						H	H	NO
X7							NO	L
X8								H

Application at WLGore

Factors	X1	X2	X3	X4	X5	X6	X7	X8
X1	H	NO	L	L	NO	NO	NO	NO
X2		H	M	L	NO	NO	L	NO
X3			NO	$\boxed{H}$	$\boxed{H}$	L	M	L
X4				NO	$\boxed{H}$	L	M	L
X5					H	L	L	NO
X6						H	$\boxed{H}$	NO
X7							NO	L
X8								H

Application at WLGore

Factors	X1	X2	X3	X4	X5	X6	X7	X8
X1	H	NO	L	L	NO	NO	NO	NO
X2		H	$\boxed{M}$	L	NO	NO	L	NO
X3			NO	H	H	L	M	L
X4				NO	H	L	M	L
X5					H	L	L	NO
X6						H	H	NO
X7							NO	L
X8								H

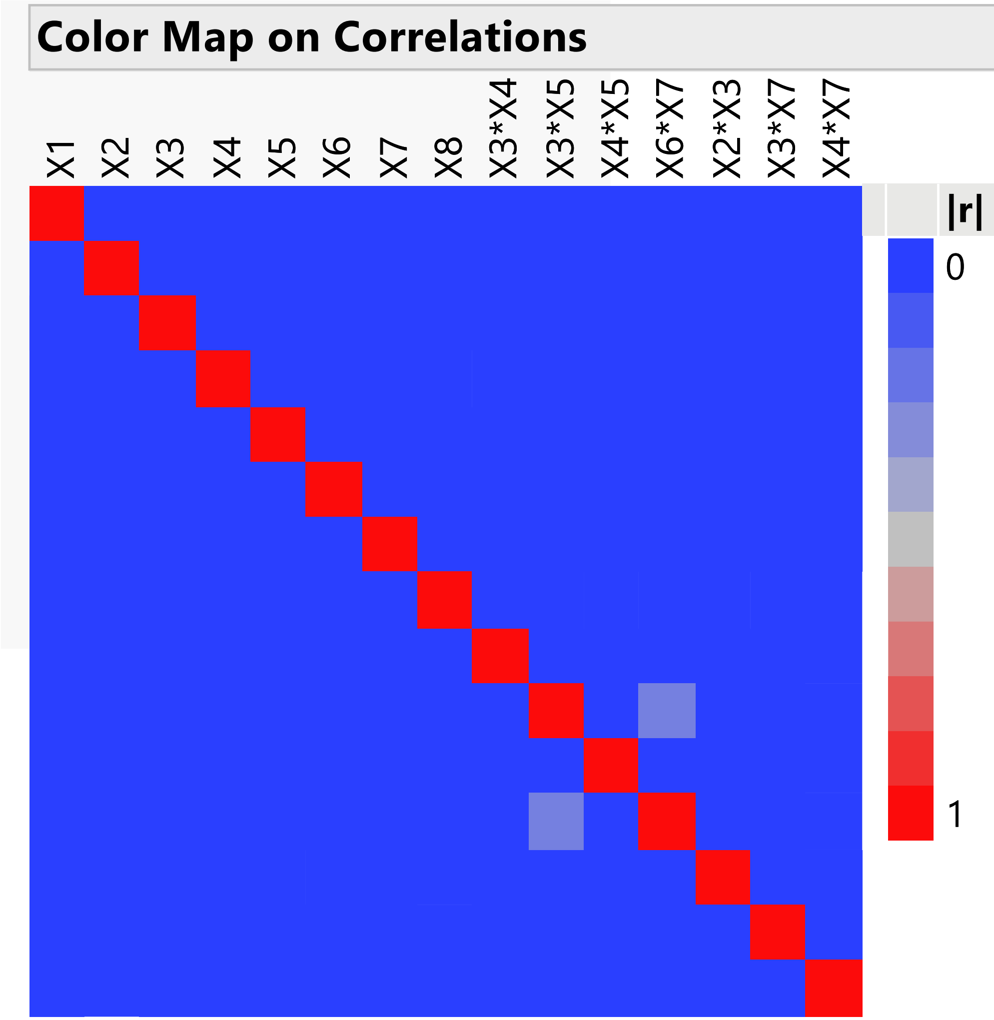
OMARS design

X1	X2	X3	X4	X5	X6	X7	X8
-1	1	1	-1	0	0	1	-1
0	1	-1	-1	1	0	-1	-1
-1	-1	-1	-1	1	1	1	0
1	-1	-1	1	0	0	-1	1
1	1	1	1	1	1	1	1
-1	0	-1	1	-1	0	1	1
1	0	1	-1	1	0	-1	-1
1	-1	-1	1	1	-1	1	-1
0	-1	1	-1	0	-1	-1	1
1	0	-1	-1	0	1	-1	1
-1	-1	1	1	1	1	-1	0
-1	-1	-1	-1	-1	-1	-1	-1
1	1	1	1	-1	-1	-1	0
-1	1	-1	1	1	-1	-1	1
0	1	-1	1	0	1	1	-1
0	-1	1	1	-1	0	1	1
-1	1	1	-1	-1	1	-1	1
1	1	-1	-1	-1	-1	1	0
0	0	-1	-1	0	0	1	1
0	0	-1	1	-1	1	-1	-1
0	0	1	-1	1	-1	1	1
0	0	1	1	0	0	-1	-1
1	-1	1	-1	-1	1	1	-1
-1	0	1	1	0	-1	1	-1

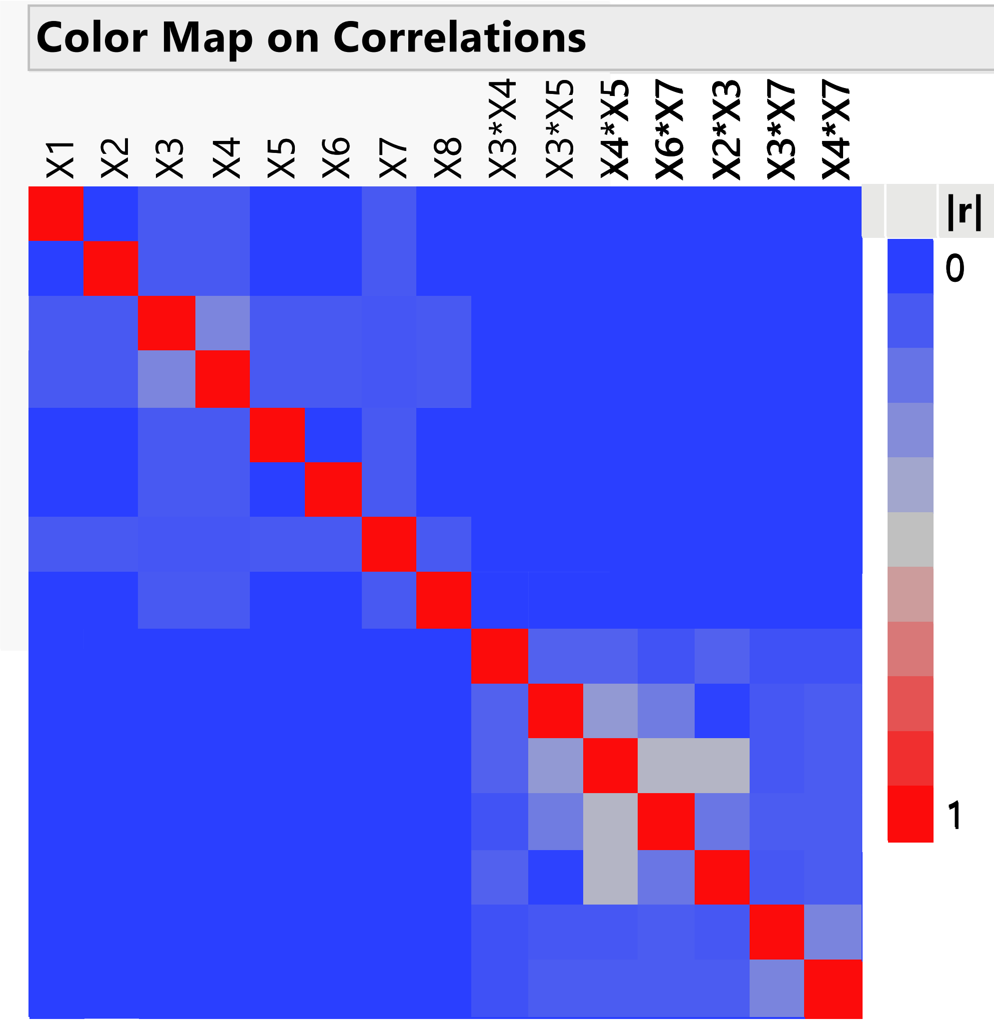
How to get the design ?

- 81 mixed-level OMARS designs involving 24 runs
- Select 15 designs with a power of 0.96 for main effects
- Select 5 designs with a minimum power of 0.9 or more for an interaction effect
- Select the one design without perfect aliasing
- Can estimate all main-effects-plus-two-factor-interactions models involving
  - any pair of three-level factors and 3 two-level factors
  - any set of 3 three-level factors and 2 two-level factors
  - any set of 4 three-level factors and one two-level factor

24-run OMARS design

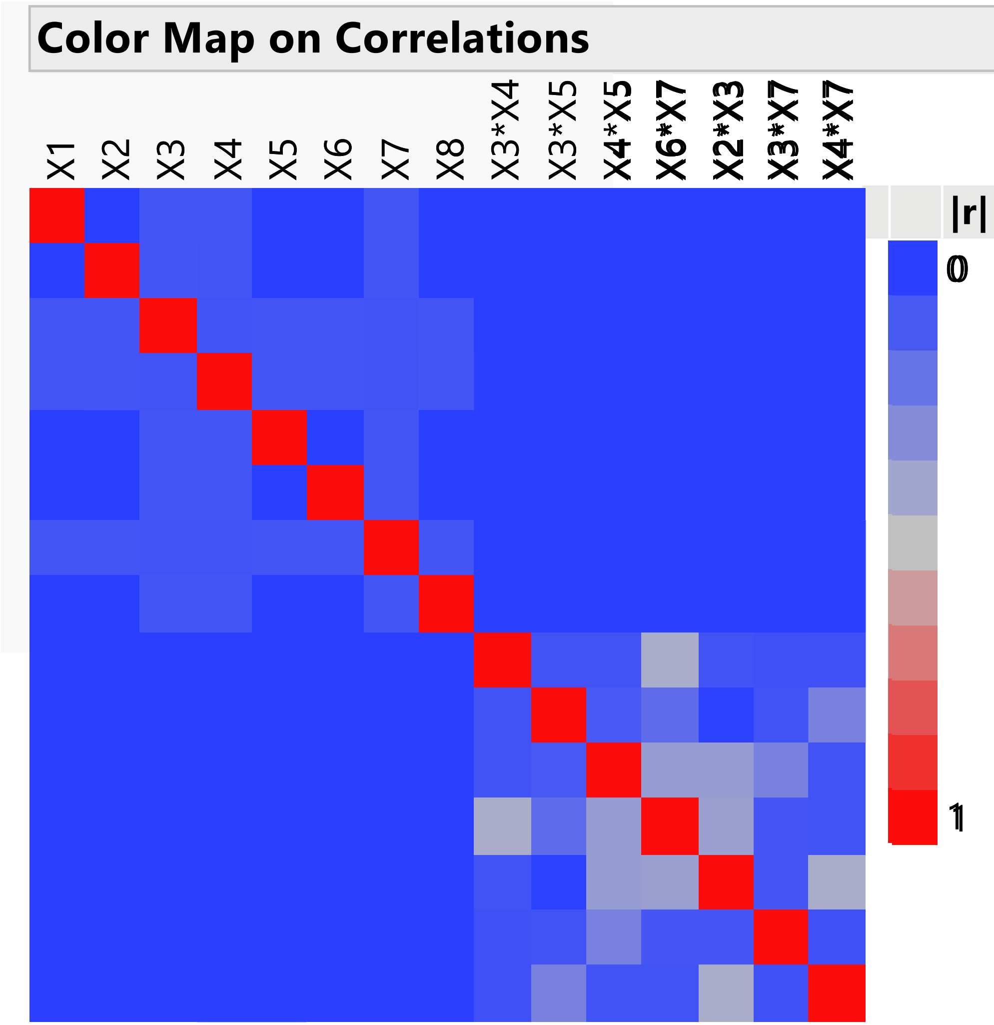


22-run DSD

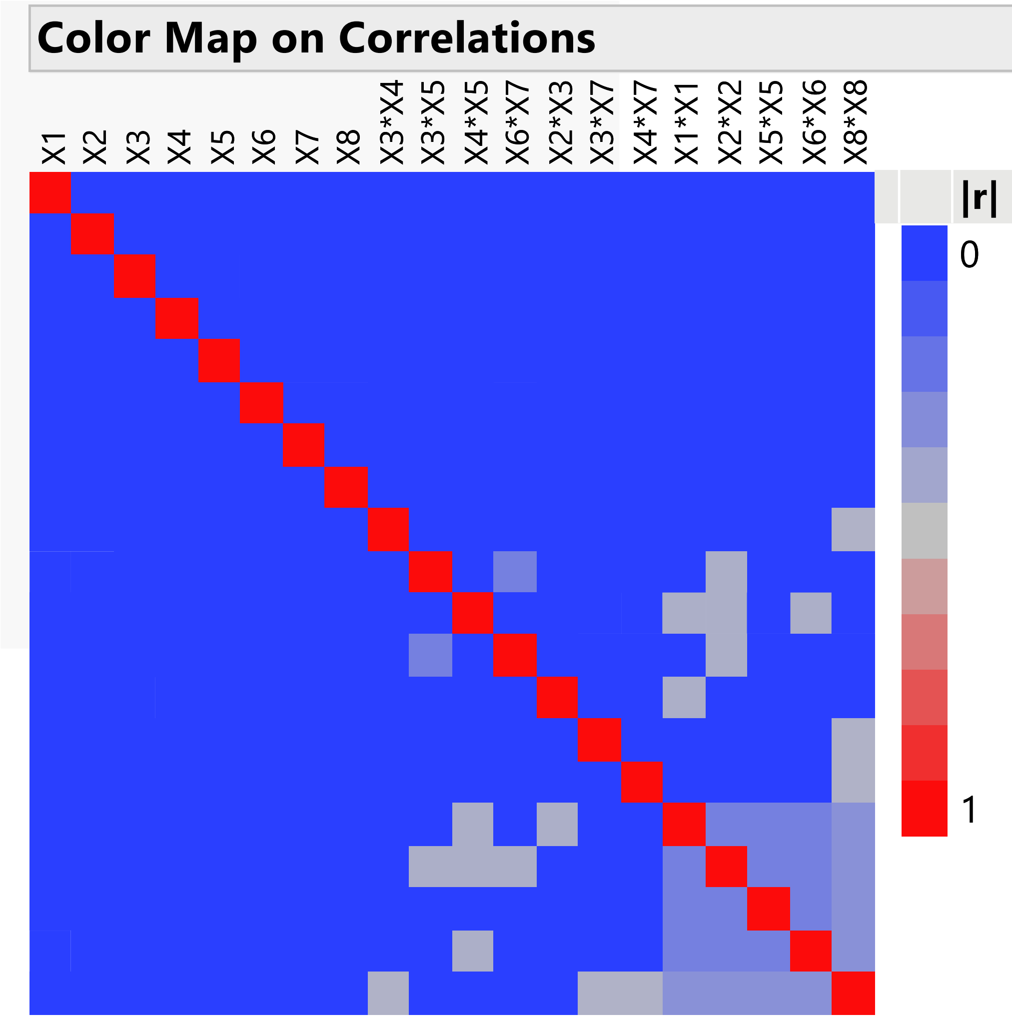


Color Map on Correlations
X1
X2
X3
X4
X5
X6
X7
X8
X3*X4
X3*X5
X4*X5
X6*X7
X2*X3
X3*X7
X4*X7
|r|
0
1

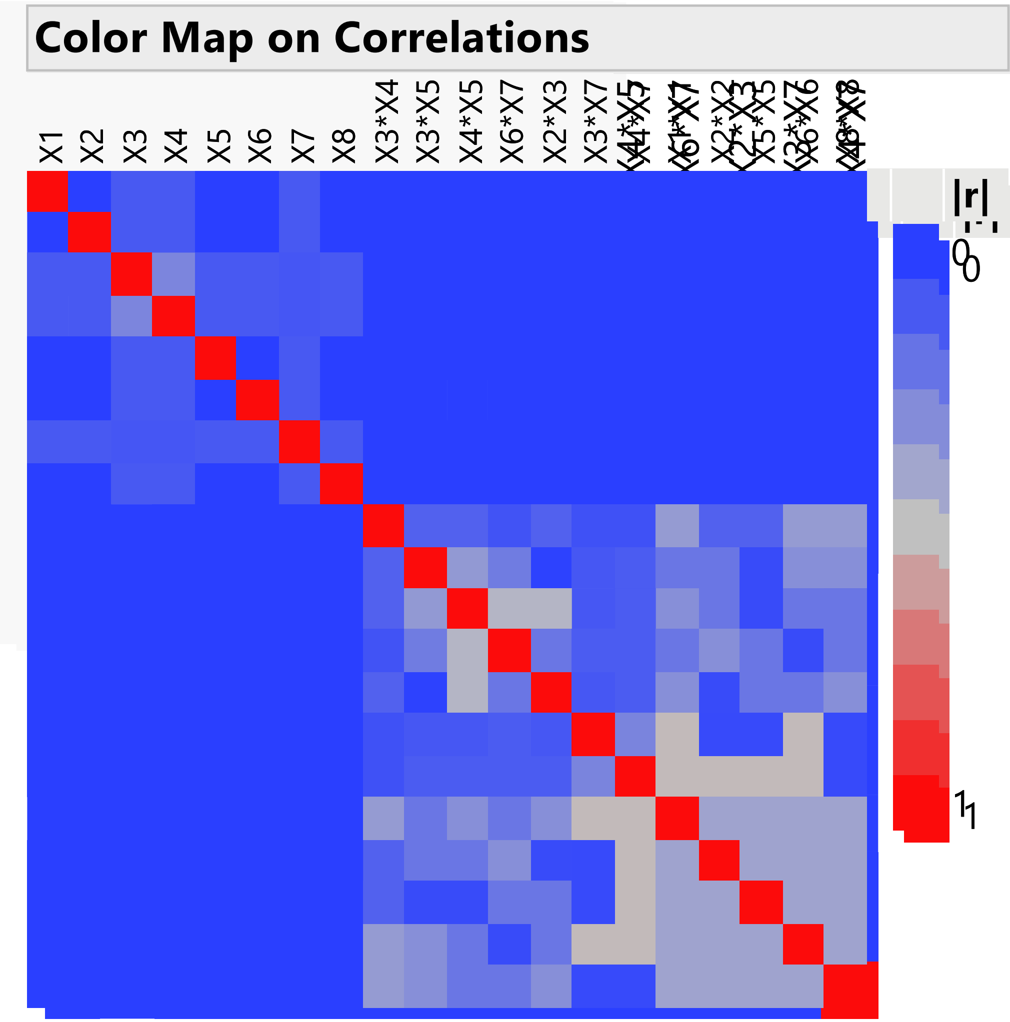
26-run DSD


Color Map on Correlations
X1
X2
X3
X4
X5
X6
X7
X8
X3*X4
X3*X5
X4*X5
X6*X7
X2*X3
X3*X7
X4*X7
|r|
0
1

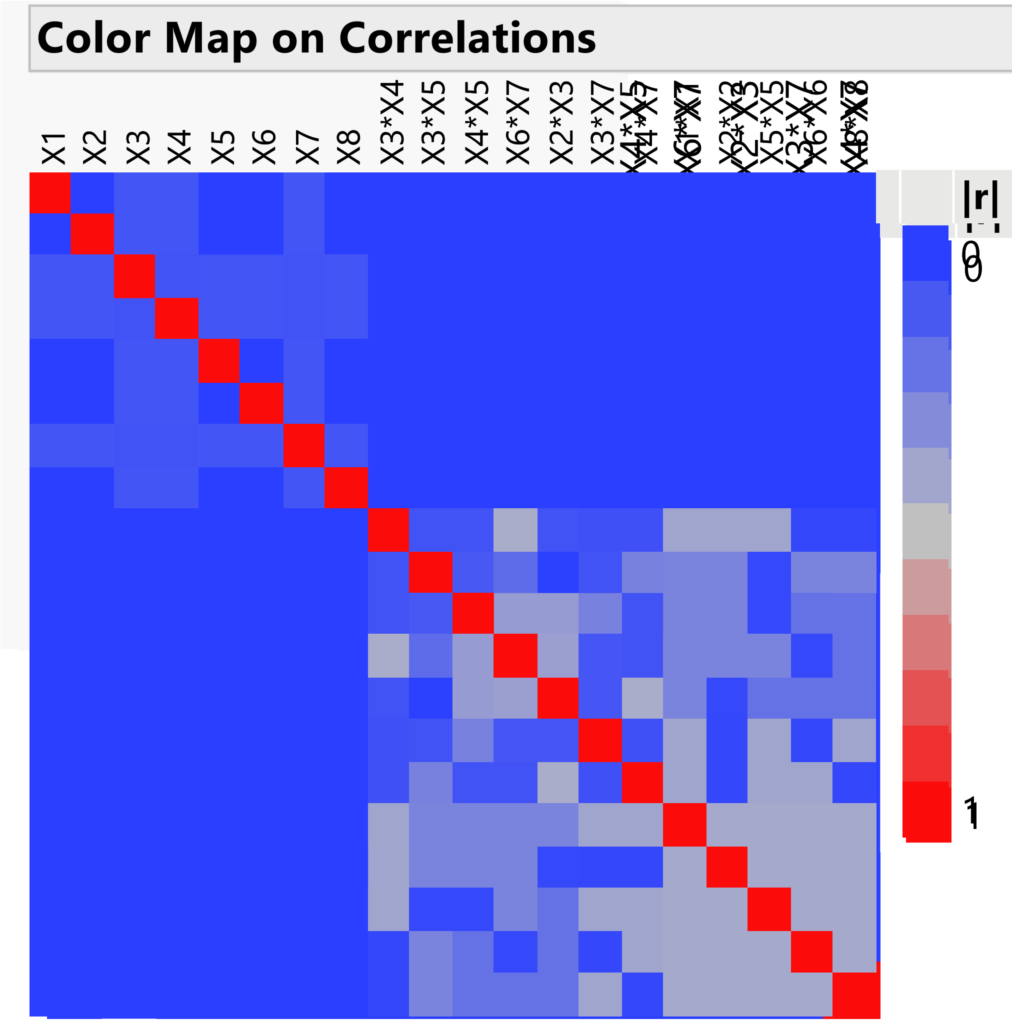
24-run OMARS design



22-run DSD


Color Map on Correlations
X1
X2
X3
X4
X5
X6
X7
X8
X3*X4
X3*X5
X4*X5
X6*X7
X2*X3
X3*X7
|r|
0
1

26-run DSD



Color Map on Correlations
X1
X2
X3
X4
X5
X6
X7
X8
X3*X4
X3*X5
X4*X5
X6*X7
X2*X3
X3*X7
|r|
0
1

References

- José Núñez Ares & Peter Goos (2020) Enumeration and Multicriteria Selection of Orthogonal Minimally Aliased Response Surface Designs, **Technometrics**, 62:1, 21-36.
- José Núñez Ares, Eric Schoen & Peter Goos (2023) Orthogonal minimally aliased response surface designs for three-level quantitative factors and two-level categorical factors. **Statistica Sinica**, 33:107–126.
- José Núñez Ares & Peter Goos (2023) Blocking OMARS designs and definitive screening designs, **Journal of Quality Technology**, 55:4, 489-509.
- Mohammed Saif Ismail Hameed, José Núñez Ares & Peter Goos (2023) Analysis of data from orthogonal minimally aliased response surface designs, **Journal of Quality Technology**, 55:3, 366-384.

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OMARS Designs: Factor Screening and Response Surface Optimization in a Single Step

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