Multicriteria Evaluation and Optimisation of Sealing Performance by DOE and Response Surface Methodology

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Structure

- Introduction
- Design Of Experiments (DOE)
  - Intuition
  - General background & principles
- Application to sealing performance
- Conclusions

Introduction

- Optimizing processes & developing new products requires experimentation
- A systematic approach is required when multiple factors are involved that potentially influence the end quality
- This systematic approach is called „Design Of Experiments“, and the field underwent a revolution during the last decade
- I will use sealing optimization as a case study (but DOE is broadly applicable)

Design of Experiments (DOE)

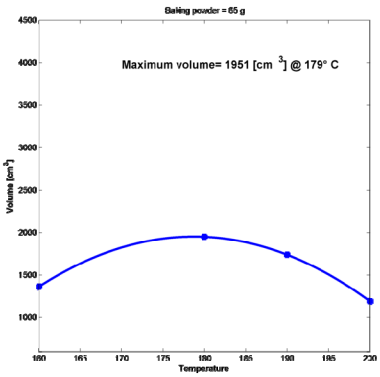
- Systematic plan to investigate the effect of multiple factors
- How can we learn most out of a minimal experimental effort?
- Often considered as an academic excercise, but this is not (anymore) the case, thanks to new classes of very flexible (tailored) designs and easy-to-use software packages

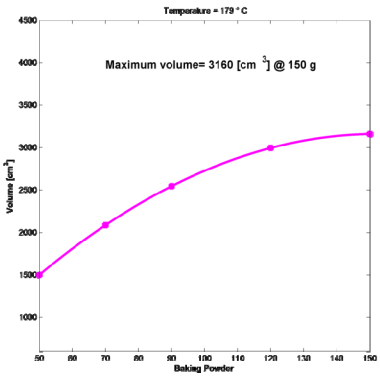
DOE – some intuition (example 1)

- Suppose we have two different parameters we can choose: time and temperature
  - Time can be chosen in between 50 and 150 minutes
  - Temperature can be chosen in between 160 and 200 degrees Celsius
- How to find the optimal combination of time and temperature that gives maximal output?

DOE – some intuition (example 1)

- How to find the optimal combination of time and temperature that gives maximal output?

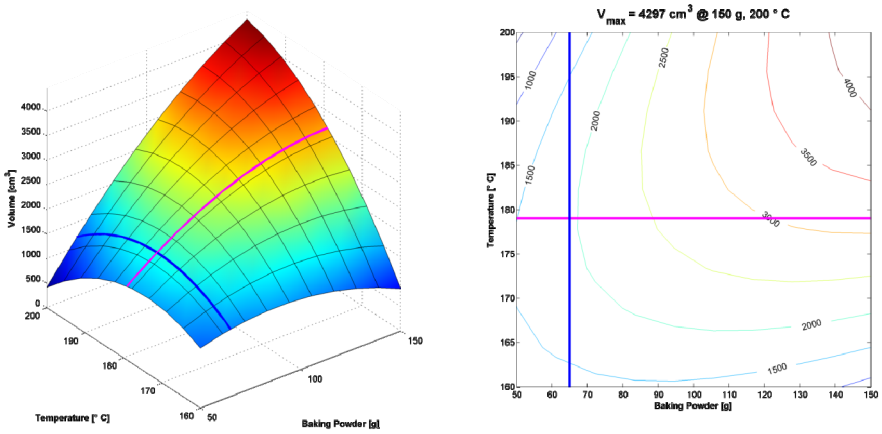




- Good approach?

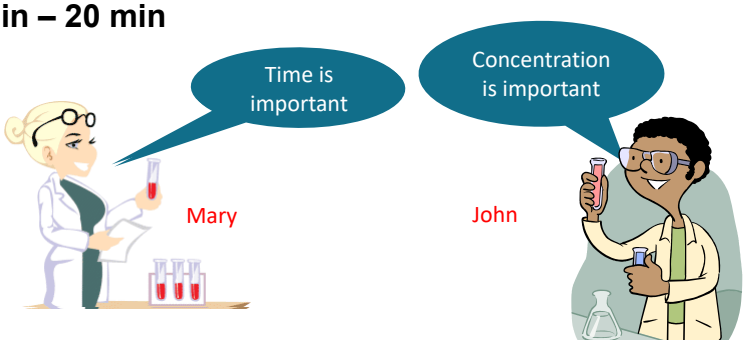
DOE – some intuition (example 1)

- Advocated approach in old textbooks and courses, but is not optimal
  - It works only in very specific situations… but mostly fails



DOE – some intuition (example 2)

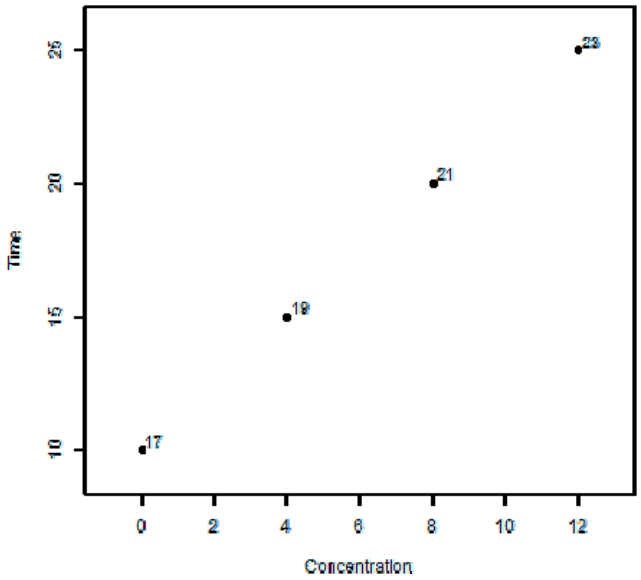
- Study about the concentration of an additive and the time of the chemical reaction
  - Concentration of additive 0 % - 12 %
  - Time of process 10 min – 20 min



- Budget for 4 experiments

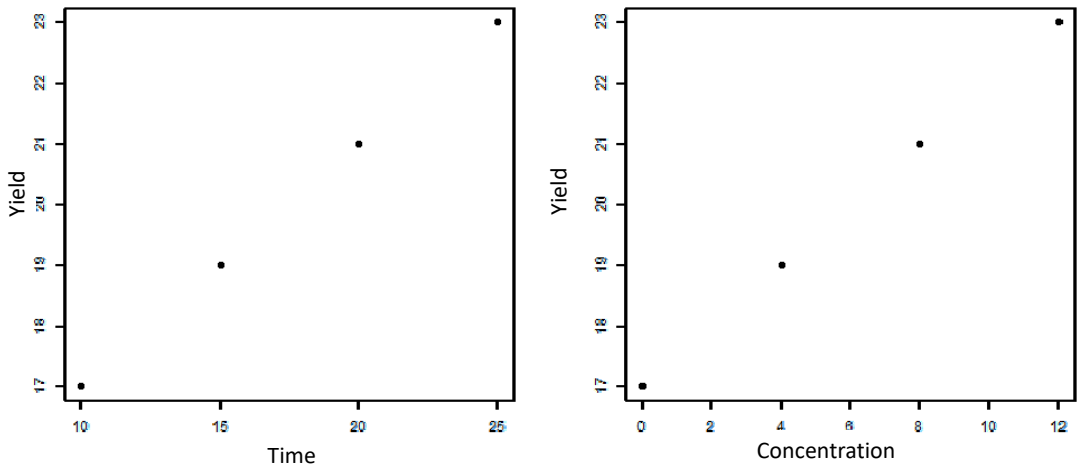
DOE – some intuition (example 2)

- **The experiment**



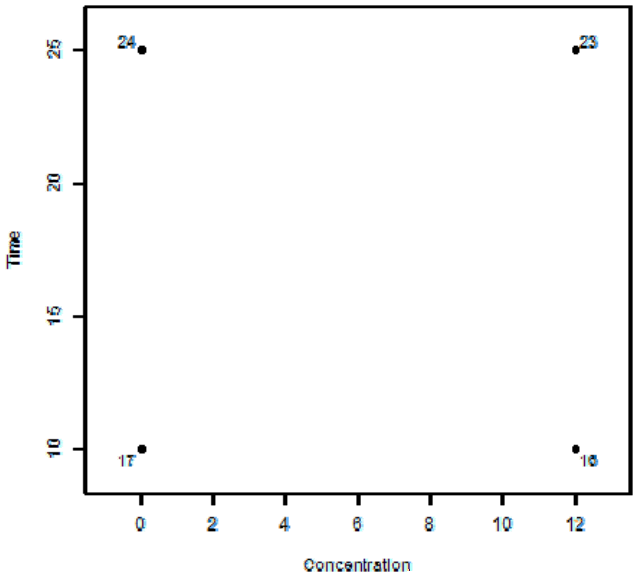
DOE – some intuition (example 2)

- **The experimental results plotted: what did we learn?**



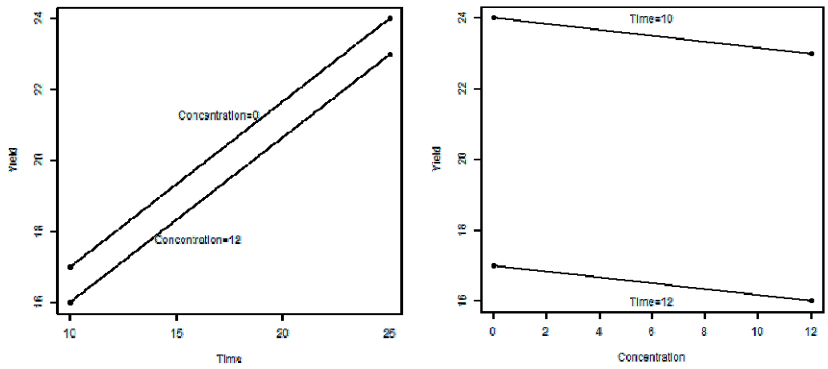
DOE – some intuition (example 2)

- **The second experiment**



DOE – some intuition (example 2)

- **The experimental results plotted: what did we learn now?**



- **Who was right?**

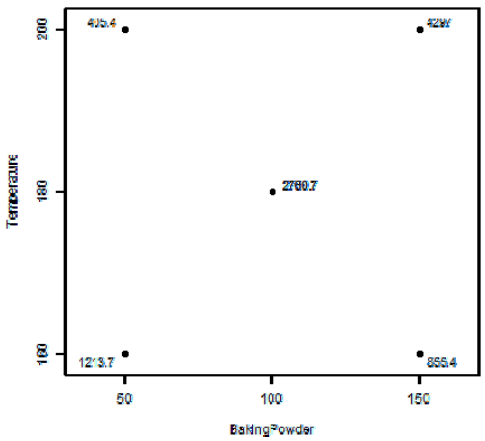
DOE – take home message

The way we perform experiments drastically influences the conclusions we can derive from it.

The goal is to learn as much as possible based on a minimal amount of experimental effort.

DOE

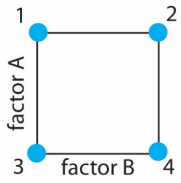
- **Changing the factors together is a good approach as we saw.**



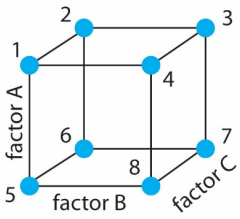
- **2^k + c experimental runs to complete**

DOE

- But what if we have many factors to consider? 2^k becomes prohibitive



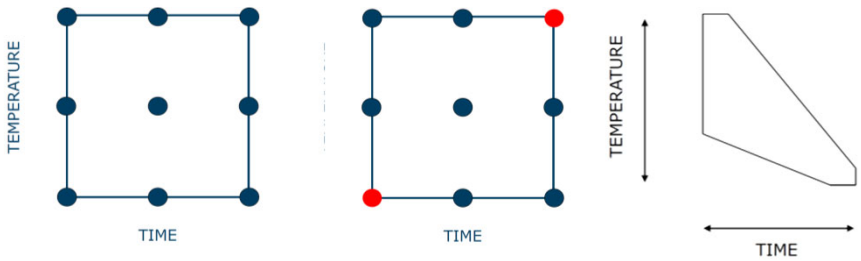
factor	points
5	32
10	1024
12	4096



- Alternatives are needed (and available – as we will see)

DOE

- Can we take into account constraints so that we only perform experiments in the "feasible" domain?



- Modern experimental design is highly flexible to include tailored requirements

- Will go through it step-by-step using sealing optimization case

Sealing optimization case

- Heat conductive sealing

- Aim
  - Evaluate effect of seal parameters on seal quality
  - Optimize seal settings towards optimal seal quality
  - Do this in a time-, labour- and material- efficient way

- Concept

Sealing optimization case

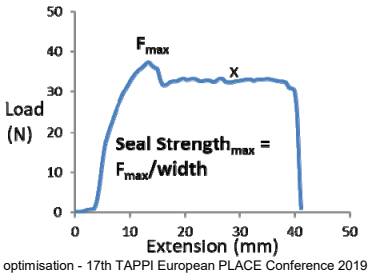
- Three inputs that can be chosen
  1. Temperature
  2. Dwell time
  3. Pressure applied on the film

- Two main responses are considered
  1. Seal strength for <u>clean</u> seals
  2. Seal strength for <u>contaminated</u> seals

- Find inputs that result in best outputs

Seal strength

- Tensile testing ASTM F88 'Standard test method for seal strength of flexible barrier materials'
  - Sample width: 15 mm
  - Rate of separation of the seal jaws: 300 mm/min
  - Distance between grips: 10 mm
  - Quantitative output: maximum seal strength



MTS 10/M
Universal testing machine

Design of Experiments approach

- Step 1: Define design space
- Step 2: Set up experimental design
- Step 3: Perform experiments
- Step 4: Fit response surface model
- Step 5: Optimize input parameters
- Step 6: Experimental validation

Step 1: Define design space

- We considered three inputs: temperature, dwell time, pressure
- Within which limits do we want to study them?
  - No strict rules
  - Definition based on:
    - Film specifications
    - Limits sealing process/device
    - Preliminary tests

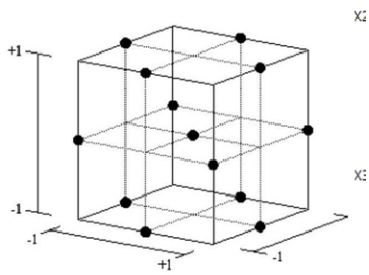
Step 1: Define design space

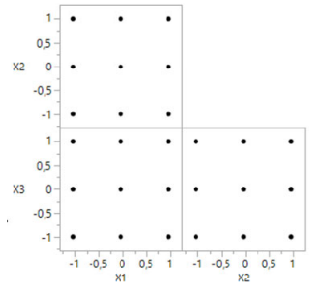
- Limits chosen here
  - Temperature: Range based on film specifications / preliminary tests
    - 200-250 °C
  - Time: Range based on film specifications / industrial conditions
    - 1-3 s
  - Pressure: Range based on film specifications / industrial conditions
    - 1-4 N/mm²

Step 2: Set up experimental design

- We need a design that allows to investigate the three input parameters

- Box-Behnken:
  - Fixed, standard design table
  - Allows to fit a quadratic model
  - Extreme conditions (corner points) not included
  - Highly efficient: 15 runs (classical full factorial design: 27 runs)





Step 2: Set up experimental design

- Fixed, standard design table → Very straight-forward to set up
- Random order of runs

Run	Parameter 1	Parameter 2	Parameter 3
1	Min	Min	Mid
2	Mid	Max	Max
3	Mid	Max	Min
4	Max	Mid	Min
5	Min	Max	Mid
6	Mid	Mid	Mid
7	Mid	Mid	Mid
8	Mid	Min	Min
9	Max	Max	Mid
10	Mid	Mid	Mid
11	Min	Mid	Max
12	Max	Mid	Max
13	Min	Mid	Min
14	Mid	Min	Max
15	Max	Min	Mid

Step 2: Set up experimental design

- Easy to generate through any statistical software, or just in EXCEL®
- Example in JMP®

	Pattern	Temperature [°C]	Time [s]	Pressure [N/mm²]	Y
1	+0−	250	2	1	•
2	++0	250	3	2,5	•
3	0−−	225	1	1	•
4	000	225	2	2,5	•
5	−0−	200	2	1	•
6	0−+	225	1	4	•
7	0+−	225	3	1	•
8	0++	225	3	4	•
9	−+0	200	3	2,5	•
10	−0+	200	2	4	•
11	+−0	250	1	2,5	•
12	000	225	2	2,5	•
13	000	225	2	2,5	•
14	−−0	200	1	2,5	•
15	+0+	250	2	4	•

Step 3: Perform measurements

1. Perform experiments as explained in 'Part 1' at the 15 parameter combinations defined by the design
2. Insert output (seal strength) for all settings in the table

	Pattern	Temperature [°C]	Time [s]	Pressure [N/mm²]	Contaminated seal strength water [N/mm]
1	+0−	250	2	1	2,404
2	++0	250	3	2,5	1,925333333
3	0−−	225	1	1	3,065333333
4	000	225	2	2,5	4,042666667
5	−0−	200	2	1	1,873333333
6	0−+	225	1	4	2,912
7	0+−	225	3	1	4,018666667
8	0++	225	3	4	1,874666667
9	−+0	200	3	2,5	3,586666667
10	−0+	200	2	4	1,501333333
11	+−0	250	1	2,5	3,277333333
12	000	225	2	2,5	3,566666667
13	000	225	2	2,5	3,650666667
14	−−0	200	1	2,5	0,492666667
15	+0+	250	2	4	1,930666667

Step 4: Fit response surface model

- **Quadratic model with interactions**

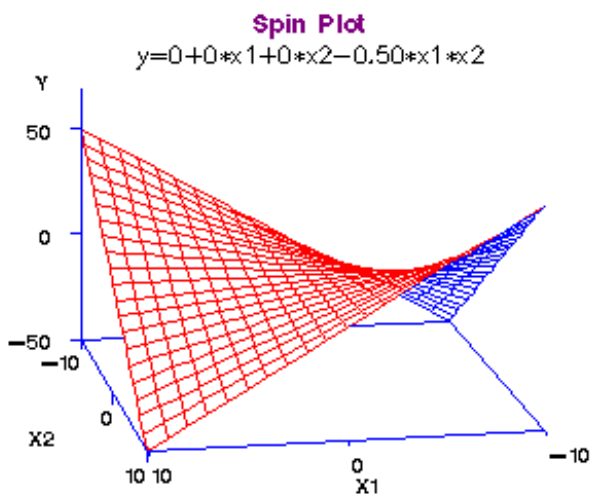
- **For 3 input variables:**

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{23} x_2 x_3 + \beta_{13} x_1 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \varepsilon$$

- **In our case:**
  - **y = seal strength;**
    - **x_1 = temperature**
    - **x_2 = time**
    - **x_3 = pressure**

Step 4: Fit response surface model

- **Interactions**



Step 4: Fit response surface model

- **Do we need this complex model, or can a more compact model do an equally good job?**
  - **Model selection process → retain only those factors that have a significant influence**
  - **E.g. through an "all possible subsets" regression procedure**

Step 4: Fit response surface model

- **Model selection process**

Please check position of green frame

All Possible Models

Ordered up to best 3 models up to 8 terms per model.

Model	Number	RSquare	RMSE	AICc	BIC	
Pressure [N/mm²](1,4)	1	0,0800	1,0453	49,9317	49,8740	●
Temperature [°C](200,250)	1	0,0351	1,0704	50,6452	50,5876	○
Time [s](1,3)	1	0,0223	1,0776	50,8442	50,7866	○
Temperature [°C](200,250),Temperature [°C]*Temperature [°C]	2	0,3721	0,8988	48,0188	46,8510	●
Pressure [N/mm²](1,4),Pressure [N/mm²]*Pressure [N/mm²]	2	0,1373	1,0535	52,7841	51,6163	○
Temperature [°C](200,250),Pressure [N/mm²](1,4)	2	0,1151	1,0670	53,1657	51,9979	○
Temperature [°C](200,250),Pressure [N/mm²](1,4),Temperature [°C]*Temperature [°C]	3	0,4521	0,8769	50,6420	47,5156	●
Temperature [°C](200,250),Time [s](1,3),Temperature [°C]*Temperature [°C]	3	0,3944	0,9219	52,1441	49,0177	○
Temperature [°C](200,250),Time [s](1,3),Temperature [°C]*Time [s]	3	0,3775	0,9347	52,5566	49,4302	○
Temperature [°C](200,250),Time [s](1,3),Temperature [°C]*Time [s],Temperature [°C]*Temperature [°C]	4	0,7145	0,6639	46,6984	40,4467	●
Temperature [°C](200,250),Pressure [N/mm²](1,4),Temperature [°C]*Temperature [°C],Pressure [N/mm²]*Pressure [N/mm²]	4	0,5314	0,8505	54,1284	47,8767	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Temperature [°C]	4	0,4743	0,9008	55,8533	49,6016	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Temperature [°C]	5	0,7944	0,5938	49,2692	38,2256	●
Temperature [°C](200,250),Time [s](1,3),Temperature [°C]*Time [s],Temperature [°C]*Temperature [°C],Time [s]*Time [s]	5	0,7200	0,6931	53,9077	42,8641	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Temperature [°C],Pressure [N/mm²]*Pressure [N/mm²]	5	0,5537	0,8750	60,8984	49,8547	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Temperature [°C],Pressure [N/mm²]*Pressure [N/mm²]	6	0,8738	0,4935	51,9511	33,6155	●
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Time [s]*Pressure [N/mm²],Temperature [°C]*Temperature [°C]	6	0,8586	0,5223	53,6556	35,3200	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Temperature [°C],Time [s]*Time [s]	6	0,7999	0,6214	58,8640	40,5284	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Time [s]*Pressure [N/mm²],Temperature [°C]*Temperature [°C],Pressure [N/mm²]*P...	7	0,9380	0,3699	55,2964	25,6689	●
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Temperature [°C],Time [s]*Time [s],Pressure [N/mm²]*Pressure [N...	7	0,8830	0,5079	64,8142	35,1867	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Pressure [N/mm²],Temperature [°C]*Temperature [°C],Pressure [...	7	0,8740	0,5272	65,9313	36,3038	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Time [s]*Pressure [N/mm²],Temperature [°C]*Temperature [°C],Time [s]*Time [s],Pr...	8	0,9472	0,3686	73,8848	25,9653	●
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Pressure [N/mm²],Time [s]*Pressure [N/mm²],Temperature [°C]*T...	8	0,9381	0,3989	76,2561	28,3366	○
Temperature [°C](200,250),Time [s](1,3),Pressure [N/mm²](1,4),Temperature [°C]*Time [s],Temperature [°C]*Pressure [N/mm²],Temperature [°C]*Temperature [°C],Time [s]*Ti...	8	0,8832	0,5482	85,7929	37,8734	○

Step 4: Fit response surface model

- **Model selection process**

All Possible Models

Ordered up to best 3 models up to 8 terms per model.

Model	Number	RSquare	RMSE	AICc	BIC
Pressure [N/mm²](1,4)	1	0,0800	1,0453	49,9317	49,8740
Temperature [°C](200,250)	1	0,0551	1,0764	50,0452	50,0876
Time [s](1,3)	1	0.0223	1.0776	50.8442	50.7866

- **<u>Rsquare</u>: as high as possible (but risk for overfitting)**
- **<u>RMSE</u>: unexplained error, as low as possible**
- **<u>AIC</u> (Akaike Information Criterion): quality of each model, relative to the other models, as low as possible**
- **<u>BIC</u> (Bayesian Information Criterion): similar to AIC, but higher penalty for number of terms, as low as possible**

Step 4: Fit response surface model

- **Final model**

Summary of Fit

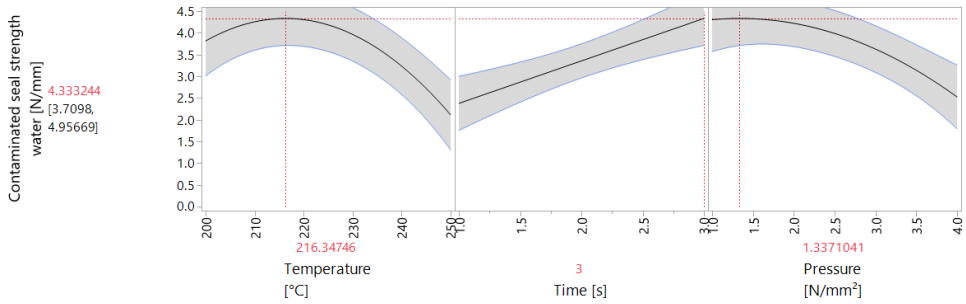
RSquare	0,937977
RSquare Adj	0,875953
Root Mean Square Error	0,369851
Mean of Response	2,6748
Observations (or Sum Wgts)	15

Effect Summary

Source	LogWorth	PValue
Temperature [°C]*Temperature [°C]	3,421	0,00038
Temperature [°C]*Time [s]	3,270	0,00054
Pressure [N/mm²](1,4)	1,703	0,01982
Pressure [N/mm²]*Pressure [N/mm²]	1,696	0,02015
Time [s]*Pressure [N/mm²]	1,508	0,03103
Temperature [°C](200,250)	1,062	0,08670 ^
Time [s](1,3)	0,804	0,15700 ^

Step 4: Fit response surface model

- Final model
  - Previous slides showed the final model. It has all required information, but it is hard to interpret
  - Can do better using a profiles (visual representation)



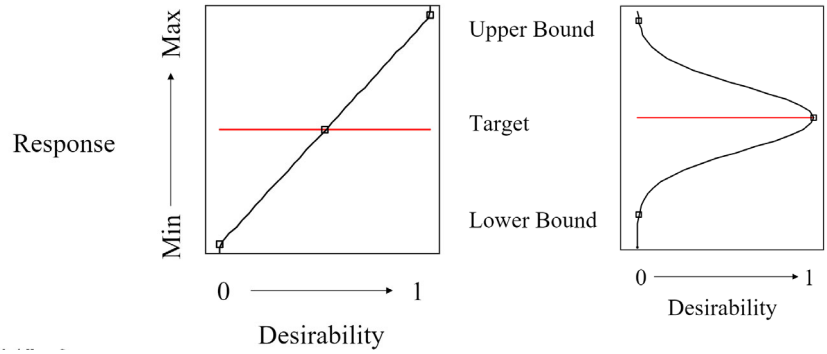
Step 5: Optimize input parameters

- Response surface model: use
  - Evaluation of effect of input variables on response
  - Optimization of input variables towards response
- 'Optimum' can mean different things:
  - Find <u>maximum</u> (E.g. seal strength as high as possible)
  - Find <u>minimum</u> (E.g. energy needed by sealing process as low as possible)
  - Match <u>specific target</u> value (E.g. a specific seal strength for a peel film)
- Optimization by means of desirability functions

Step 5: Optimize input parameters

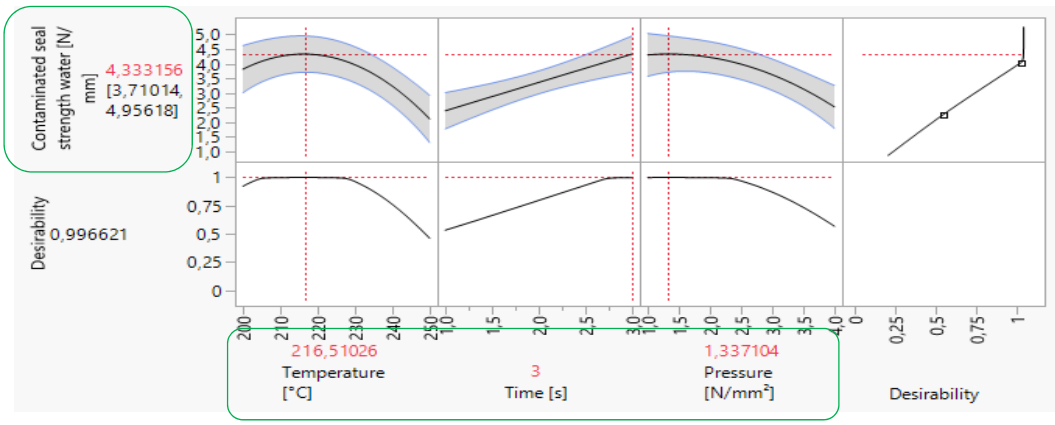
- **Desirability functions: maps the response in a range from 0 (undesired) to 1 (highly desirable)**

- **Can do it for**
  - **Maximizing**
  - **Minimizing**
  - **Matching target**



Step 5: Optimize input parameters

Max. seal strength



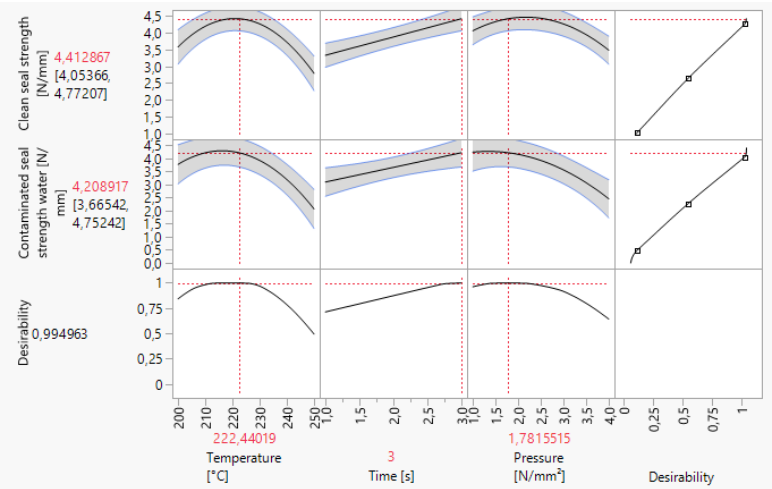
Optimal seal settings

Step 5: Optimize input parameters

- Can define a desirability function for more than one response, and optimize them altogether to obtain the best overall solution
- Example
  - ‘Clean seal strength [N/mm]’
  - ‘Contaminated seal strength water [N/mm]
- Both need to be high

Step 5: Optimize input parameters

- Can define a desirability function for more than one response, and optimize them altogether to obtain the <u>best overall desirability</u>



Step 6: Experimental validation

- **Confirmation runs at optimal settings (e.g. 10 repeated measurements)**
- **Calculate confidence interval based on confirmation runs (CICon approach as suggested by Antony (2003) and Jensen (2016))**

$$\bar{y}_c \pm t_{1-\alpha/2,c-1}\, s_c/\sqrt{c}$$

with c the number of confirmation runs, $\bar{y}_c$ the mean of the confirmation runs and s_c their standard deviation.

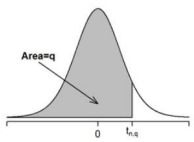
- **Predicted optimum in confidence interval → OK**

Step 6: Experimental validation

- **E.g. for α = 0.05 and c=10 →** $t_{1-\frac{\alpha}{2},c-1} = t_{0.975,9} = 2.262$

Quartiles of the t Distribution

The table gives the value if $t_{n;q}$ - the qth quantile of the t distribution for n degrees of freedom



	q = 0.6	0.75	0.9	0.95	0.975	0.99	0.995	0.9975	0.999	0.9995
n = 1	0.3249	1.0000	3.078	6.314	12.706	31.821	63.657	127.321	318.309	636.619
2	0.2887	0.8165	1.886	2.920	4.303	6.965	9.925	14.089	22.327	31.599
3	0.2767	0.7649	1.638	2.353	3.182	4.541	5.841	7.453	10.215	12.924
4	0.2707	0.7407	1.533	2.132	2.776	3.747	4.604	5.598	7.173	8.610
5	0.2672	0.7267	1.476	2.015	2.571	3.365	4.032	4.773	5.893	6.869
6	0.2648	0.7176	1.440	1.943	2.447	3.143	3.707	4.317	5.208	5.959
7	0.2632	0.7111	1.415	1.895	2.365	2.998	3.499	4.029	4.785	5.408
8	0.2619	0.7064	1.397	1.860	2.306	2.896	3.355	3.833	4.501	5.041
9	0.2610	0.7027	1.383	1.833	2.262	2.821	3.250	3.690	4.297	4.781
10	0.2602	0.6998	1.372	1.812	2.228	2.764	3.169	3.581	4.144	4.587
11	0.2596	0.6974	1.363	1.796	2.201	2.718	3.106	3.497	4.025	4.437
12	0.2590	0.6955	1.356	1.782	2.179	2.681	3.055	3.428	3.930	4.318
13	0.2586	0.6938	1.350	1.771	2.160	2.650	3.012	3.372	3.852	4.221
14	0.2582	0.6924	1.345	1.761	2.145	2.624	2.977	3.326	3.787	4.140

Conclusions

- **Design Of Experiments is a highly flexible, powerful framework for optimizing products and processes**
- **It allows to investigate the influence of many factors on a response**
- **Modern software allows to implement the framework without too much background needed**

"Thank You"
for your patience

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