# DoE for Scale-Up

***… using MODDE® and DoE-DiVa®***

**Session 2: Scale Up and the Similarity Principle -- 25.01. 2023**

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umesoft

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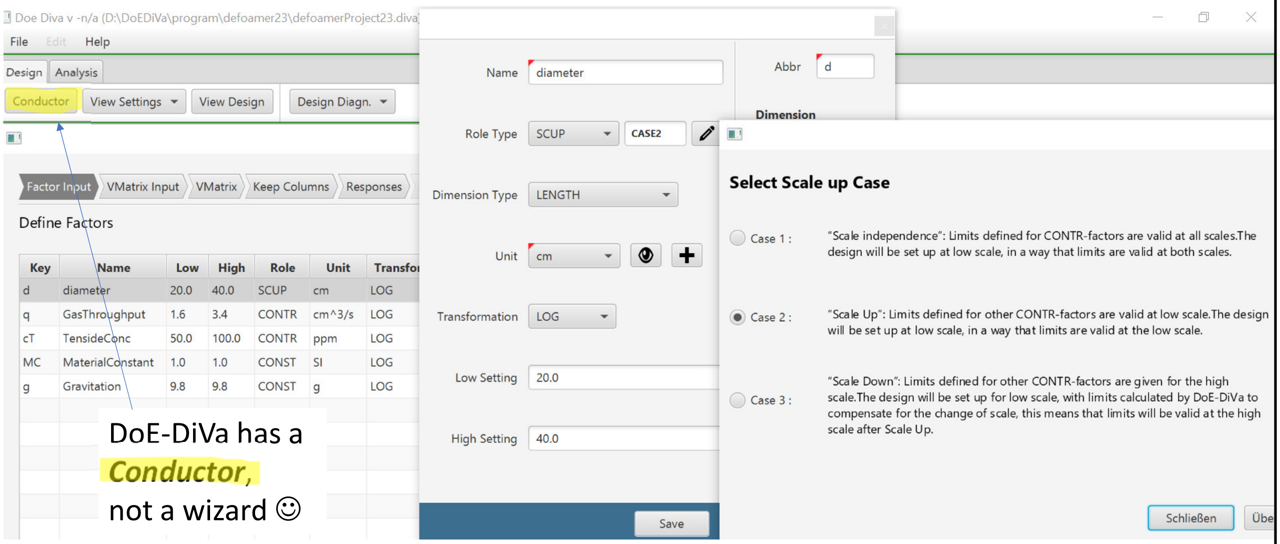
Bundesministerium für Wirtschaft und Klimaschutz
aufgrund eines Beschlusses des Deutschen Bundestages

## Refresh on ***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* ***o****f* ***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***

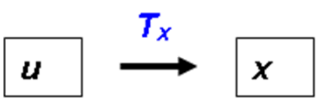
# This is how the ***DoE-DiVa*** looks.

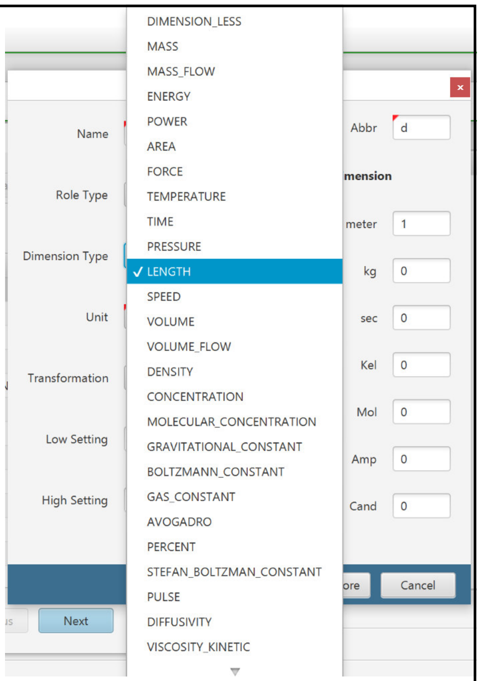




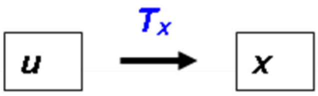

# ***DoE-DiVa's conductor*** is easy

- ***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
- ***u**-factors and **x**-factors*



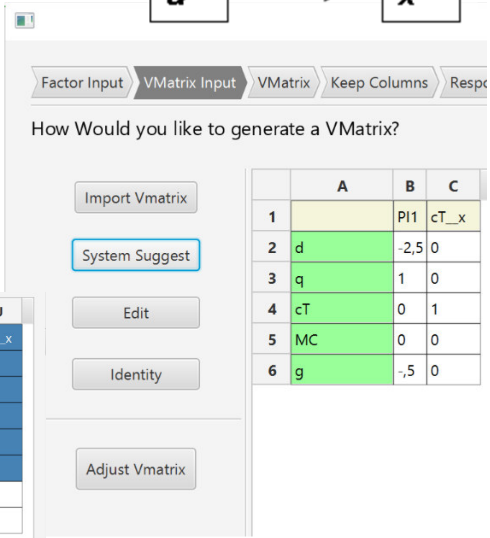
# ***DoE-DiVa's conductor*** is flexible




- Based on factor dimensions ***DoE-DiVa*** *suggests* the ***Tr****ansformation to get dimensionless* ***x****-factors,*
- *allows adjusting these,*
- *allows editing them*

| | A | B | C |
|---|---|---|---|
| 1 | | PI1 | cT__x |
| 2 | Fr | 2 | 0 |
| 3 | cT__x | 0 | 1 |

| | A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | factorKey | m | k | s | Kel | mol | amp | cand | Fr | cT__x |
| 2 | d | 1 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | 0 |
| 3 | q | 3 | 0 | -1 | 0 | 0 | 0 | 0 | 2 | 0 |
| 4 | cT | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| 5 | MC | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | g | 1 | 0 | -2 | 0 | 0 | 0 | 0 | -1 | 0 |
| 7 | Fr | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | cT__x | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |




| | A | B | C |
|---|---|---|---|
| 1 | | PI1 | cT__x |
| 2 | d | -2,5 | 0 |
| 3 | q | 1 | 0 |
| 4 | cT | 0 | 1 |
| 5 | MC | 0 | 0 |
| 6 | g | -,5 | 0 |



# ***DoE-DiVa's conductor*** is communicative

- ***DoE-DiVa*** exports x-factors and x-designs to MODDE®
- ***DoE-DiVa*** exports formulae for ***u****-designs* to MODDE® for ***optimization*** at low and high scale

| | Fr | cT__x | d | ncr | Q_1 |
|---|---|---|---|---|---|
| R0 | -9,398 | -4,30 | 20 | 0,046 | 2,519 |
| R1 | -9,072 | -4,30 | 20 | 0,053 | 2,411 |
| R2 | -8,800 | -4,30 | 20 | 0,057 | 2,311 |
| R3 | -8,605 | -4,30 | 20 | 0,060 | 2,233 |
| R4 | -8,451 | -4,30 | 20 | 0,063 | 2,178 |
| R5 | -9,056 | -4,00 | 20 | 0,062 | 2,478 |
| R6 | -8,800 | -4,00 | 20 | 0,069 | 2,392 |
| R7 | -8,608 | -4,00 | 20 | 0,074 | 2,331 |

| | |
|---|---|
| d_C | (10^( - 0.172414*v1+((Log10(0.01*v3) - ( - 0.172414* |
| q_C | (10^(0.068966*v1+2.5*((Log10(0.01*v3) - ( - 0.17241 |
| cT_C | (10^(v2))/1.0E-6 |
| ncr_C | (10^(v6+( - 0.172414*v1+((Log10(0.01*v3) - ( - 0.1724 |
| Q_1_C | Log10(v4)+( - 0.172414*v1+((Log10(0.01*v3) - ( - 0.17 |

1. ***Dimensional Analysis and Similarity Principle***
2. Dimensionless e***X***plaining factors vs. ***U***ser factors
3. Using DoE-DiVa for preparing simple Scale Up
4. Using MODDE to perform the Scale Up

# *SI system: Base Dimensions and Base Units*

"The ***International System of Units***, known by the international abbreviation ***SI*** in all languages and sometimes … as the ***SI system***, is the modern form of the ***metric system*** and the world's most widely used ***system of measurement***.

It is the only system of measure-ment with an official status in nearly every country in the world, employed in science, technology, industry, and everyday commerce".

| Symbol | Base Unit | Base Dimension |
|---|---|---|
| **m** | metre | length |
| **kg** | kilogram | mass |
| **s** | second | time |
| **A** | ampere | electric current |
| **Kel** | kelvin | thermodynamic temperature |
| **mol** | mole | amount of substance |
| **cd** | candela | luminous intensity |

***https://en.wikipedia.org/wiki/International_System_of_Units***

# *SI system: Derived Dimensions and Units*

"The system allows for an unlimited number of additional units, called ***derived units***, which can always be represented as ***products of powers of the base units***, possibly with a nontrivial numeric multiplier. When that multiplier is one, the unit is called a coherent derived unit."

| Symbol | Unit | Derived Dimension | Relation | m | kg | s | A | Kel | mol | cd |
|---|---|---|---|---|---|---|---|---|---|---|
| **1/s** | hertz | frequency | 1/time(s) | | | -1 | | | | |
| **N** | newton | force | mass(kg)*acceleration ($m/s^2$) | 1 | 1 | -2 | | | | |
| **Pas** | pascal | pressure | force(N)/area($m^2$) | -1 | 1 | -2 | | | | |
| **J** | joule | energy | force(N)*distance(m) | 2 | 1 | -2 | | | | |
| **W** | watt | power | energy(J)/time(s) | 2 | 1 | -3 | | | | |
| **V** | volt | potential difference | power(W)/electric current(A) | 2 | 1 | -3 | -1 | | | |
| **C** | coulomb | electric charge | electric current(A)*time(s) | | | 1 | 1 | | | |
| **M** | kg/mol ( !! ) | molar mass | mass(kg)*amount of substance(mol) | | 1 | | | | -1 | |
| **$c_p$** | J/kg-Kel | specific heat capacity | energy(J)/mass(kg)/Kel | 2 | | -2 | | -1 | | |

***https://en.wikipedia.org/wiki/International_System_of_Units***



# *Permitted non-SI units (in our words „User"-Units)*

"There is a special group of units that are called "non-SI units that are accepted for use with the SI". Most of these, in order to be converted to the corresponding SI unit, require ***conversion factors*** that are not necessarily powers of ten."

| Symbol | Non-SI "User"-Unit | Dimension | Relation to SI-Unit gradient * SI-Unit + offset | m | kg | s | A | Kel | mol | cd |
|---|---|---|---|---|---|---|---|---|---|---|
| **min** | min | time | min = **60** * s + 0 | | | 1 | | | | |
| **rpm** | rpm | frequency | 1/min = **0,0166666667** * 1/s + 0 | | | -1 | | | | |
| **°C** | °Celsius | temperature | °C = **1** * Kel + **273,15** | | | | | 1 | | |
| **$cm^3$ / s** | ccm/sec | volume or gas flow | $cm^3$/sec = **0,000001** * $m^3$/s + 0 | 3 | | -1 | | | | |
| **M [g/mol]** | gr/mol | molar mass | M[g/mol] = **0,001***kg/mol + 0 | | 1 | | | | -1 | |
| **atm** | atmosphere | pressure | atm = **101325** * Pas + 0 | -1 | 1 | -2 | | | | |

***https://en.wikipedia.org/wiki/International_System_of_Units***

# *Buckingham π theorem of Dimensional Analysis*

“The ***Buckingham π theorem*** describes how every physically meaningful equation involving n variables can be equivalently rewritten as an equation of n − m ***dimensionless parameters***, where m is the rank of the dimensional matrix. … provides a method for computing these … from the given variables.”

| Symbol | Unit | Dimension | Relation | m | kg | s | A | Kel | mol | cd | Froude | cT | inv Gasflow |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **rpm** | rpm | frequency | 1/min = **0,0166666667** * 1/s + 0 | | | **-1** | | | | | | | **1** |
| **°C** | °Celsius | temperature | °C = **1** * Kel + **273,15** | | | | | **1** | | | | | |
| **cm³ / s** | ccm/sec | volume or gas flow | cm³/sec = **0,000001** * m³/s + 0 | **3** | | **-1** | | | | | **2** | | **-1** |
| **g** | gravity consant | acceleration | acceleration (m/s²) | **1** | | **-2** | | | | | **-1** | | |
| **d** | cm | length | cm = 0,01 * m | **1** | | | | | | | **-5** | | **3** |
| **c** | dimensionless | vol/vol concentration | volume(m³)/volume(m³) | 0 | 0 | 0 | | | | | | **1** | |
| **Fr** | dimensionless | power number | power/density/frequency³/length^5 | 0 | 0 | 0 | | | | | | | |
| **Q_1** | dimensionless | Reynolds number | area*frequency*density/viscosity | 0 | 0 | 0 | | | | | | | |

***https://en.wikipedia.org/wiki/Dimensional_analysis***



# *Similarity theory – Ähnlichkeitstheorie*

***Similarity theory*** is a technique in physics and engineering that describes how a ***physical process (large scale original)*** is traced back to a ***model process (small scale model)*** with the help of ***dimensionless ratios***. This theory is both used for theoretical considerations as well as for experimentation.

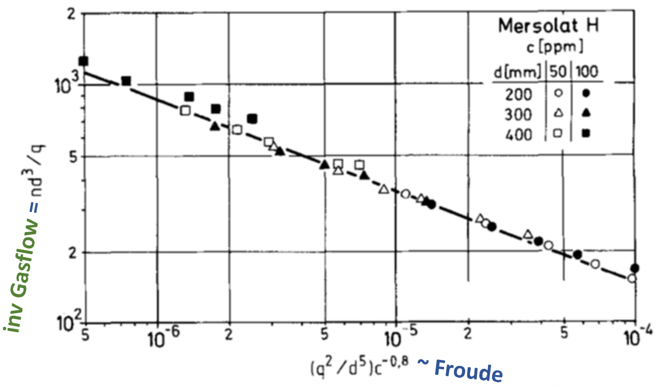



Abb. 7. Prozeß-Charakteristik des Schaumzerstörers für unterschiedliche Konzentrationen von Mersolat H.

***Marco Zlokarnik: Auslegung und Dimensionierung eines mechanischen Schaumzerstörers. Chem-Ing.-Tech. (56) 1984 Nr. 11, S. 842***

## *The Similarity Principle and its Contraposition*

*If the state of a system can be* ***completely described*** *by the dimensionless factors,*

*then two manifestations of a system* ***behave the same****, if they have the* ***same settings of the dimensionless factors*** *(**x**-factors).*

*even if the* ***real factors*** *(**u**-factors)* ***have different setting values****.*

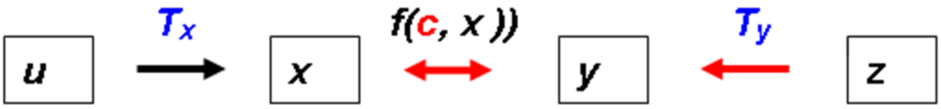
*Contraposition: Influencing* ***factors that induce the most change*** *in a system must be* ***dimensionless.***

*Therefore:* ***optimal experimental design****, with* ***maximal information (=variation)****, and with* ***minimal experimental effort*** *must be for* ***dimensionless factors.***



1. Dimensional Analysis and Similarity Principle
2. ***Dimensionless eXplaining factors vs. User factors***
3. Using DoE-DiVa for preparing simple Scale Up
4. Using MODDE to perform the Scale Up

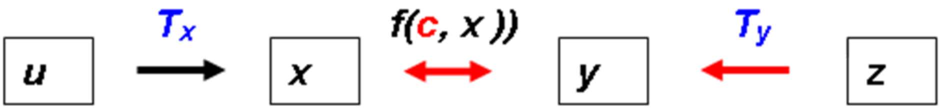
# The general ***DoE-DiVa***-approach




***u:*** *User-factor,* to be set in the experiment, e.g. *Temp, pressure etc.*
***x:*** *e**X**plaining-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*



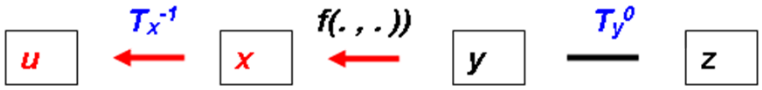
# Todays ***Scale-Up***-example:



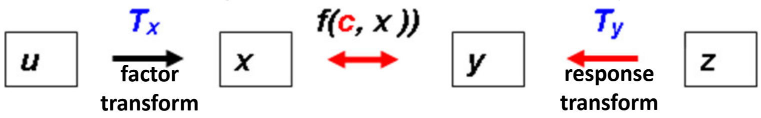

***u:*** *User-factors,* ***d****=diameter (to scale up),* ***q****=volume flow,* ***cT****=tenside conc.*
***x: dimensionless*** *e**X**plaining-factor: Froude number and cT_x (vol/vol)*
***$T_x$:*** *transformation:* ***$Fr = q^2/d^5g$, cT_x = cT***. *(g = gravitational constant)*
***c:*** *coefficients or parameters in the model,* ***f***, *to be determined by model FIT*
***z:*** *measured response value,* ***ncr*** *= critical revolution number*
***y: dimensionless*** *response value,* ***Q_1***
***$T_y$:*** *transformation* to get from ***z*** to ***y***, ***Q_1 = ncr / q * $d^3$***

## The role of the *Transformations*

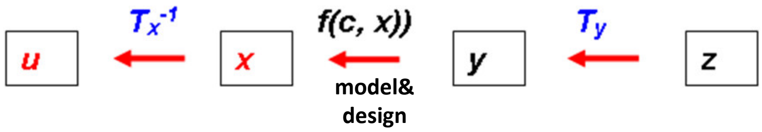
**Design: How to get *u* from *f* and the *tr*ansformation**




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




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



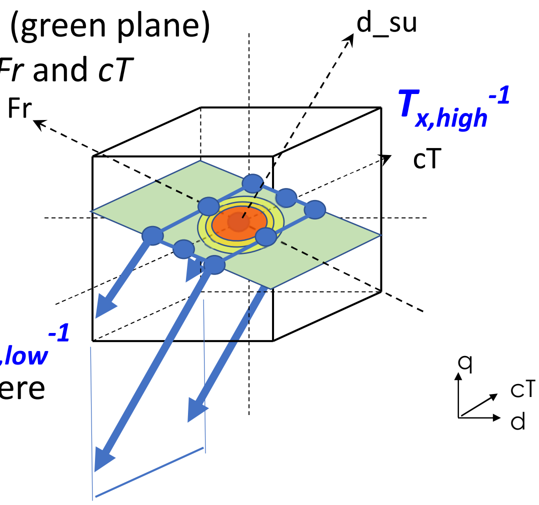



## The *Scale-Up* principle – using similarity

***Fit the model*** here (green plane) for dimensionless *Fr* and *cT*

$T_x^{-1}$ ***Formulae for MODDE!***

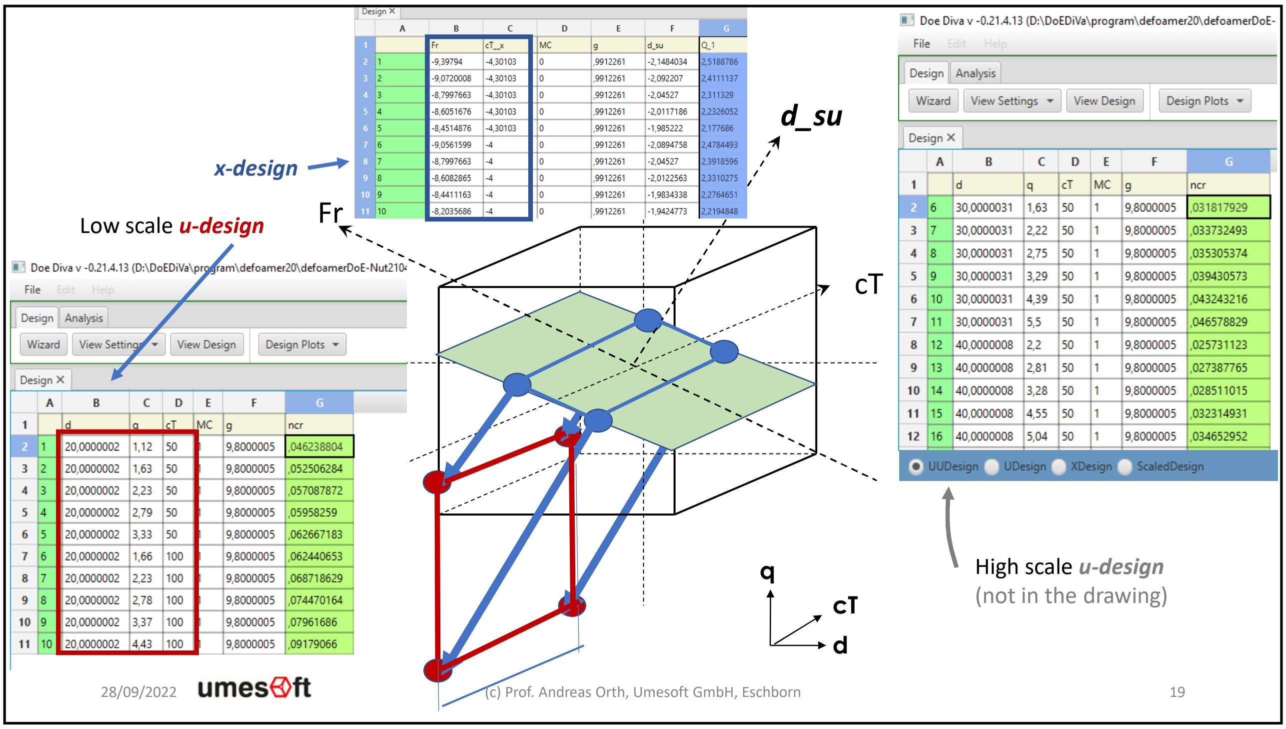
| | |
|---|---|
| d_C | (10^( - 0.172414*v1+((L |
| q_C | (10^(0.068966*v1+2.5*( |
| cT_C | (10^(v2))/1.0E-6 |
| ncr_C | (10^(v6+( - 0.172414*v1 |
| Q_1_C | Log10(v4)+( - 0.172414* |




$T_{x,low}^{-1}$

Do experiments here at the left where *diameter is low*

***Transfer the optimum*** to the high scale, here at the right where diameter is high




1. Dimensional Analysis and Similarity Principle
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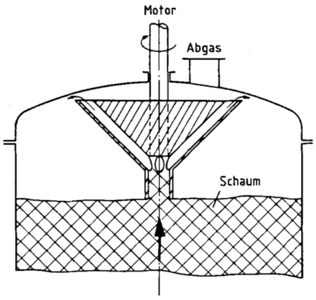
# Auslegung und Dimensionierung eines mechanischen Schaumzerstörers*

Marko Zlokarnik**




**Design and dimensions of a mechanical defoamer.** This paper presents a newly developed powerful mechanical defoamer which exploits centrifugal force and, thanks to circular channels, also Coriolis force for destruction of foam. It is incorporated into containers such that the expelled foam concentrate is deflected by the lid without producing fresh foam. Model experiments with three geometrically similar but different sized laboratory models led to dimensional-theoretically formulated process-relations of the defoamer for various material systems (five chemical foamers, two biological substrates). Such process-relations represent a reliable basis for design and dimensions of the defoamer presented, on the one hand, and permit determination of an "intermediate characteristic", having the dimensions of acceleration, which represents the mechanical degradability of the foam.

Chem.-Ing.-Tech. 56 (1984) Nr. 11, S. 839 – 844



0009-286X/84/1111-0839$02.50/0



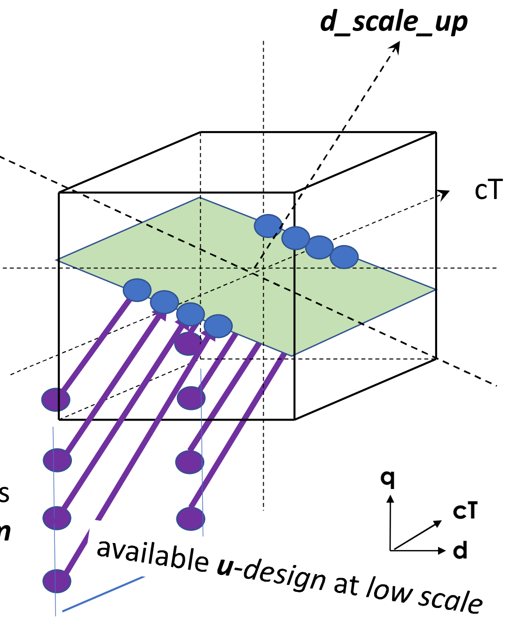
## Scale-Up example: Defoamer

$u_1$ = d = diameter, 20 to 40 cm (Scale-Up)
$u_2$ = q = gasThroughput, 1.6 to 3.4 cm³/s
$u_3$ = cT = tensileConc, 50 to 100 ppm
$u_4$ = g = gravity, const 9.81 m/s²

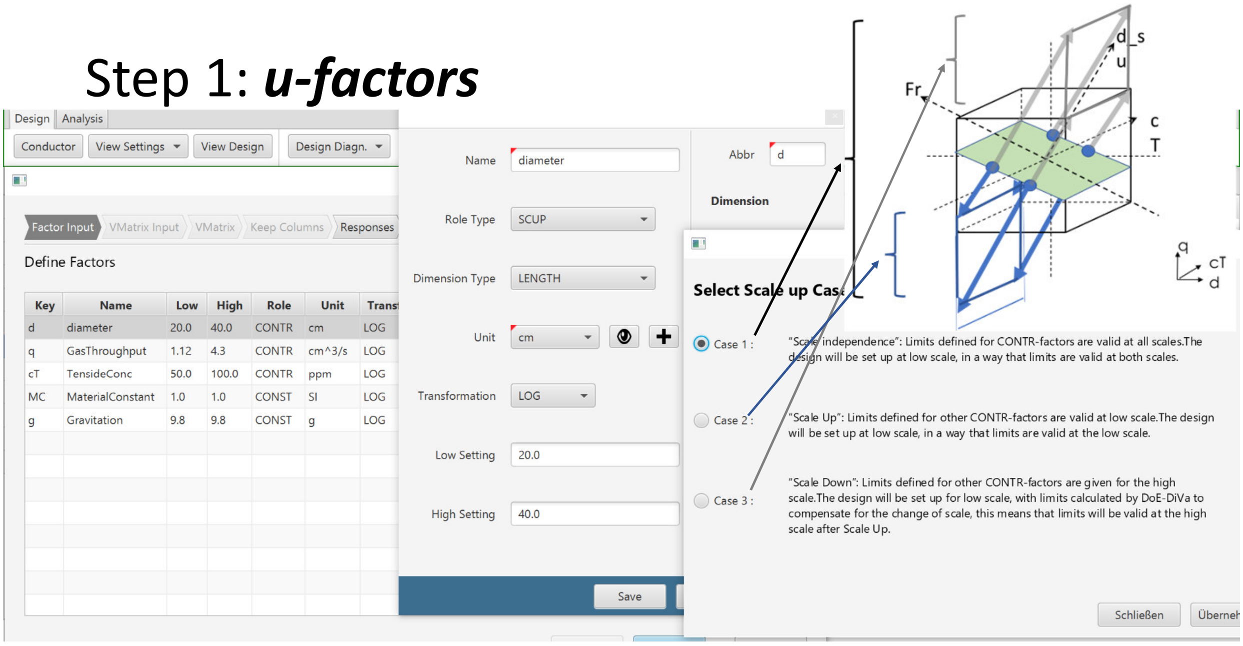
Exponent V-Matrix (for factors)

| | *Fr* | *cT_x* |
|---|---|---|
| $u_1$ | -5 | 0 |
| $u_2$ | 2 | 0 |
| $u_3$ | 0 | 1 |
| $u_4$ | -1 | 0 |

By the ***Similarity Principle of DA***, moving orthogonally to dimensionless plane, along ***d_su***, leaves the system invariant. Experiments for fitting $\boldsymbol{y = f_{causal}(x)}$ can be done at ***d = 20 cm***



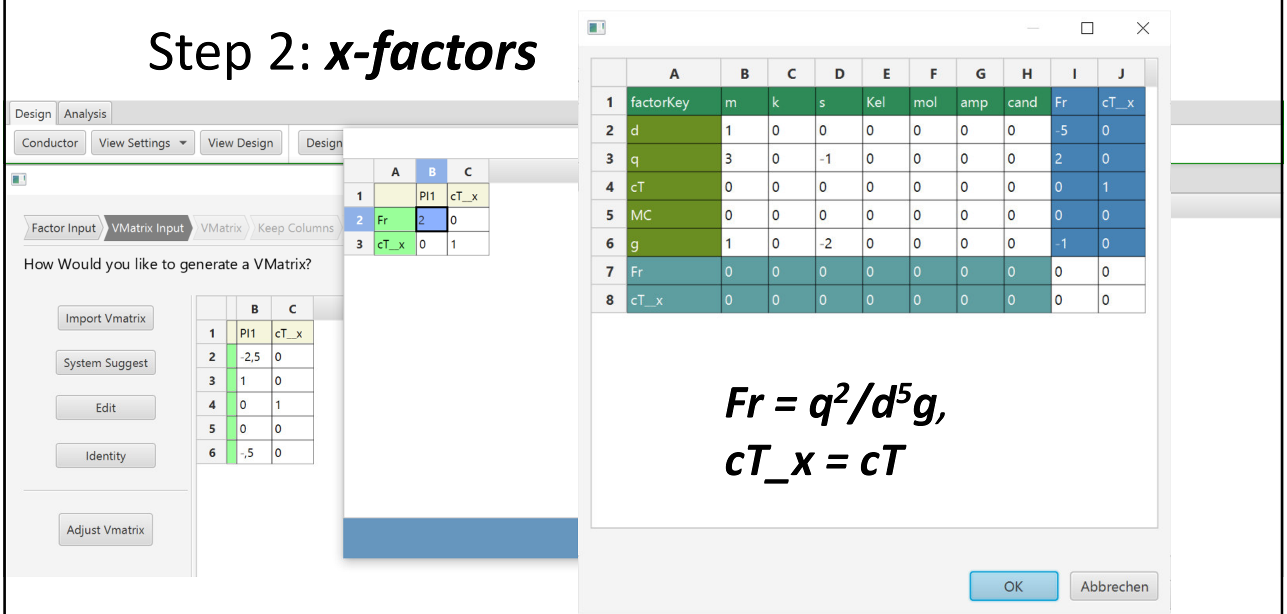
# Step 1: *u-factors*




| Key | Name | Low | High | Role | Unit | Trans |
|---|---|---|---|---|---|---|
| d | diameter | 20.0 | 40.0 | CONTR | cm | LOG |
| q | GasThroughput | 1.12 | 4.3 | CONTR | cm^3/s | LOG |
| cT | TensideConc | 50.0 | 100.0 | CONTR | ppm | LOG |
| MC | MaterialConstant | 1.0 | 1.0 | CONST | SI | LOG |
| g | Gravitation | 9.8 | 9.8 | CONST | g | LOG |



# Step 2: *x-factors*



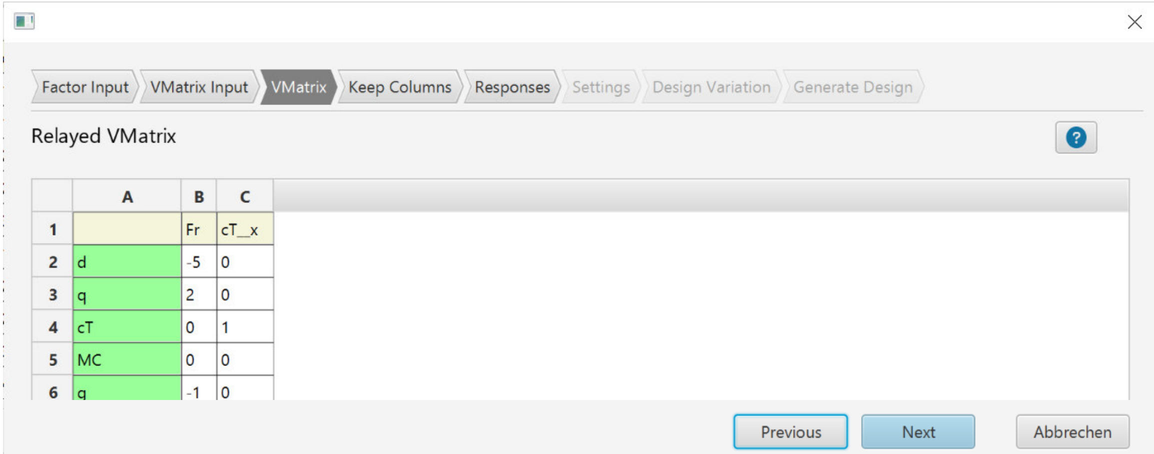

| | B | C |
|---|---|---|
| 1 | PI1 | cT_x |
| 2 | -2,5 | 0 |
| 3 | 1 | 0 |
| 4 | 0 | 1 |
| 5 | 0 | 0 |
| 6 | -,5 | 0 |

| | A | B | C |
|---|---|---|---|
| 1 | | PI1 | cT_x |
| 2 | Fr | 2 | 0 |
| 3 | cT_x | 0 | 1 |

| | A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | factorKey | m | k | s | Kel | mol | amp | cand | Fr | cT_x |
| 2 | d | 1 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | 0 |
| 3 | q | 3 | 0 | -1 | 0 | 0 | 0 | 0 | 2 | 0 |
| 4 | cT | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| 5 | MC | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | g | 1 | 0 | -2 | 0 | 0 | 0 | 0 | -1 | 0 |
| 7 | Fr | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | cT_x | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

$$Fr = q^2/d^5 g,$$
$$cT\_x = cT$$

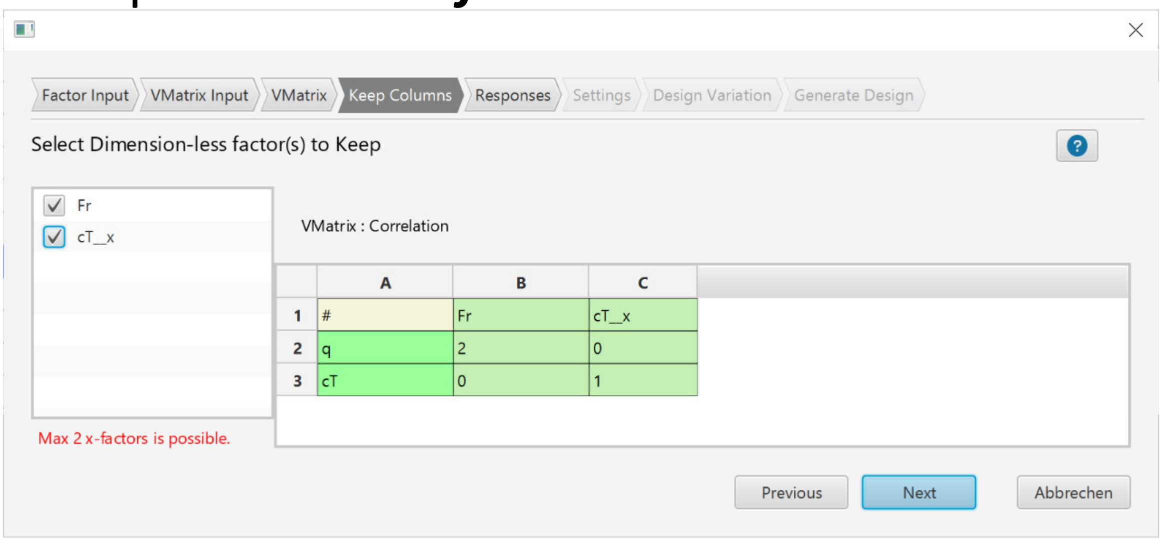
# Info, ***T – transformation as a matrix,***
# this *T* is easily invertible for fixed *d = low or high*




| | A | B | C |
|---|---|---|---|
| 1 | | Fr | cT_x |
| 2 | d | -5 | 0 |
| 3 | q | 2 | 0 |
| 4 | cT | 0 | 1 |
| 5 | MC | 0 | 0 |
| 6 | g | -1 | 0 |

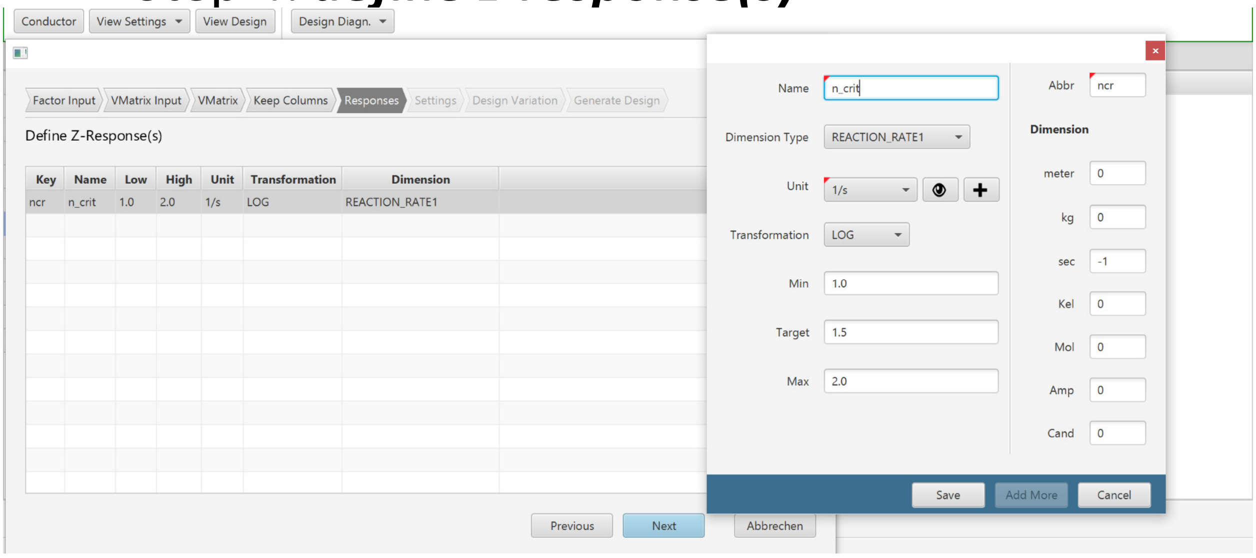


# Step 3: ***choose x-factors to use***



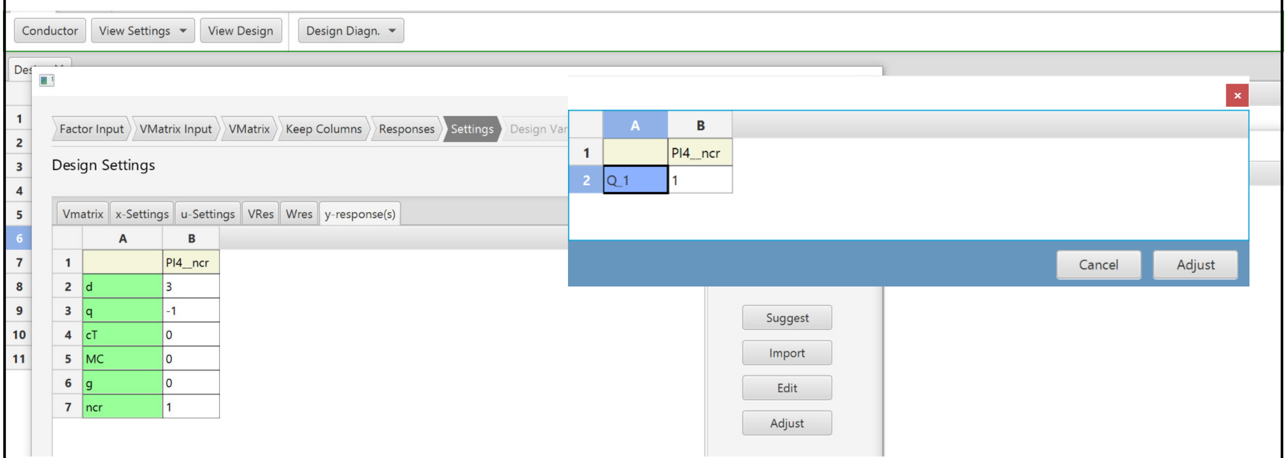

| | A | B | C |
|---|---|---|---|
| 1 | # | Fr | cT_x |
| 2 | q | 2 | 0 |
| 3 | cT | 0 | 1 |

# Step 4: ***define z-response(s)***






# Step 5: ***define y-response(s)***



# Step 6: ***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 |
|---|---|---|---|---|---|---|---|---|
| Fr | 1.0 | -9.08814 | -9.08814 | -9.08814 | -8.76078 | -8.43342 | -8.43342 | -8.43342 |
| cT_x | 1.0 | -4.30103 | -4.30103 | -4.30103 | -4.15052 | -4.0 | -4.0 | -4.0 |
| MC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| g | 0.0 | 0.991226 | 0.991226 | 0.991226 | 0.991226 | 0.991226 | 0.991226 | 0.991226 |
| d_su | 0.0 | -0.69897 | -0.69897 | -0.69897 | -0.69897 | -0.69897 | -0.69897 | -0.69897 |

Transformation: (•) LOG ( ) back-transform

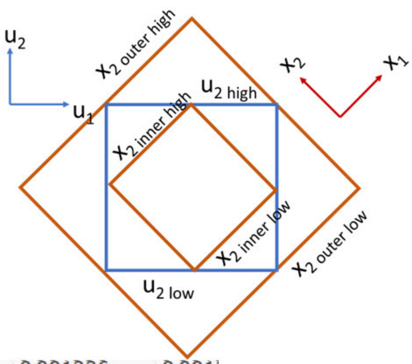
Use: (•) Inner ( ) Outer ( ) Inbetween ( ) User

Setting | Generate x-Settings

Previous | Next | Abbrechen



# Step 6ff: ***x-settings***




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

| # | Weight | Outer Low | User Low | Inner Low | Mean | | |
|---|---|---|---|---|---|---|---|
| Fr | 1.0 | -9.08814 | -9.08814 | -9.08814 | -8.76078 | | |
| cT_x | 1.0 | -4.30103 | -4.30103 | -4.30103 | -4.15052 | | |
| MC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | |
| g | 0.0 | 0.991226 | 0.991226 | 0.991226 | 0.991226 | 0.991226 | 0.991: |
| d_su | 0.0 | -0.69897 | -0.69897 | -0.69897 | -0.69897 | -0.69897 | -0.698 |

Transformation: (•) LOG ( ) back-transform

Use: (•) Inner ( ) Outer ( ) Inbetween ( ) User

Setting | Generate x-Settings

In this example ***inner limits*** and ***outer limits*** are ***the same***

Previous | Next | Abbrechen

# Step 7: ***select the design variation***

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

Select Design Variation

- ( ) Generate Design
- (•) Import Design
- ( ) Generate Candidate Set
- ( ) Performed Design for Analysis (and Prediction)

Previous | Next | Abbrechen

| | A | B | C |
|---|---|---|---|
| 1 | | q | cT |
| 2 | 2 | 1,63 | 50 |
| 3 | 3 | 2,23 | 50 |
| 4 | 4 | 2,79 | 50 |
| 5 | 5 | 3,33 | 50 |
| 6 | 6 | 1,66 | 100 |
| 7 | 7 | 2,23 | 100 |
| 8 | 8 | 2,78 | 100 |
| 9 | 9 | 3,37 | 100 |



# Step 7f: ***Look at the design (u-... and x-...)***

Design | Analysis

Conductor | View Settings | View Design | Design Diagn.

Design ×

| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| 1 | | d | q | cT | MC | g | ncr |
| 2 | R0 | 20,0000002 | 1,63 | 49,9999995 | 1 | 9,8000005 | 0 |
| 3 | R1 | 20,0000002 | 2,2300002 | 49,9999995 | 1 | 9,8000005 | 0 |
| 4 | R2 | 20,0000002 | 2,79 | 49,9999995 | 1 | 9,8000005 | 0 |
| 5 | R3 | 20,0000002 | 3,3299997 | 49,9999995 | 1 | 9,8000005 | 0 |
| 6 | R4 | 20,0000002 | 1,66 | 100 | 1 | 9,8000005 | 0 |
| 7 | R5 | 20,0000002 | 2,2300002 | 100 | 1 | 9,8000005 | 0 |
| 8 | R6 | 20,0000002 | 2,78 | 100 | 1 | 9,8000005 | 0 |
| 9 | R7 | 20,0000002 | 3,37 | 100 | 1 | 9,8000005 | 0 |

(•) uu ( ) u ( ) xx ( ) x ( ) scaled

Design | Analysis

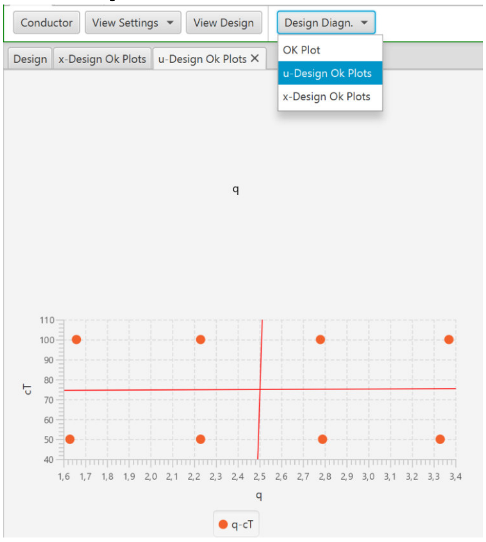
Conductor | View Settings | View Design | Design Diagn.

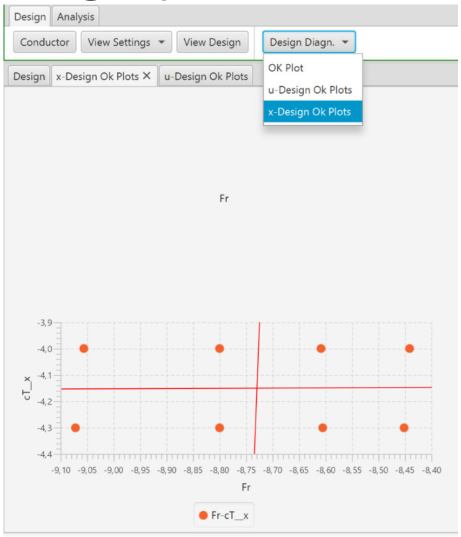
Design ×

| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| 1 | | Fr | cT__x | MC | g | d_su | Q_1 |
| 2 | R0 | -9,0720008 | -4,30103 | 0 | ,9912261 | -2,092207 | 0 |
| 3 | R1 | -8,7997663 | -4,30103 | 0 | ,9912261 | -2,04527 | 0 |
| 4 | R2 | -8,6051676 | -4,30103 | 0 | ,9912261 | -2,0117186 | 0 |
| 5 | R3 | -8,4514876 | -4,30103 | 0 | ,9912261 | -1,985222 | 0 |
| 6 | R4 | -9,0561599 | -4 | 0 | ,9912261 | -2,0894758 | 0 |
| 7 | R5 | -8,7997663 | -4 | 0 | ,9912261 | -2,04527 | 0 |
| 8 | R6 | -8,6082865 | -4 | 0 | ,9912261 | -2,0122563 | 0 |
| 9 | R7 | -8,4411163 | -4 | 0 | ,9912261 | -1,9834338 | 0 |

( ) uu ( ) u ( ) xx (•) x ( ) scaled

## Step 7ff: ***Look at the design (u-… and x-…)***

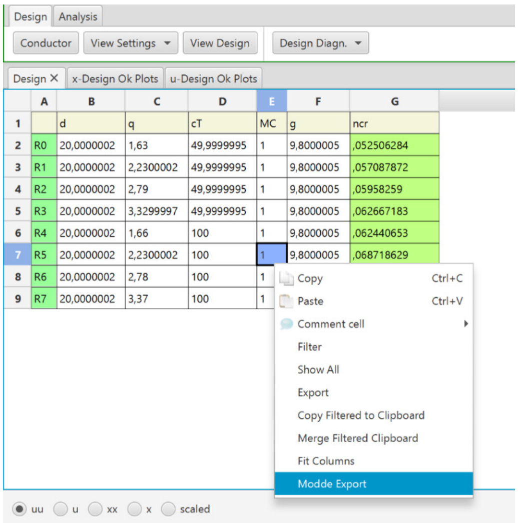


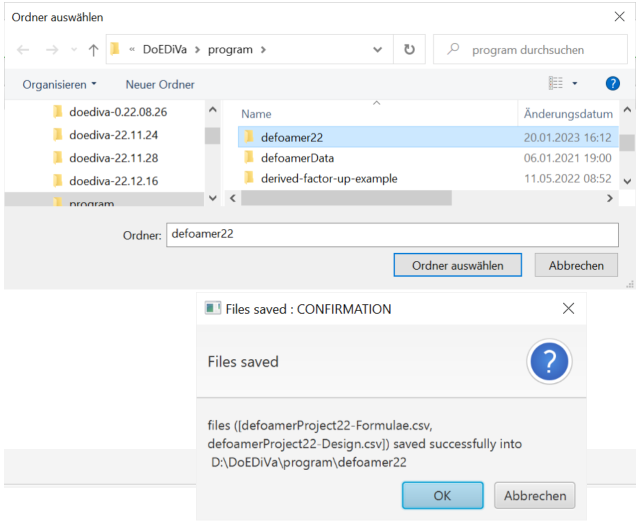



1. Dimensional Analysis and Similarity Principle
   Dimensionless eXplaining factors vs. User factors
2. Using DoE-DiVa for preparing simple Scale Up
3. ***Using MODDE to perform the Scale Up***

# Step 8: *Enter (z-)results; Export to MODDE®*

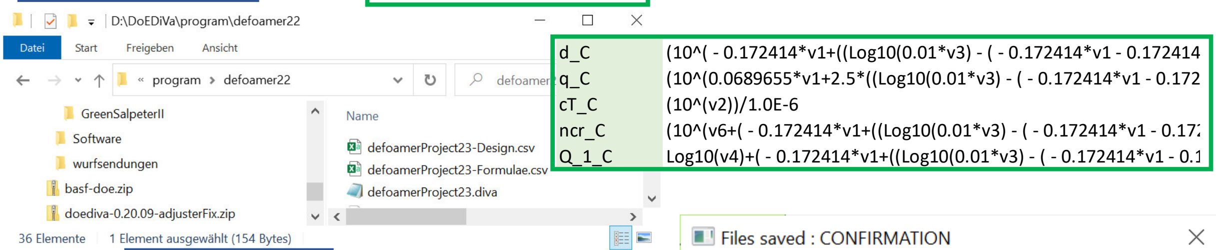



| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| 1 | | d | q | cT | MC | g | ncr |
| 2 | R0 | 20,0000002 | 1,63 | 49,9999995 | 1 | 9,8000005 | ,052506284 |
| 3 | R1 | 20,0000002 | 2,2300002 | 49,9999995 | 1 | 9,8000005 | ,057087872 |
| 4 | R2 | 20,0000002 | 2,79 | 49,9999995 | 1 | 9,8000005 | ,05958259 |
| 5 | R3 | 20,0000002 | 3,3299997 | 49,9999995 | 1 | 9,8000005 | ,062667183 |
| 6 | R4 | 20,0000002 | 1,66 | 100 | 1 | 9,8000005 | ,062440653 |
| 7 | R5 | 20,0000002 | 2,2300002 | 100 | 1 | 9,8000005 | ,068718629 |
| 8 | R6 | 20,0000002 | 2,78 | 100 | 1 | | |
| 9 | R7 | 20,0000002 | 3,37 | 100 | 1 | | |

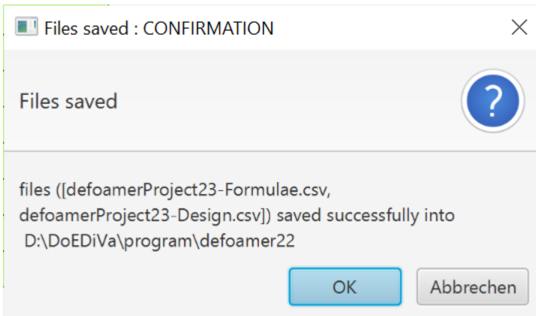




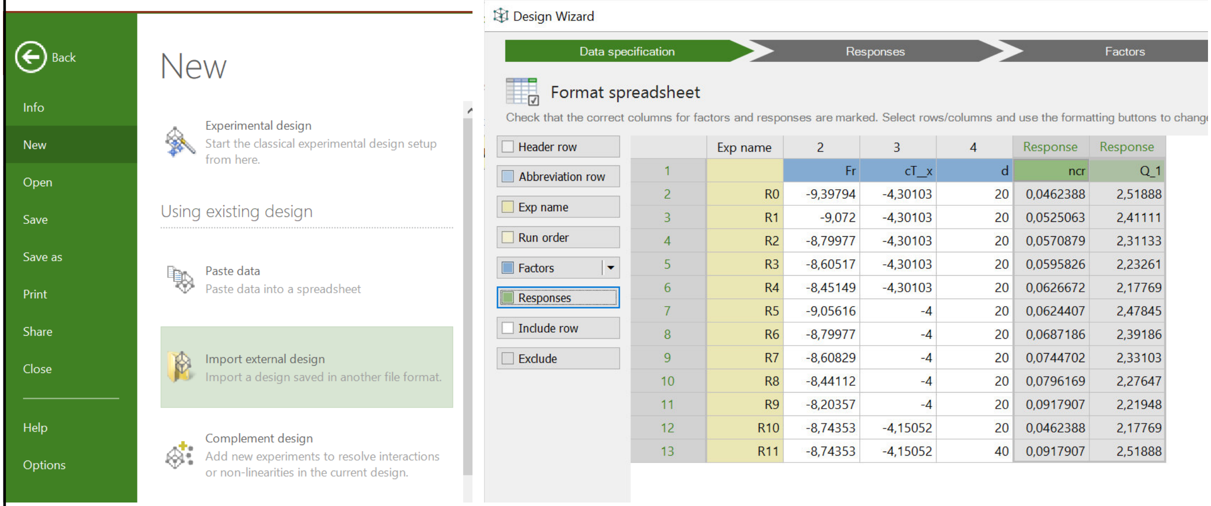

# *x-Design and u-formulae exported to MODDE®*




| | Fr | cT__x | d | ncr | Q_1 |
|---|---|---|---|---|---|
| R0 | -9,0720008 | -4,30103 | 20 | 0,0525063 | 2,4111137 |
| R1 | -8,7997663 | -4,30103 | 20 | 0,0570879 | 2,311329 |
| R2 | -8,6051676 | -4,30103 | 20 | 0,0595826 | 2,2326052 |
| R3 | -8,4514876 | -4,30103 | 20 | 0,0626672 | 2,177686 |
| R4 | -9,0561599 | -4 | 20 | 0,0624407 | 2,4784493 |
| R5 | -8,7997663 | -4 | 20 | 0,0687186 | 2,3918596 |
| R6 | -8,6082865 | -4 | 20 | 0,0744702 | 2,3310275 |
| R7 | -8,4411163 | -4 | 20 | 0,0796169 | 2,2764651 |
| R8 | -8,7292189 | -4,150515 | 20 | 0,0525063 | 2,177686 |
| R9 | -8,7292189 | -4,150515 | 40 | 0,0796169 | 2,4784493 |



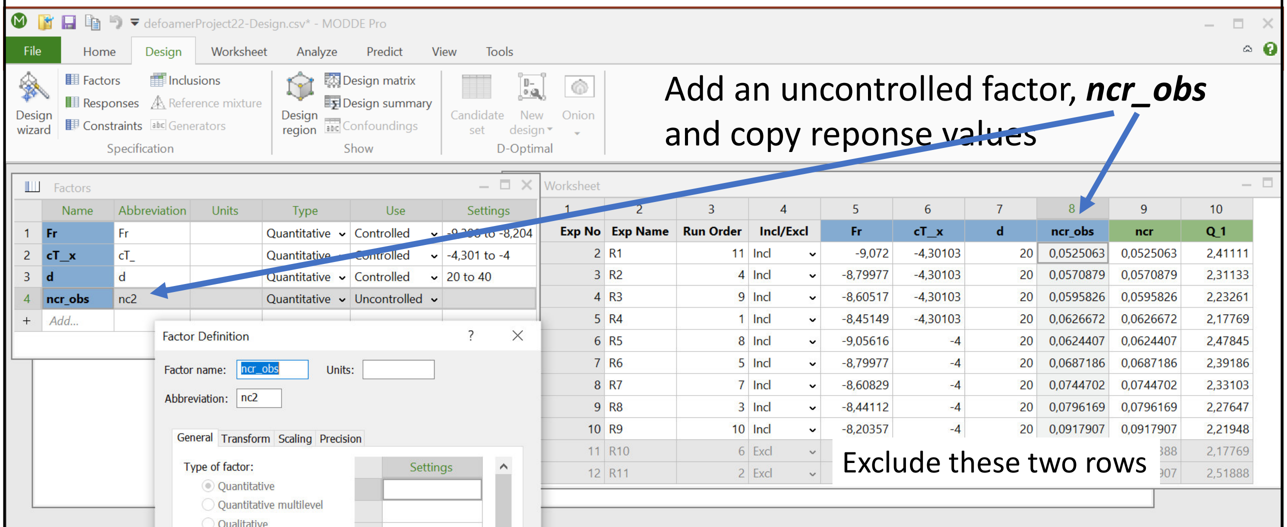
# Step 9: ***Use MODDE® to Analyse and Optimize***




| | Exp name | 2 | 3 | 4 | Response | Response |
|---|---|---|---|---|---|---|
| 1 | | Fr | cT_x | d | ncr | Q_1 |
| 2 | R0 | -9,39794 | -4,30103 | 20 | 0,0462388 | 2,51888 |
| 3 | R1 | -9,072 | -4,30103 | 20 | 0,0525063 | 2,41111 |
| 4 | R2 | -8,79977 | -4,30103 | 20 | 0,0570879 | 2,31133 |
| 5 | R3 | -8,60517 | -4,30103 | 20 | 0,0595826 | 2,23261 |
| 6 | R4 | -8,45149 | -4,30103 | 20 | 0,0626672 | 2,17769 |
| 7 | R5 | -9,05616 | -4 | 20 | 0,0624407 | 2,47845 |
| 8 | R6 | -8,79977 | -4 | 20 | 0,0687186 | 2,39186 |
| 9 | R7 | -8,60829 | -4 | 20 | 0,0744702 | 2,33103 |
| 10 | R8 | -8,44112 | -4 | 20 | 0,0796169 | 2,27647 |
| 11 | R9 | -8,20357 | -4 | 20 | 0,0917907 | 2,21948 |
| 12 | R10 | -8,74353 | -4,15052 | 20 | 0,0462388 | 2,17769 |
| 13 | R11 | -8,74353 | -4,15052 | 40 | 0,0917907 | 2,51888 |



# Step 9f: ***Prepare the worksheet (… obs-column)***

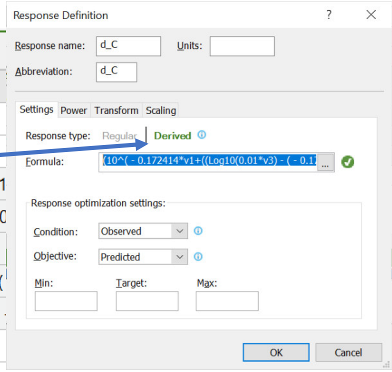



| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|
| Exp No | Exp Name | Run Order | Incl/Excl | Fr | cT_x | d | ncr_obs | ncr | Q_1 |
| 2 | R1 | 11 | Incl | -9,072 | -4,30103 | 20 | 0,0525063 | 0,0525063 | 2,41111 |
| 3 | R2 | 4 | Incl | -8,79977 | -4,30103 | 20 | 0,0570879 | 0,0570879 | 2,31133 |
| 4 | R3 | 9 | Incl | -8,60517 | -4,30103 | 20 | 0,0595826 | 0,0595826 | 2,23261 |
| 5 | R4 | 1 | Incl | -8,45149 | -4,30103 | 20 | 0,0626672 | 0,0626672 | 2,17769 |
| 6 | R5 | 8 | Incl | -9,05616 | -4 | 20 | 0,0624407 | 0,0624407 | 2,47845 |
| 7 | R6 | 5 | Incl | -8,79977 | -4 | 20 | 0,0687186 | 0,0687186 | 2,39186 |
| 8 | R7 | 7 | Incl | -8,60829 | -4 | 20 | 0,0744702 | 0,0744702 | 2,33103 |
| 9 | R8 | 3 | Incl | -8,44112 | -4 | 20 | 0,0796169 | 0,0796169 | 2,27647 |
| 10 | R9 | 10 | Incl | -8,20357 | -4 | 20 | 0,0917907 | 0,0917907 | 2,21948 |
| 11 | R10 | 6 | Excl | | | | | 388 | 2,17769 |
| 12 | R11 | 2 | Excl | | | | | 907 | 2,51888 |

# Step 9ff: ***Prepare the worksheet (u-T^-1 ransforms)***

Responses

| | Name | Abbreviation | Units | Type |
|---|---|---|---|---|
| 1 | ncr | ncr | | Regular |
| 2 | Q_1 | Q_1 | | Regular |
| 3 | d_C | d_C | | Derived: (10^( - 0.172414*v1+((Log10(0.01*v3) - ( - 0.1 |
| 4 | q_C | q_C | | Derived: (10^(0.068966*v1+2.5*((Log10(0.01*v3) - ( - 0 |
| 5 | cT_C | cT2 | | Derived: (10^(v2))/1.0E-6 |
| 6 | ncr_C | nc2 | | Derived: (10^(v6+( - 0.172414*v1+((Log10(0.01*v3) - ( |
| 7 | Q_1_C | Q_2 | | Derived: Log10(v4)+( - 0.172414*v1+((Log10(0.01*v3) |
| + | Add... | | | |




Add „***derived responses***" for the u-factors: ***d_C, q_C, cT_C,***
then add „*derived responses*" for the responses, ***ncr_C, Q_1_C,***
using the formulae that the *DoE-DiVa* provided.



# Step 9fff: ***Check the worksheet (u-T^-1 ransforms)***

Responses

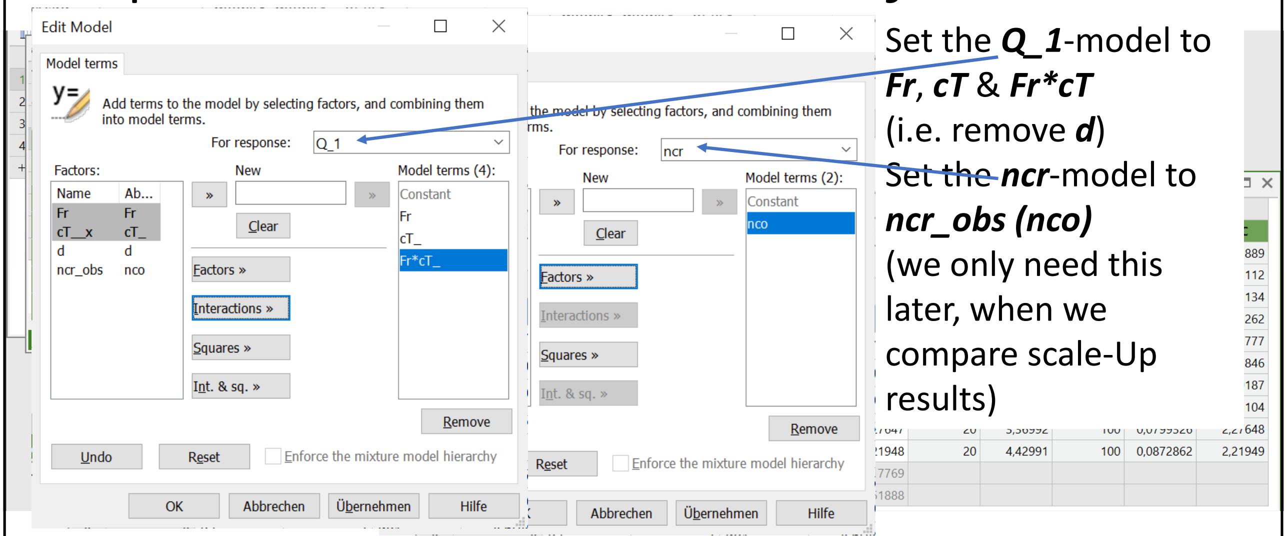
| | Name | Abbreviation | Units | Type | Condition | Objective | Min | Target | Max | Predicted min |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | ncr | ncr | | Regular | Required | Inside | | | | -- |
| 2 | Q_1 | Q_1 | | Regular | Required | Inside | | | | -- |
| 3 | d_C | d_C | | Derived: (10^( - 0.172414*v1+((Log10(0.01*v3) - ( - 0.172414*v1 - 0.17241 | Observed | Predicted | | | | -- |
| 4 | q_C | q_C | | Derived: (10^(0.068966*v1+2.5*((Log10(0.01*v3) - ( - 0.172414*v1 - 0.172 | Observed | Predicted | | | | |
| 5 | cT_C | cT2 | | | | | | | | |
| 6 | ncr_C | nc2 | | | | | | | | |
| 7 | Q_1_C | Q_2 | | | | | | | | |
| + | Add... | | | | | | | | | |

Worksheet

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Exp No | Exp Name | Run Order | Incl/Excl | Fr | cT_x | d | ncr_obs | ncr | Q_1 | d_C | q_C | cT_C | ncr_C | Q_1_C |
| 1 | 1 | R0 | 7 | Incl | -9,39794 | -4,30103 | 20 | 0,0462388 | 0,0462388 | 2,51888 | 20 | 1,11998 | 50 | 0,0454014 | 2,51889 |
| 2 | 2 | R1 | 2 | Incl | -9,072 | -4,30103 | 20 | 0,0525063 | 0,0525063 | 2,41111 | 20 | 1,62997 | 50 | 0,0512287 | 2,41112 |
| 3 | 3 | R2 | 9 | Incl | -8,79977 | -4,30103 | 20 | 0,0570879 | 0,0570879 | 2,31133 | 20 | 2,22995 | 50 | 0,0566649 | 2,31134 |
| 4 | 4 | R3 | 10 | Incl | -8,60517 | -4,30103 | 20 | 0,0595826 | 0,0595826 | 2,23261 | 20 | 2,78994 | 50 | 0,0609012 | 2,23262 |
| 5 | 5 | R4 | 11 | Incl | -8,45149 | -4,30103 | 20 | 0,0626672 | 0,0626672 | 2,17769 | 20 | 3,32993 | 50 | 0,0644693 | 2,1777 |
| 6 | 6 | R5 | 6 | Incl | -9,05616 | -4 | 20 | 0,0624407 | 0,0624407 | 2,47845 | 20 | 1,65997 | 100 | 0,0636451 | 2,47846 |
| 7 | 7 | R6 | 8 | Incl | -8,79977 | -4 | 20 | 0,0687186 | 0,0687186 | 2,39186 | 20 | 2,22995 | 100 | 0,0699869 | 2,39187 |
| 8 | 8 | R7 | 3 | Incl | | | | | | | | | | | 2,33104 |
| 9 | 9 | R8 | 1 | Incl | | | | | | | | | | | 2,27648 |
| 10 | 10 | R9 | 4 | Incl | | | | | | | | | | | 2,21949 |
| 11 | 11 | R10 | 12 | Excl | | | | | | | | | | | |
| 12 | 12 | R11 | 5 | Excl | -8,74353 | -4,15052 | 40 | 0,0917907 | 0,0917907 | 2,51888 | | | | | |

Remove the last two rows from the worksheet,
they were needed for MODDE to not set ***d*** to constant.

# Step 10: ***Edit the model to be used for FIT***

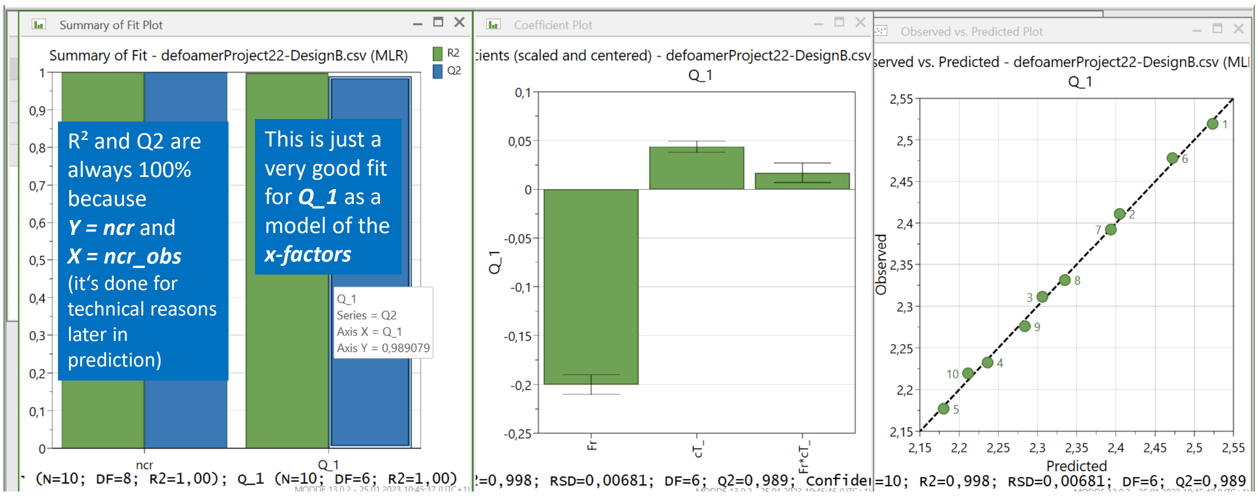



Set the ***Q_1***-model to ***Fr, cT*** & ***Fr*cT*** (i.e. remove ***d***)

Set the ***ncr***-model to ***ncr_obs (nco)*** (we only need this later, when we compare scale-Up results)



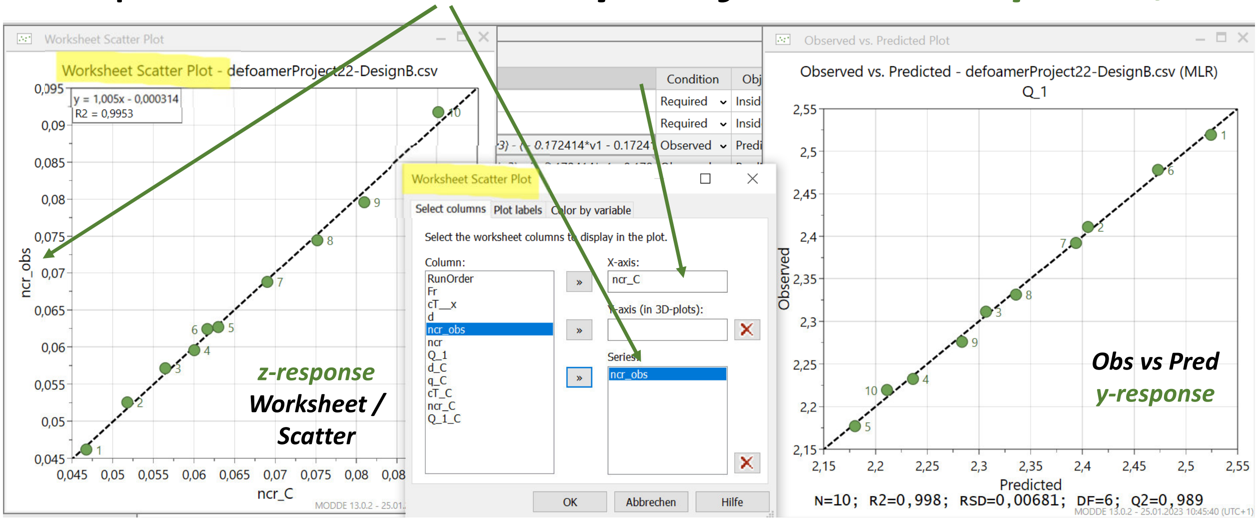
# Step 10f: ***FIT the model – y-response to x-design***




$R^2$ and Q2 are always 100% because ***Y = ncr*** and ***X = ncr_obs*** (it's done for technical reasons later in prediction)

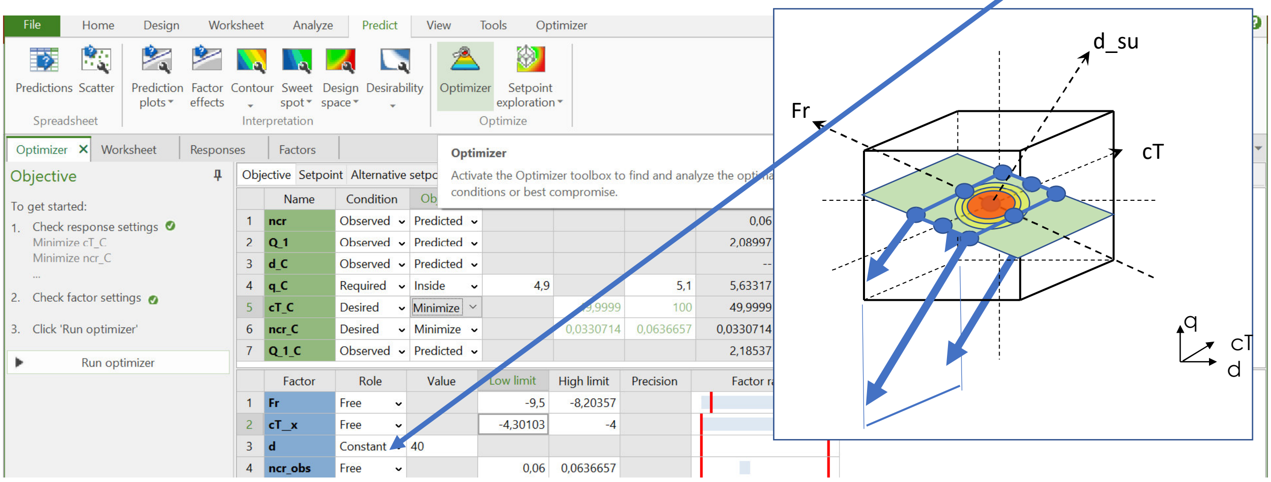
This is just a very good fit for ***Q_1*** as a model of the ***x-factors***

# Step 10ff: *Check obs vs pred for the z-response,*





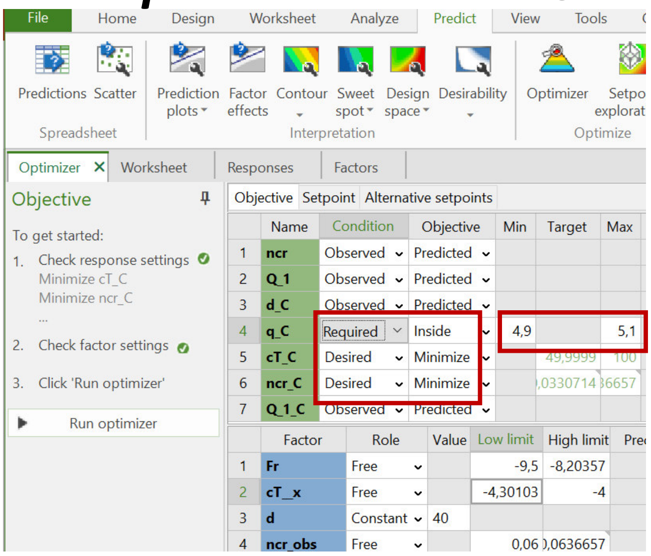

# Step 11: *Optimize for the high Scale, d = 40*



# Step 11f: ***Before we optimize: Think*** ☺

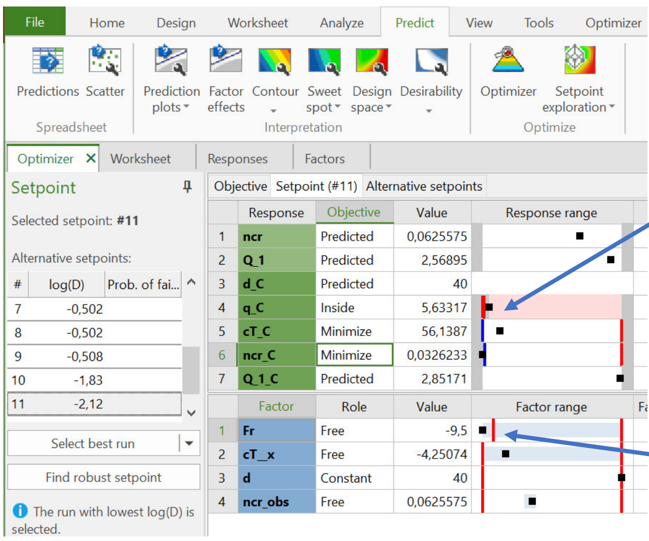
***ncr*** was (already) ***minimal rotation***, for which de-foaming works. We in fact ***control n***, ***n** must be* ***> ncr.***

What we probably want: Given a gas throughput, ***q***, (that causes formation of foam), what ***ncr*** should we use, and how much tenside, ***cT***?






# Step 11ff: ***Optimization result at*** ***d = 40***

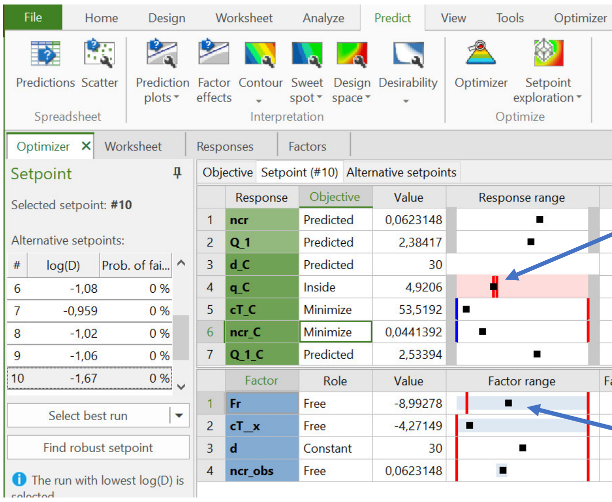



Gas throughput, ***q***, is too high

Maybe we don't need the big defoamer, ***d = 30*** cm may suffice

And the model extrapolates for ***Fr = -9,5*** ☹

## Step 11fff: ***Optimization result at d = 30***



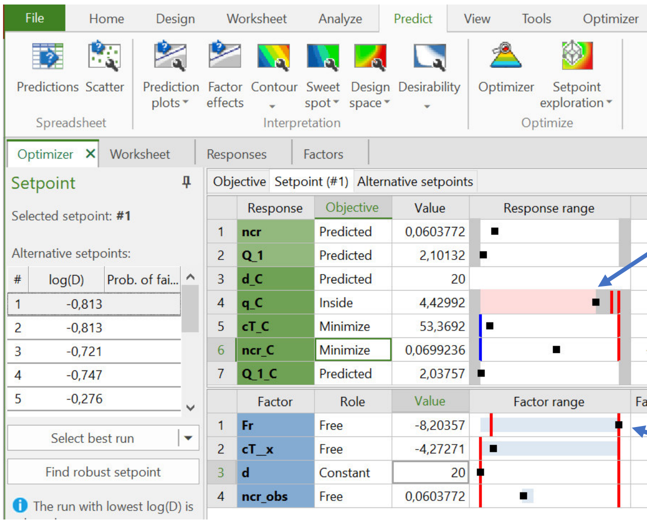

Gas throughput, ***q***, is ok now!

Indeed, it seems, the defoamer with ***d = 30*** cm is better

And the model is not extrapolated ***Fr = -8,99*** is good ☺



## Step 11ffff: ***Optimization result at d = 20***




Gas throughput, ***q***, is now too low!

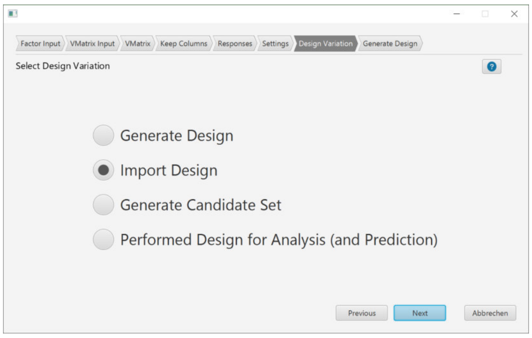
So, a defoamer with ***d = 20*** cm is also unsuited

And the model wants to extrapolate ***Fr = -8,204*** is limit ☹

# Step 12: ***Validating Scale Up, when data are available***

*We have data* for d=30/40!*

*Import the* ***u-factor data*** *into the* ***DoE-DiVa***




Import csv

Input Csv Se

Input Data

| | A | B | C | D |
|---|---|---|---|---|
| 1 | | d | q | cT |
| 2 | 6 | 30 | 1,63 | 50 |
| 3 | 7 | 30 | 2,22 | 50 |
| 4 | 8 | 30 | 2,75 | 50 |
| 5 | 9 | 30 | 3,29 | 50 |
| 6 | 10 | 30 | 4,39 | 50 |
| 7 | 11 | 30 | 5,5 | 50 |
| 8 | 12 | 40 | 2,2 | 50 |
| 9 | 13 | 40 | 2,81 | 50 |
| 10 | 14 | 40 | 3,28 | 50 |

* Chem.-Ing.-Tech. 56 (1984) Nr. 11, S. 839 – 844



0009-286X/84/1111-0839$02.50/0



# Step 12f: ***Validating Scale Up***

*Enter **z**-response data* for d=30/40, then Copy/Paste to MODDE®*

Design | Analysis — Conductor | View Settings | View Design | Design Diagn.

Design × | u-Design Ok Plots | x-Design Ok Plots | Coefficients -Q_1

| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| 1 | | d | q | cT | MC | g | ncr |
| 2 | R0 | 30,0000031 | 1,63 | 50 | 1 | 9,8000005 | ,031817929 |
| 3 | R1 | 30,0000031 | 2,22 | 50 | 1 | 9,8000005 | ,033732493 |
| 4 | R2 | 30,0000031 | 2,75 | 50 | 1 | 9,8000005 | ,035305374 |
| 5 | R3 | 30,0000031 | 3,29 | 50 | 1 | 9,8000005 | ,039430573 |
| 6 | R4 | 30,0000031 | 4,39 | 50 | 1 | 9,8000005 | ,043243216 |
| 7 | R5 | 30,0000031 | 5,5 | 50 | 1 | 9,8000005 | ,046578829 |
| 8 | R6 | 40,0000008 | 2,2 | 50 | 1 | 9,8000005 | ,025731123 |
| 9 | R7 | 40,0000008 | 2,81 | 50 | 1 | 9,8000005 | ,027387765 |

uu u xx x scaled

Design × | u-Design Ok Plots | x-Design Ok Plots | Coefficients -Q_1 | Fit-Q_1

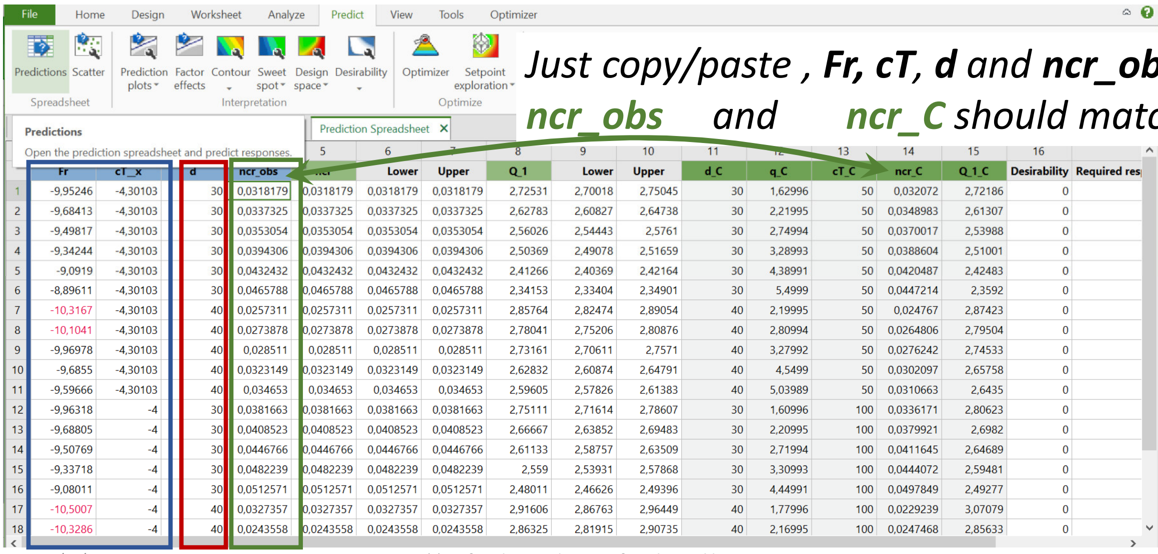
| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| 1 | | Fr | cT__x | MC | g | d_su | Q_1 |
| 2 | R0 | -9,9524571 | -4,30103 | | ,9912261 | -2,0679186 | 2,72184820839 |
| 3 | R1 | -9,6841264 | -4,30103 | | ,9912261 | -2,0216547 | 2,61305933891 |
| 4 | R2 | -9,498167 | -4,30103 | | ,9912261 | -1,9895927 | 2,53987201646 |
| 5 | R3 | -9,3424406 | -4,30103 | | ,9912261 | -1,9627433 | 2,51000108823 |
| 6 | R4 | -9,0919033 | -4,30103 | | ,9912261 | -1,9195472 | 2,42481738498 |
| 7 | R5 | -8,896107 | -4,30103 | | ,9912261 | -1,8857892 | 2,35918976609 |
| 8 | R6 | -10,3166807 | -4,30103 | | ,9912261 | -2,005777 | 2,87421604081 |
| 9 | R7 | -10,1041134 | -4,30103 | | ,9912261 | -1,9691275 | 2,79503029275 |
| 10 | R8 | -9,9697783 | -4,30103 | | ,9912261 | -1,9459663 | 2,74531887858 |
| 11 | R9 | -9,6855032 | -4,30103 | | ,9912261 | -1,8969533 | 2,65757183293 |

uu u xx x scaled

# Step 12ff: ***Use MODDE® Prediction set***

*Just copy/paste , **Fr, cT, d** and **ncr_obs***

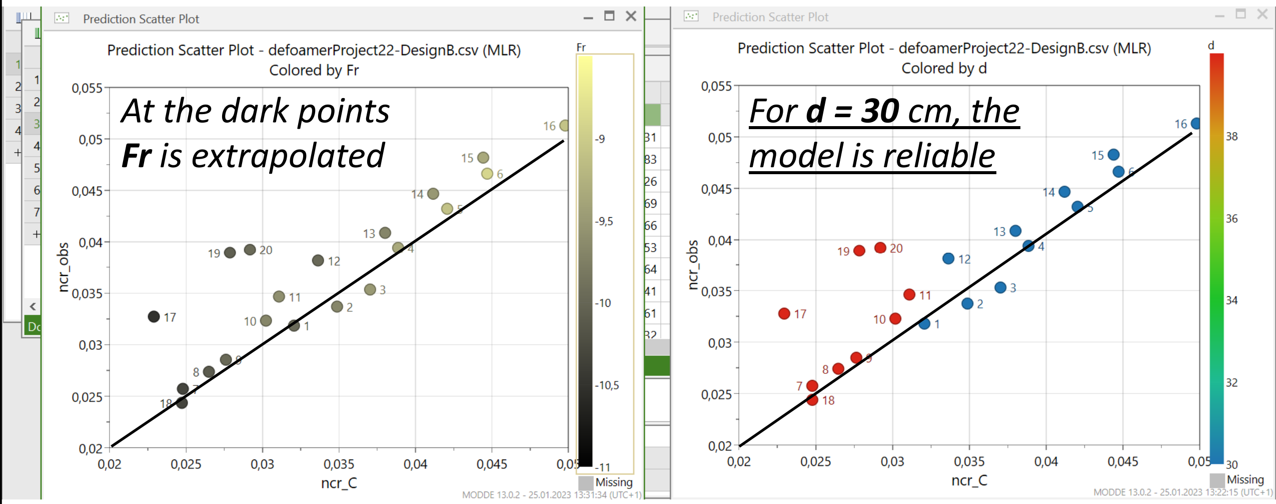
***ncr_obs*** *and* ***ncr_C*** *should match!*




| | Fr | cT_x | d | ncr_obs | [illegible] | Lower | Upper | Q_1 | Lower | Upper | d_C | q_C | cT_C | ncr_C | Q_1_C | Desirability | Required res |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -9,95246 | -4,30103 | 30 | 0,0318179 | 0,0318179 | 0,0318179 | 0,0318179 | 2,72531 | 2,70018 | 2,75045 | 30 | 1,62996 | 50 | 0,032072 | 2,72186 | 0 | |
| 2 | -9,68413 | -4,30103 | 30 | 0,0337325 | 0,0337325 | 0,0337325 | 0,0337325 | 2,62783 | 2,60827 | 2,64738 | 30 | 2,21995 | 50 | 0,0348983 | 2,61307 | 0 | |
| 3 | -9,49817 | -4,30103 | 30 | 0,0353054 | 0,0353054 | 0,0353054 | 0,0353054 | 2,56026 | 2,54443 | 2,5761 | 30 | 2,74994 | 50 | 0,0370017 | 2,53988 | 0 | |
| 4 | -9,34244 | -4,30103 | 30 | 0,0394306 | 0,0394306 | 0,0394306 | 0,0394306 | 2,50369 | 2,49078 | 2,51659 | 30 | 3,28993 | 50 | 0,0388604 | 2,51001 | 0 | |
| 5 | -9,0919 | -4,30103 | 30 | 0,0432432 | 0,0432432 | 0,0432432 | 0,0432432 | 2,41266 | 2,40369 | 2,42164 | 30 | 4,38991 | 50 | 0,0420487 | 2,42483 | 0 | |
| 6 | -8,89611 | -4,30103 | 30 | 0,0465788 | 0,0465788 | 0,0465788 | 0,0465788 | 2,34153 | 2,33404 | 2,34901 | 30 | 5,4999 | 50 | 0,0447214 | 2,3592 | 0 | |
| 7 | -10,3167 | -4,30103 | 40 | 0,0257311 | 0,0257311 | 0,0257311 | 0,0257311 | 2,85764 | 2,82474 | 2,89054 | 40 | 2,19995 | 50 | 0,024767 | 2,87423 | 0 | |
| 8 | -10,1041 | -4,30103 | 40 | 0,0273878 | 0,0273878 | 0,0273878 | 0,0273878 | 2,78041 | 2,75206 | 2,80876 | 40 | 2,80994 | 50 | 0,0264806 | 2,79504 | 0 | |
| 9 | -9,96978 | -4,30103 | 40 | 0,028511 | 0,028511 | 0,028511 | 0,028511 | 2,73161 | 2,70611 | 2,7571 | 40 | 3,27992 | 50 | 0,0276242 | 2,74533 | 0 | |
| 10 | -9,6855 | -4,30103 | 40 | 0,0323149 | 0,0323149 | 0,0323149 | 0,0323149 | 2,62832 | 2,60874 | 2,64791 | 40 | 4,5499 | 50 | 0,0302097 | 2,65758 | 0 | |
| 11 | -9,59666 | -4,30103 | 40 | 0,034653 | 0,034653 | 0,034653 | 0,034653 | 2,59605 | 2,57826 | 2,61383 | 40 | 5,03989 | 50 | 0,0310663 | 2,6435 | 0 | |
| 12 | -9,96318 | -4 | 30 | 0,0381663 | 0,0381663 | 0,0381663 | 0,0381663 | 2,75111 | 2,71614 | 2,78607 | 30 | 1,60996 | 100 | 0,0336171 | 2,80623 | 0 | |
| 13 | -9,68805 | -4 | 30 | 0,0408523 | 0,0408523 | 0,0408523 | 0,0408523 | 2,66667 | 2,63852 | 2,69483 | 30 | 2,20995 | 100 | 0,0379921 | 2,6982 | 0 | |
| 14 | -9,50769 | -4 | 30 | 0,0446766 | 0,0446766 | 0,0446766 | 0,0446766 | 2,61133 | 2,58757 | 2,63509 | 30 | 2,71994 | 100 | 0,0411645 | 2,64689 | 0 | |
| 15 | -9,33718 | -4 | 30 | 0,0482239 | 0,0482239 | 0,0482239 | 0,0482239 | 2,559 | 2,53931 | 2,57868 | 30 | 3,30993 | 100 | 0,0444072 | 2,59481 | 0 | |
| 16 | -9,08011 | -4 | 30 | 0,0512571 | 0,0512571 | 0,0512571 | 0,0512571 | 2,48011 | 2,46626 | 2,49396 | 30 | 4,44991 | 100 | 0,0497849 | 2,49277 | 0 | |
| 17 | -10,5007 | -4 | 40 | 0,0327357 | 0,0327357 | 0,0327357 | 0,0327357 | 2,91606 | 2,86763 | 2,96449 | 40 | 1,77996 | 100 | 0,0229239 | 3,07079 | 0 | |
| 18 | -10,3286 | -4 | 40 | 0,0243558 | 0,0243558 | 0,0243558 | 0,0243558 | 2,86325 | 2,81915 | 2,90735 | 40 | 2,16995 | 100 | 0,0247468 | 2,85633 | 0 | |



# Step 12fff: ***Use MODDE® Prediction Scatter Plot***



Thank You!

Gefördert durch:

Bundesministerium
für Wirtschaft
und Energie

aufgrund eines Beschlusses
des Deutschen Bundestages

and in particular to:

Chhawang Lama
Anthony Orth