**H-JG Consulting**

**Dr. Hans-Joachim Graf**

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www.hans-joachim-graf.com

www.grafcompounder.com

# All About Compounding

## Artificial Intelligence [AI] in Rubber Compounding:

### Introduction of GrafCompounder 4.0.6

## Content of this presentation

1. Introduction
2. Tools in Compounding
    1. Design of Experiment and AI Program
    2. Compounding and Artificial Intelligence
3. Program GrafCompounder 4.0.6
4. Program tools
5. Confirmation of Simulation
6. Conclusion

## ➔ Computer Aided Compound Development

- **Bridgestone Patent 1994**
  **Inventor: Akihiko Abe**
- **Bridgestone Patent 2002**

**Inventor: Yukio Nakajima**

- ***Colour Matching***
  ***Patents from***
  ***BASF, CyanAmid, DuPONT***

- ***Empirical DoE Patent:***
  ***Honeywell***

- ***Recipe Libary Search and***
  ***Comparison***
  ***CombiChem, GE, Hunt (Private)***

(12) **United States Patent**
**Nakajima**

US006411945B1

(10) **Patent No.: US 6,411,945 B1**
(45) **Date of Patent: Jun. 25, 2002**

(54) **METHOD AND APPARATUS FOR DESIGNING MULTI-COMPONENT MATERIAL, OPTIMIZATION ANALYZER AND STORAGE MEDIUM USING LEARNING PROCESS**

(75) Inventor: **Yukio Nakajima**, Tokyo (JP)

(73) Assignee: **Bridgestone Corporation**, Tokyo (JP)

( * ) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

(21) Appl. No.: **09/051,416**

(22) PCT Filed: **Aug. 8, 1997**

(86) PCT No.: **PCT/JP97/02784**

§ 371 (c)(1),
(2), (4) Date: **Apr. 6, 1998**

(87) PCT Pub. No.: **WO98/06550**

PCT Pub. Date: **Feb. 19, 1998**

(30) **Foreign Application Priority Data**

JP 9-16654 1/1997
WO WO 94/16877 8/1994

OTHER PUBLICATIONS

Goldberg, David E., "Genetic Algorithm in Search, Optimization and Machine Learning", Addison–Wesley, 1989.*
Oda, Juhachi; Okada, Hiroyasu; "Design method of materials composed of some ingredients by using neural network"; Optimization Symposium '94; pp. 57–63, 1994.*
A formulation tool, Alan H. Bohl, *Chemtech*, May 1988 pp. 284–289.
The Role of Integrated AI Technologies in Product Formulation, *ISA Transactions*, 1992, vol. 31, No. 2, pp. 151–157.
Design Method of Materials Composed of Some Ingredients by Using Neural Network, Juhachi Oda and Hiroyasu Okada, *Optimization Symposium '94*, pp. 57–62.
Non–Linear Multi–Variate Analysis—Approach by Neural Network, Hideki Toyota, *Asakura Book Store*, 1996, pp. 11–13 and 162–166.
Design and Analysis in Mixed Experiments, Manabu Iwasaki, *Scientist Co.*.

* cited by examiner

*Primary Examiner*—George B. Davis
(74) *Attorney, Agent, or Firm*—Sughrue Mion, PLLC

(71) Applicant: **10-1, Kyobashi 1-Chome**
**Chuo-Ku**
**Tokyo 104 (JP)**

(54) **Method for designing pneumatic tires.**

(57) In order to perform tire design and development highly efficiently and provide a tire at low cost, a tire basic model for representing a tire cross-sectional shape including an internal structure and being divided into a plurality of elements, an objective function for representing

FIG.2A

START

MODELING OF TIRE

100

ition number : **0 647 911 A2**

**LICATION**

Cl.[6]: **G06F 17/50**

Inventor : **Abe, Akihiko**
**3-5-5, Ogawa-higashi-cho**
**Kodaira-shi, Tokyo (JP)**

Representative : **Whalley, Kevin**
**MARKS & CLERK,**
**57-60 Lincoln's Inn Fields**
**London WC2A 3LS (GB)**

# ➔Tools in Compound Development

## ➔Database Oriented

- **Better utilization of historic compound data base**
- **Faster results - minimizes efforts and time in development**
- **Increases creativity through compound simulation**

## ➔Experimentation Oriented

- **Evaluation of New Material without History**
- **Correlation between effect of factors on response**
- **Creates statistically sound knowledge about ingredients and processes**

## ➔ Tools in Compound Development

### ➔ Experimentation oriented

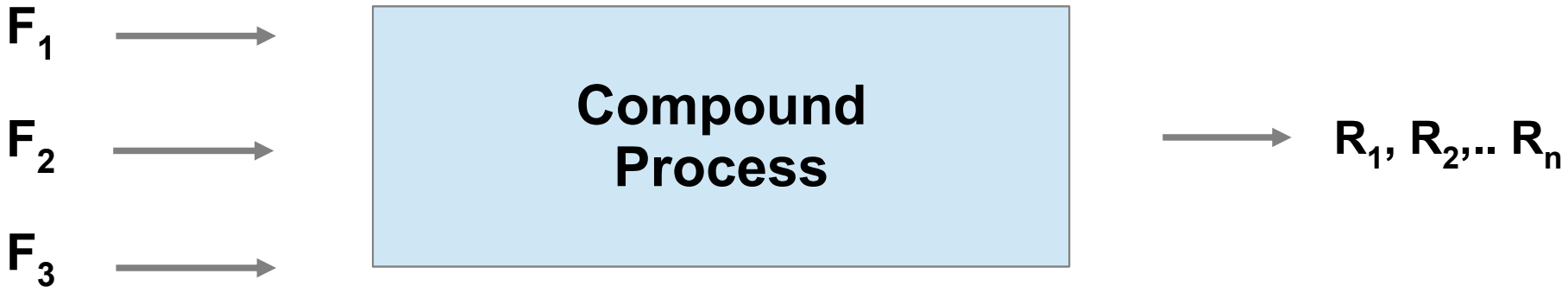
### ➔ Input: Factor Variation

- Experiments according DoE systematic
- Testing
- Data treatment: ANOVA, Regression, Correlation between factor variation and response

### ➢ Output: Recipe, Correlation Maps, Overlay Plots

**Experimentation:**
**Variation of Factors**

**Measurements:**
**Responses**




**Objective of the Experiment is the identification of the factors ($F_{1,}..F_n$) type of influence on the responses ($R_{1,}...R_n$) and description with mathematical equations for further processing.**

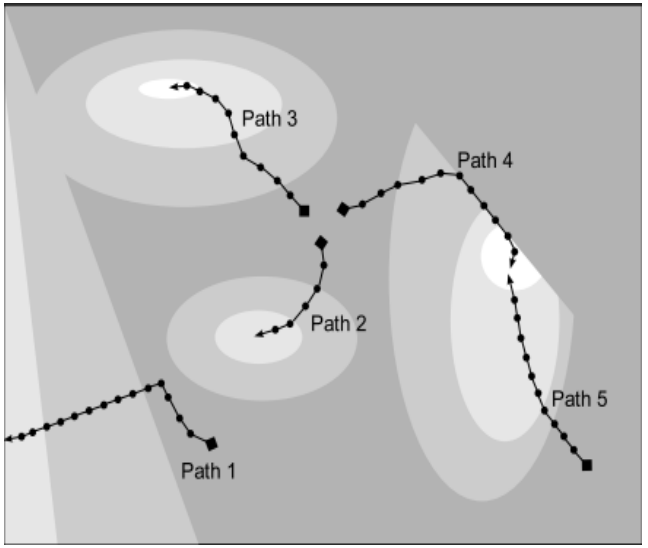
$$R_{i(1...n)} = f(A_0 + A_1F_1 + ....A_nF_n + ....)$$

# Tools in Compound Development

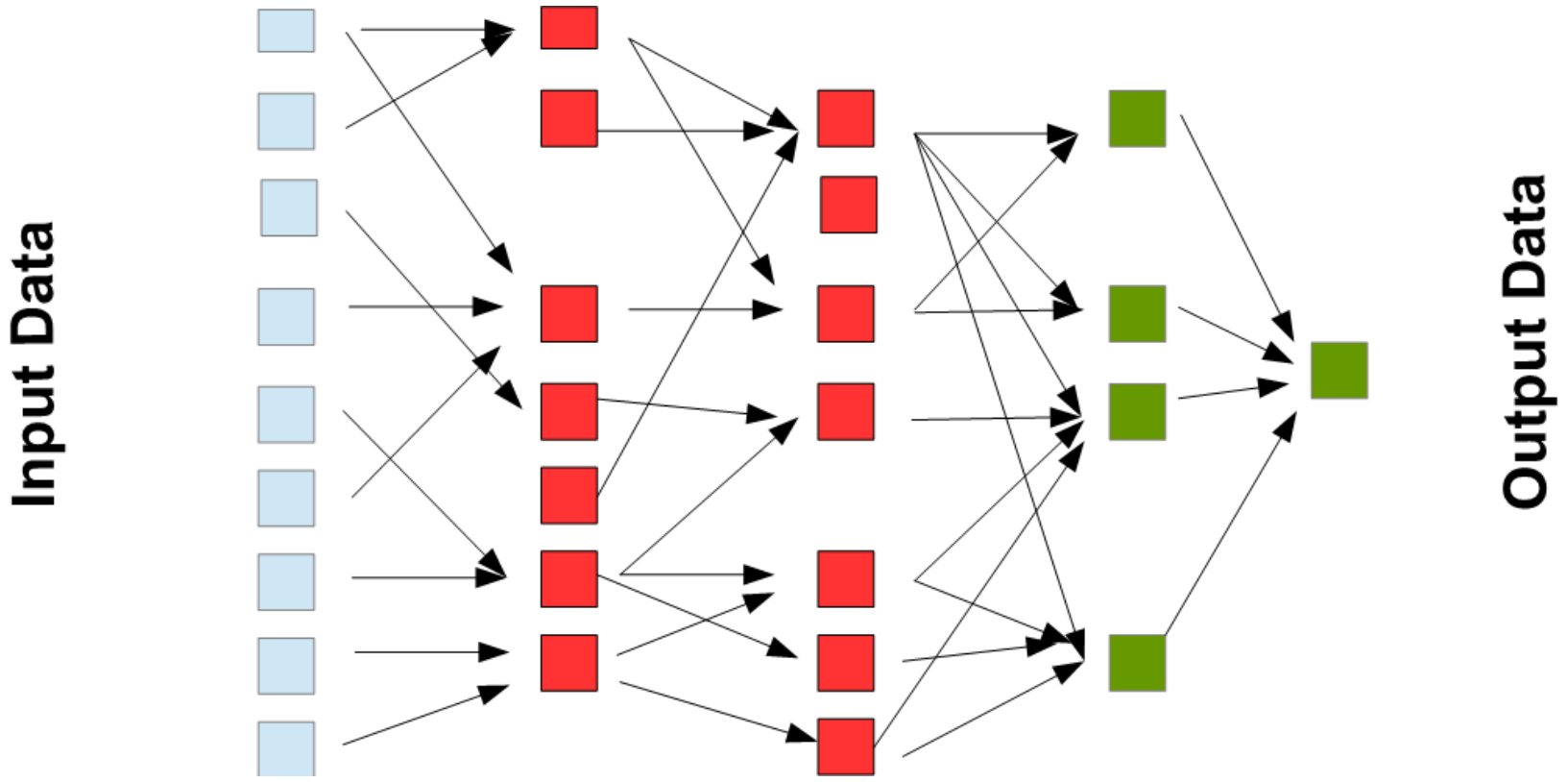
## ➔Database Oriented

## ➔Input: Data + Multi target query

- Data treatment with Multi Objective Evolutionary Algorithm (MOEA)
- Numerical Solution with a Gradient Walking Method and data treatment simultaneously.
- Approximation Function calculates distance from target.




## ➔Output: Recipe with Ingredients and its Properties




- Each square represents a data column: Recipe and property information
- Simultaneous treatment of all data columns in small steps

# Algorithm used in AI Programming

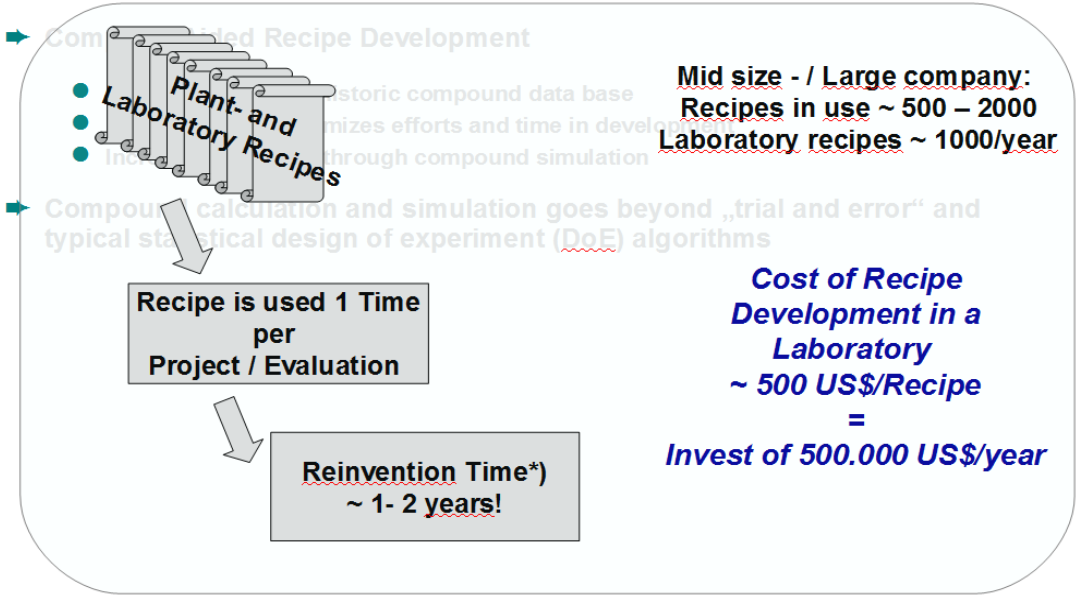
- **k-Means-Algorithm**
  - **Creates cluster, calculates mean (Centroide) reoganization, Iteration**

- **Genetic Algorithm**
  - **Proposed Solution, iteration and mutation towards optimum, selection of results**

- **Neuronal Net**
  - **Complex algorithm (Neuron): Calculation of a weighted sum, normalisation to emphazise or dampen the summands. „Input – Hidden – Output“ layer. Feed Forward Networks / Recurrent Neuronal Networks**

# Compound Database

- **Unorganized**
- **Incomplete**
- **Inhomogeneous**




## Solution

**Inclusion / Exclusion of Recipes from query.**

**Analytical tools for transparency**

**Addition of Data with merger function**

**Confirmation Experiment for Result verification**

➔ **Database created with Statistic Experimental Design (DoE)**

- **Organized / limited size**
- **Variation of few factors according DoE scheme**
- **Optimization, numerical and graphical / prediction Tool available in the software**

➔ **Computer Aided Recipe Development with GrafCompounder using Database created historically**

- **Unorganized / Unlimited**
- **Multiple Factor Query**
- **Compound Simulation according Multi Targets**

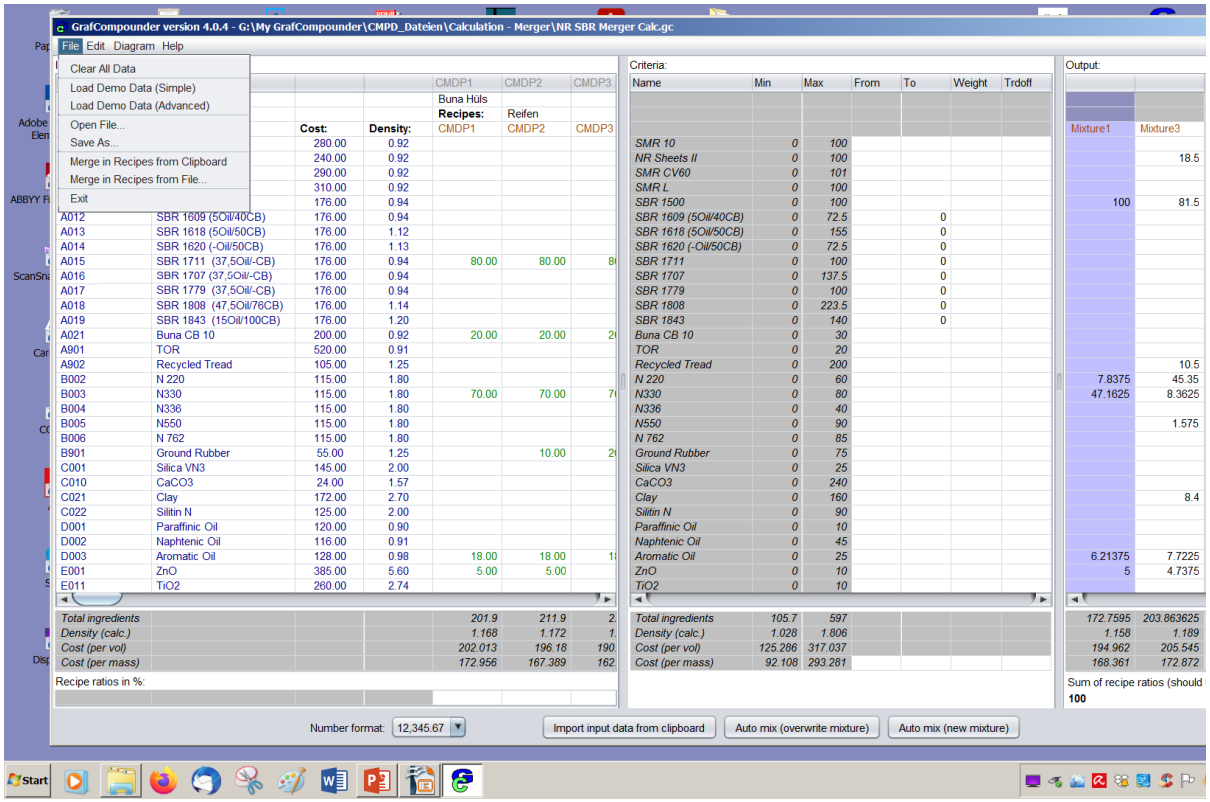
- **Calculation in multiple small steps excludes none linear effects.**
- **Accurate Property Data yield Output in 95% confidence interval.**

# Pull Down Menue

- **Clear all data**
- **Load Demo Data**
  - ✓ **Simple**
  - ✓ **Advanced**
- **Openfile**

***Data.gc File***

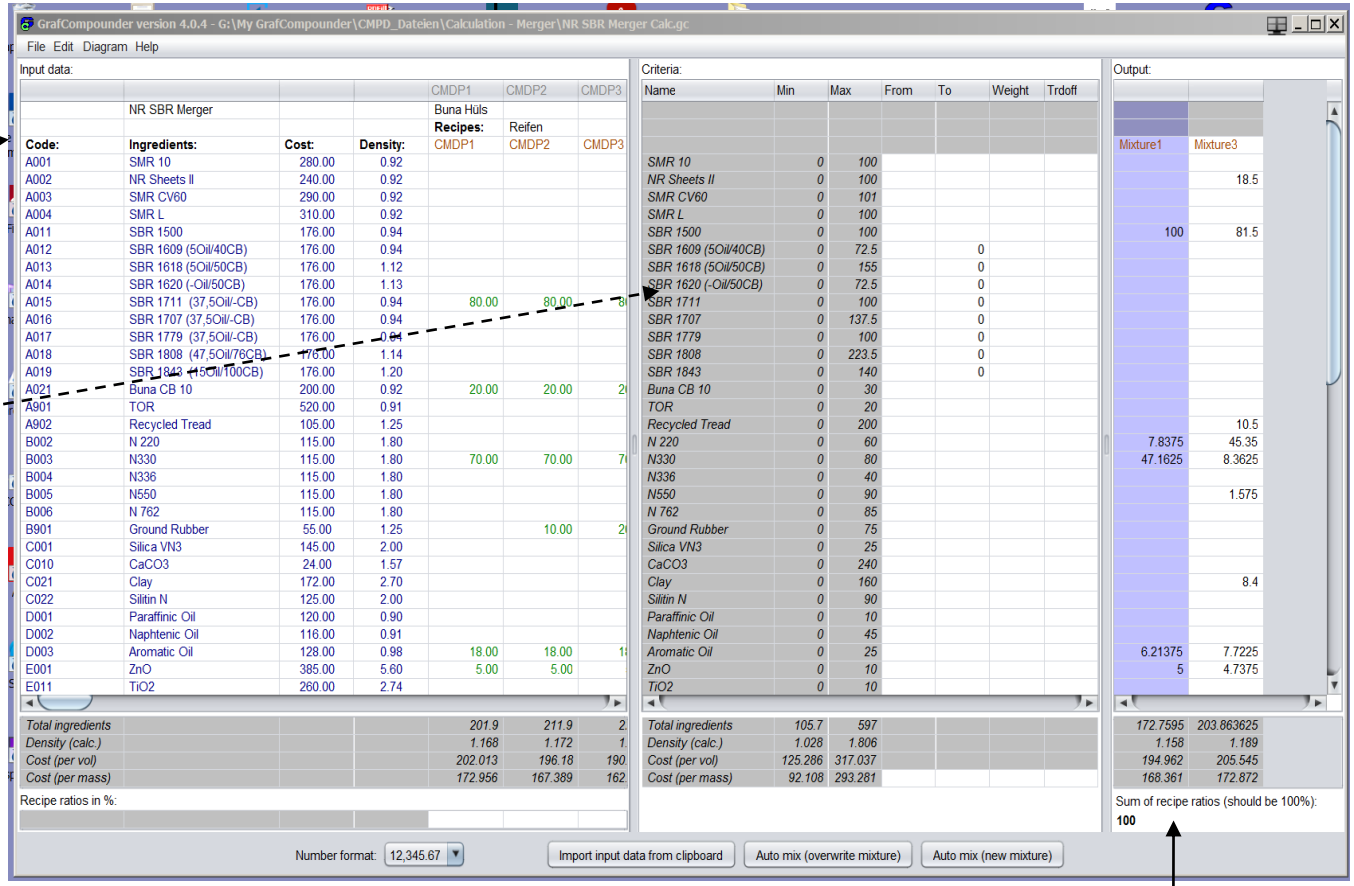
- **Merge Recipes from**
  - ***Clipboard***
  - ***File***
- **Exit**




- **Paste file from any table calculation program with Button: *Import Data from Clipboard***

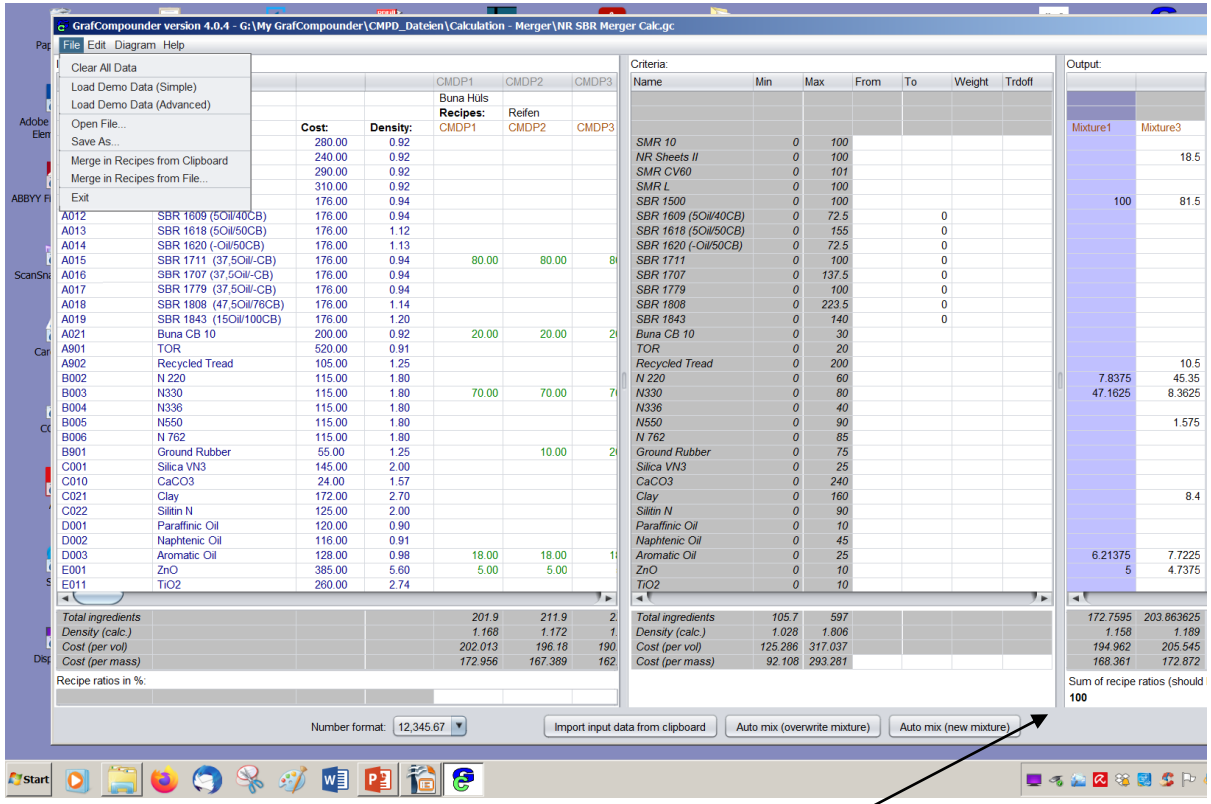
## GrafCompounder Screen

- **Data field**
  - Code
  - Ingredient name
  - Cost information
  - Density
- **Criteria field**
  - Min/Max Value
  - Query column:
    - From
    - To
    - Weight
    - TrdOff
- **Output field**



# Information Area

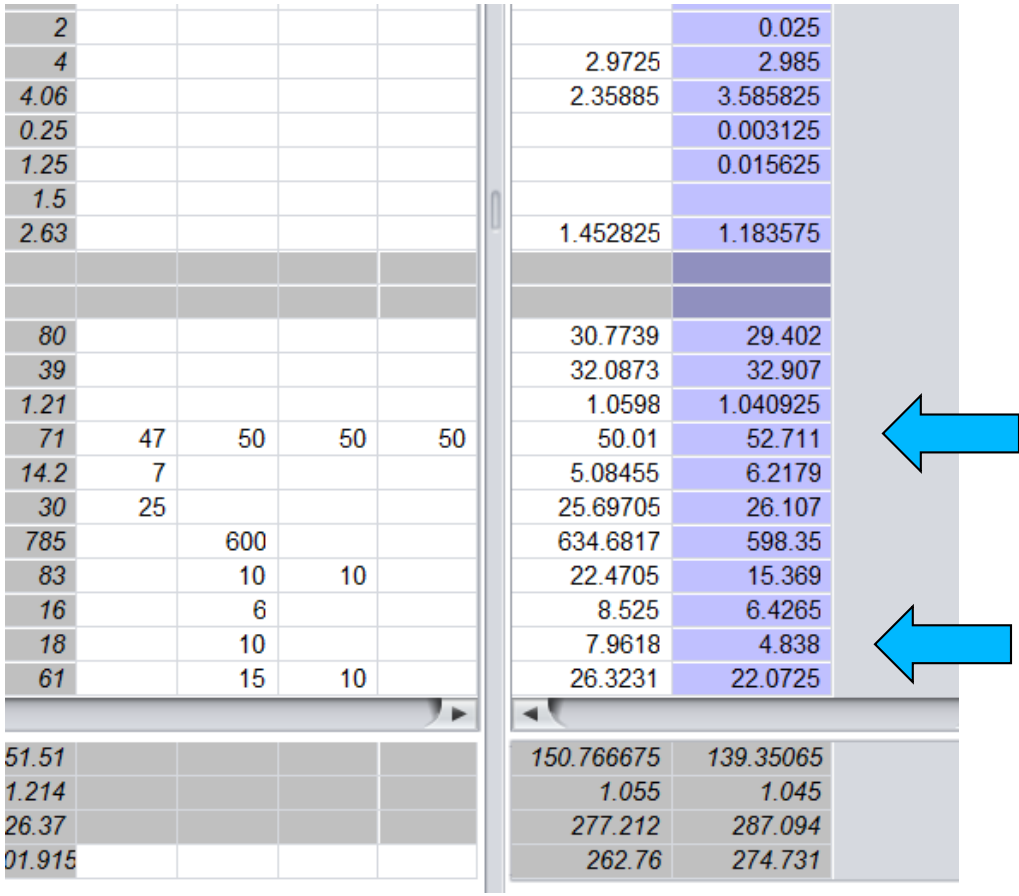
- **Total Sum of Ingredients**
- **Density (calc)**
  **According to density information in Column**
- **Cost (per volume)**
- ***Cost (per mass)***
- ***Recipe ratio in %***




***Control: Sum of recipes used for calculation should be always 100%.***

# How to do a query:

1. **Ingredients**
   **Exclude with target = 0**
2. **Properties**
   - ✓ **Target from Min value to Max value**
   - ✓ **Put a weight on property target,**
     **if more important than others**
   - ✓ **In case of conflicting target:**
     **Give a preference with Trdoff:**
     **Back off a bit from the target in favour**
     **of others**



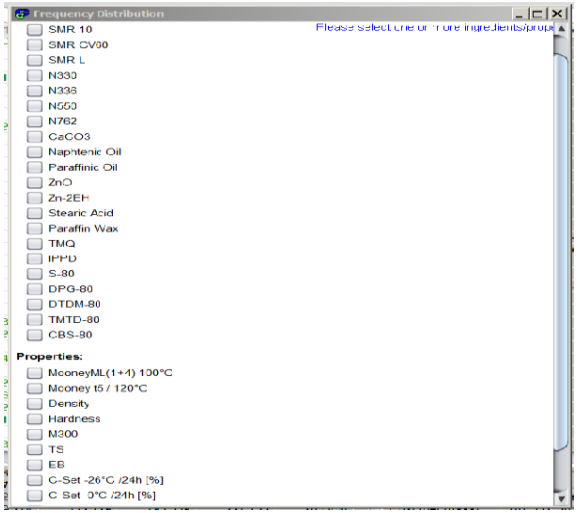
| | | | | | | |
|---|---|---|---|---|---|---|
| 2 | | | | | | 0.025 |
| 4 | | | | | 2.9725 | 2.985 |
| 4.06 | | | | | 2.35885 | 3.585825 |
| 0.25 | | | | | | 0.003125 |
| 1.25 | | | | | | 0.015625 |
| 1.5 | | | | | | |
| 2.63 | | | | | 1.452825 | 1.183575 |
| | | | | | | |
| | | | | | | |
| 80 | | | | | 30.7739 | 29.402 |
| 39 | | | | | 32.0873 | 32.907 |
| 1.21 | | | | | 1.0598 | 1.040925 |
| 71 | 47 | 50 | 50 | 50 | 50.01 | 52.711 |
| 14.2 | 7 | | | | 5.08455 | 6.2179 |
| 30 | 25 | | | | 25.69705 | 26.107 |
| 785 | | 600 | | | 634.6817 | 598.35 |
| 83 | | 10 | 10 | | 22.4705 | 15.369 |
| 16 | | 6 | | | 8.525 | 6.4265 |
| 18 | | 10 | | | 7.9618 | 4.838 |
| 61 | | 15 | 10 | | 26.3231 | 22.0725 |
| 51.51 | | | | | 150.766675 | 139.35065 |
| 1.214 | | | | | 1.055 | 1.045 |
| 26.37 | | | | | 277.212 | 287.094 |
| 01.915 | | | | | 262.76 | 274.731 |

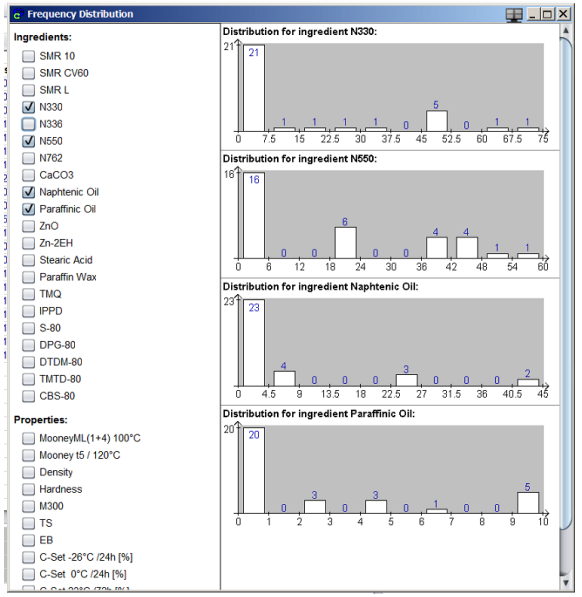
# Database Diagnose Tool

- **Frequency distribution of**
  - **Ingredient**
  - **Property**

  **can be chosen**

- **Scale is automatically selected according**
  **Minimum and Maximum value in the database**

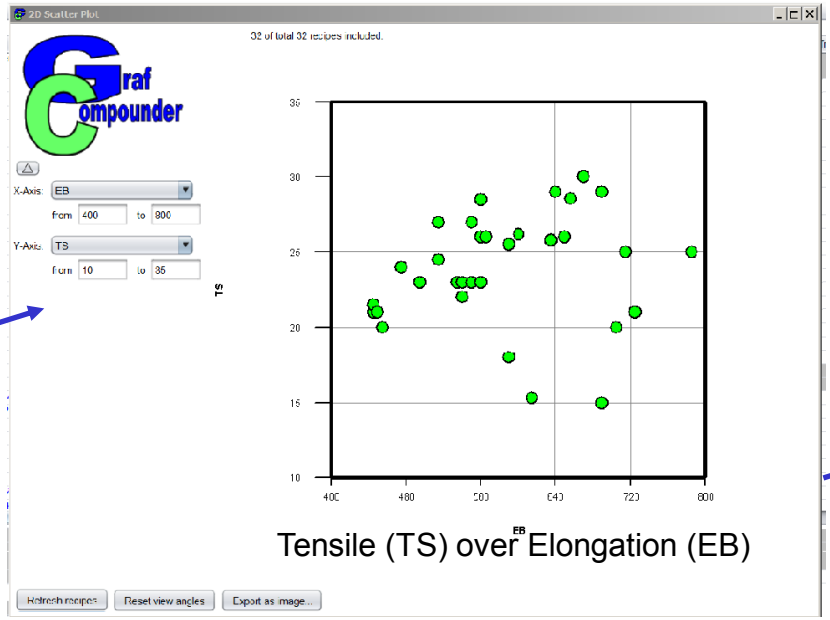


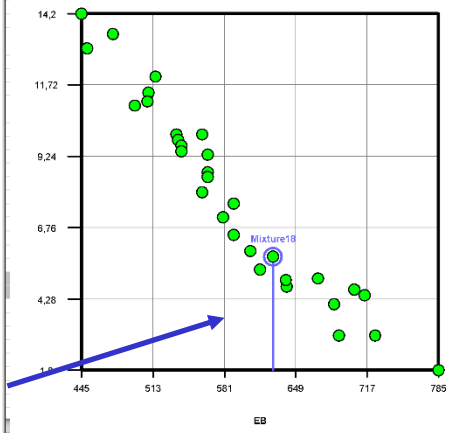
# Database Diagnose Tool

- **Correlation Diagram**


- **Example:**
  **Tensile (TS) over Elongation at Break (EB)**
  - **Scale for axis**
    **Selected**
    **- automatically**
    **or**
    **- manually**
  - **Highlight recipe for evaluation or exclusion**




Tensile (TS) over Elongation (EB)




Modulus M300 over Elongation (EB)

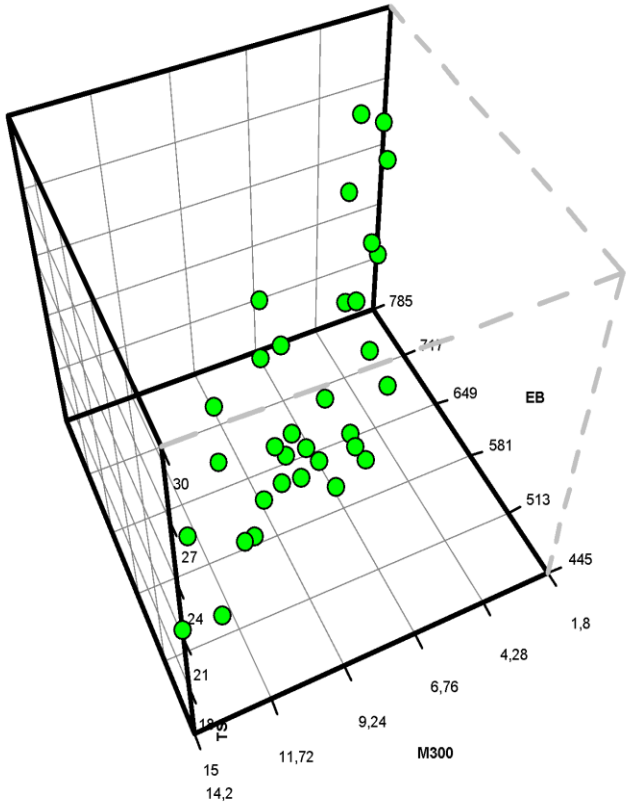
# Database Diagnose Tool

- **3D Correlation Diagram**

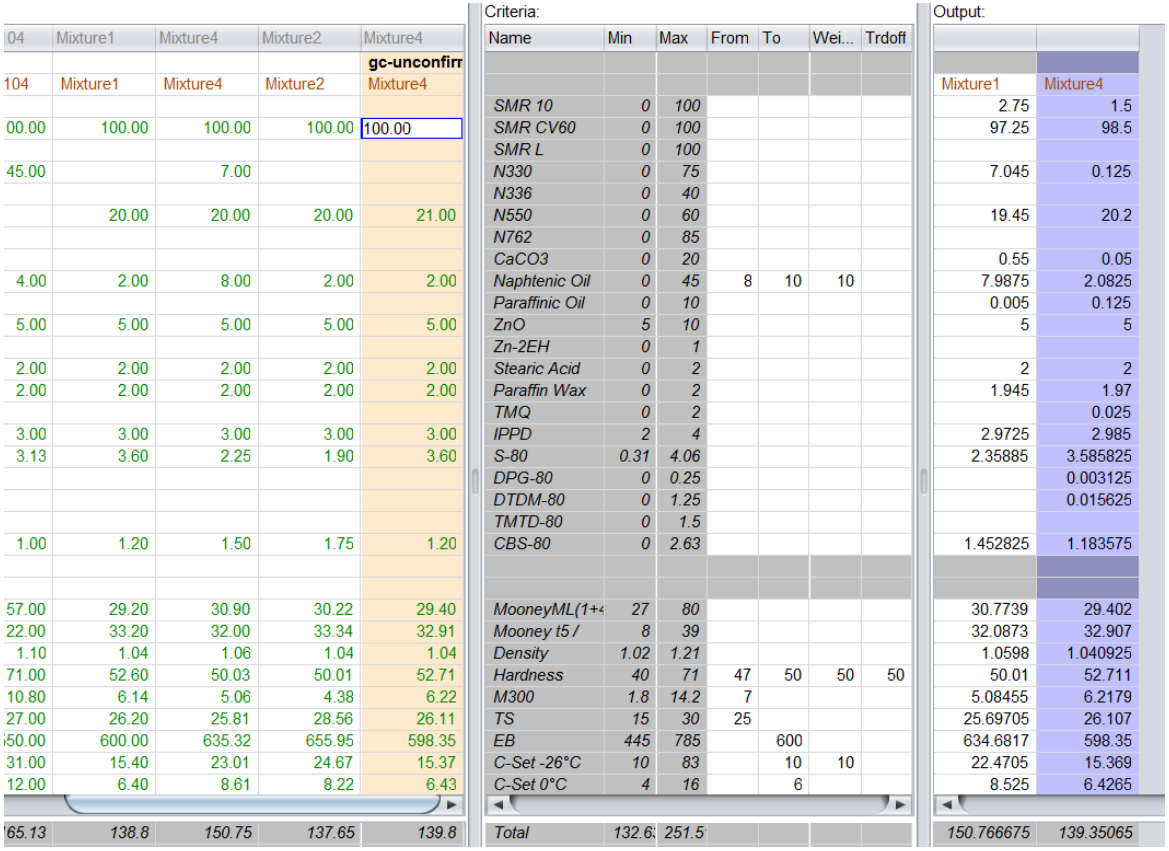
- **Example:**
  - **X- axis: Elongation at Break (EB)**
  - **Y- axis: Modulus 300 (M300)**
  - **Z-axis: Tensile at break (TS)**

  - **Scale for axis: Selected automatically**

    **can be changed manually**



- **Recipe for confirmation experiment**
  - **Append selected recipe in “Input data” field**
    - **It is highlighted as “gc-unconfirmed”**
  - **Eliminate nonsense values and consolidate**
  - **Round values to two decimal places**
- **Confirmation**
  - **Experiment: Change property values to confirmed values**



| 04 | Mixture1 | Mixture4 | Mixture2 | Mixture4 |
|---|---|---|---|---|
| | | | | gc-unconfirr |
| 104 | Mixture1 | Mixture4 | Mixture2 | Mixture4 |
| 00.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| 45.00 | | 7.00 | | |
| | 20.00 | 20.00 | 20.00 | 21.00 |
| 4.00 | 2.00 | 8.00 | 2.00 | 2.00 |
| 5.00 | 5.00 | 5.00 | 5.00 | 5.00 |
| 2.00 | 2.00 | 2.00 | 2.00 | 2.00 |
| 2.00 | 2.00 | 2.00 | 2.00 | 2.00 |
| 3.00 | 3.00 | 3.00 | 3.00 | 3.00 |
| 3.13 | 3.60 | 2.25 | 1.90 | 3.60 |
| 1.00 | 1.20 | 1.50 | 1.75 | 1.20 |
| 57.00 | 29.20 | 30.90 | 30.22 | 29.40 |
| 22.00 | 33.20 | 32.00 | 33.34 | 32.91 |
| 1.10 | 1.04 | 1.06 | 1.04 | 1.04 |
| 71.00 | 52.60 | 50.03 | 50.01 | 52.71 |
| 10.80 | 6.14 | 5.06 | 4.38 | 6.22 |
| 27.00 | 26.20 | 25.81 | 28.56 | 26.11 |
| 50.00 | 600.00 | 635.32 | 655.95 | 598.35 |
| 31.00 | 15.40 | 23.01 | 24.67 | 15.37 |
| 12.00 | 6.40 | 8.61 | 8.22 | 6.43 |
| *65.13* | *138.8* | *150.75* | *137.65* | *139.8* |

Criteria:

| Name | Min | Max | From | To | Wei... | Trdoff |
|---|---|---|---|---|---|---|
| *SMR 10* | *0* | *100* | | | | |
| *SMR CV60* | *0* | *100* | | | | |
| *SMR L* | *0* | *100* | | | | |
| *N330* | *0* | *75* | | | | |
| *N336* | *0* | *40* | | | | |
| *N550* | *0* | *60* | | | | |
| *N762* | *0* | *85* | | | | |
| *CaCO3* | *0* | *20* | | | | |
| *Naphtenic Oil* | *0* | *45* | 8 | 10 | 10 | |
| *Paraffinic Oil* | *0* | *10* | | | | |
| *ZnO* | *5* | *10* | | | | |
| *Zn-2EH* | *0* | *1* | | | | |
| *Stearic Acid* | *0* | *2* | | | | |
| *Paraffin Wax* | *0* | *2* | | | | |
| *TMQ* | *0* | *2* | | | | |
| *IPPD* | *2* | *4* | | | | |
| *S-80* | *0.31* | *4.06* | | | | |
| *DPG-80* | *0* | *0.25* | | | | |
| *DTDM-80* | *0* | *1.25* | | | | |
| *TMTD-80* | *0* | *1.5* | | | | |
| *CBS-80* | *0* | *2.63* | | | | |
| *MooneyML(1+* | *27* | *80* | | | | |
| *Mooney t5 /* | *8* | *39* | | | | |
| *Density* | *1.02* | *1.21* | | | | |
| *Hardness* | *40* | *71* | 47 | 50 | 50 | 50 |
| *M300* | *1.8* | *14.2* | 7 | | | |
| *TS* | *15* | *30* | 25 | | | |
| *EB* | *445* | *785* | | 600 | | |
| *C-Set -26°C* | *10* | *83* | | 10 | 10 | |
| *C-Set 0°C* | *4* | *16* | | 6 | | |
| *Total* | *132.6* | *251.5* | | | | |

Output:

| Mixture1 | Mixture4 |
|---|---|
| 2.75 | 1.5 |
| 97.25 | 98.5 |
| 7.045 | 0.125 |
| 19.45 | 20.2 |
| 0.55 | 0.05 |
| 7.9875 | 2.0825 |
| 0.005 | 0.125 |
| 5 | 5 |
| 2 | 2 |
| 1.945 | 1.97 |
| | 0.025 |
| 2.9725 | 2.985 |
| 2.35885 | 3.585825 |
| | 0.003125 |
| | 0.015625 |
| 1.452825 | 1.183575 |
| 30.7739 | 29.402 |
| 32.0873 | 32.907 |
| 1.0598 | 1.040925 |
| 50.01 | 52.711 |
| 5.08455 | 6.2179 |
| 25.69705 | 26.107 |
| 634.6817 | 598.35 |
| 22.4705 | 15.369 |
| 8.525 | 6.4265 |
| *150.766675* | *139.35065* |

## Confirmation experiments

- **To proove calculation of recipe using a database or even historic data from literature three experiments were coosen**
  - **Recalculation of Filler / Oil DoE (Cabot Compounding Tables)**
  - **EPDM ENB / Accelerator DoE recalculation (published by DuPont 1998) for optimum ENB content and None n-nitrosamine Acceleratorsystem**
  -

# Properties of MB is determined by Polymer, CB and Oil content and the ratio or CB and Oil.

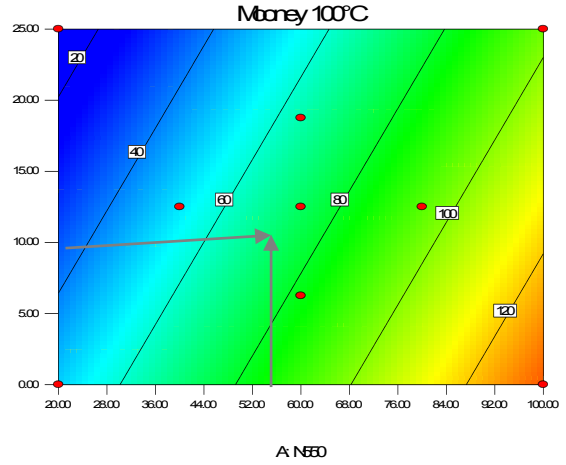
- Unit 2 as a reference (based on Cabot TG RG-135
- …

- CB 550: 55 phr
- Oil: 10 phr

- Mooney Viscosity: 71 M-Units
- Hardness: 60 ° ShA
- Tensile: 21 MPa
- Elongation: 460 %
- C-Set: 28%

**NR Compound**

- *SMR 5CV – 100 phr*
- *CB – Var*
- *Oil – Var*
- *ZnO – 5 phr*
- *StAc – 1 phr*
- *AO – 1 phr*
- *NR 100 phr*
- *MBTS – 0.6*
- *S – 2.5 phr*



# Calculation method confirmation

- **Prove with**
  1. **NR Filler / Oil DoE – most of basic physicals are linear**
  2. **Filler / Oil DoE**
  3. **Accelerator DoE**

**DoE with 4 Factors**

**Polymer used: EPDM (Vistalon 8600)**

1.

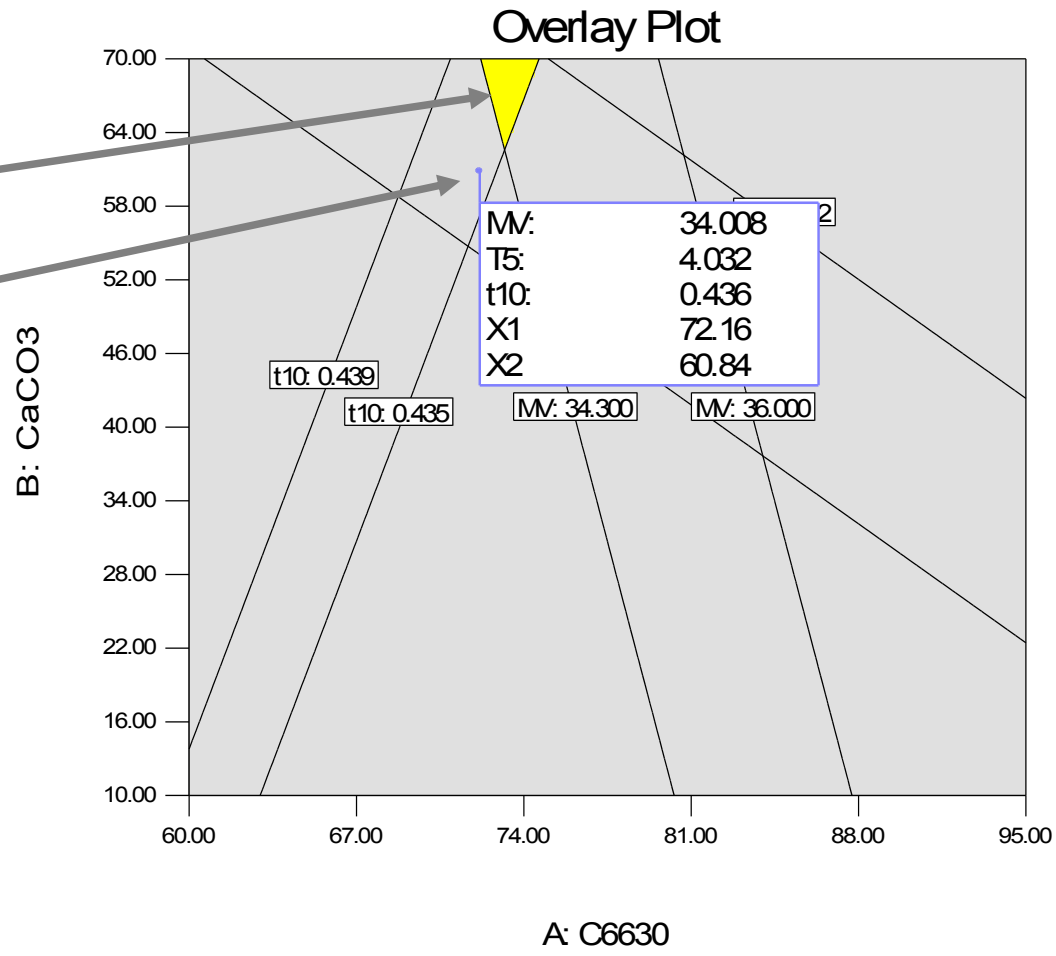
| Factor | Name | Units | Min | Max |
|---|---|---|---|---|
| A | C6630 | phr | 60.00 | 95.00 |
| B | CaCO3 | phr | 10.00 | 70.00 |
| C | Clay | phr | 10.00 | 50.00 |
| D | Oil | phr | 70.00 | 95.00 |

- **A fractional factorial DoE with 11 compounds only!**

**Optimization area calculated with Design Expert**

**Solution given by GrafCompounder**

**with the additional condition (CC 6630 – 73 phr)**



**2.**

**DoE published by DuPont Dow in 1998**

- **Factors: ENB, DTDC, S, MBT, TiTBD, ZdiBC, DTP**
- **DoE with 41 Experiments**

**Tensile at break is significant with linear model**

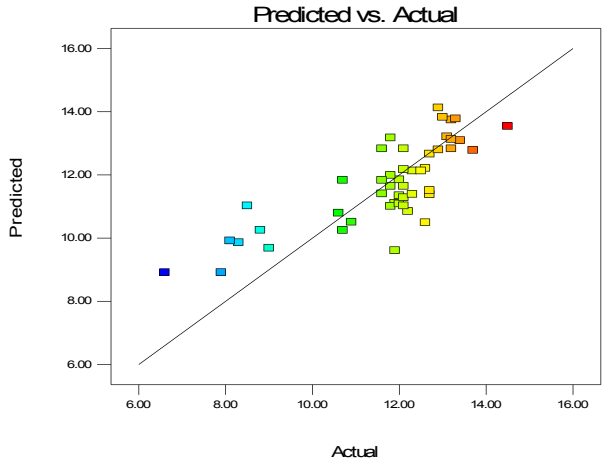
- **Sulfur has larger influence followed by DTDC and TiBTD, but negative**

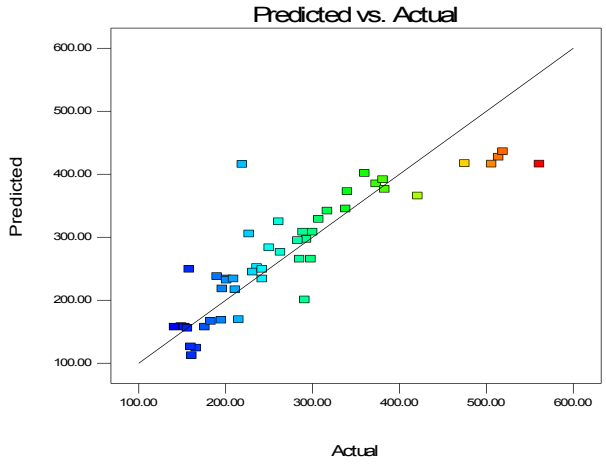
**Elongation is significant with quadratic model, but linear model is a more than sufficient fit**

- **Sulfur has the largest influence followed by DTDC**

**Hardness is sufficient significant with linear model as well**

- **Main influence Sulfur, DTDC**



- **Boundary Conditions**
  - **Select boundaries**

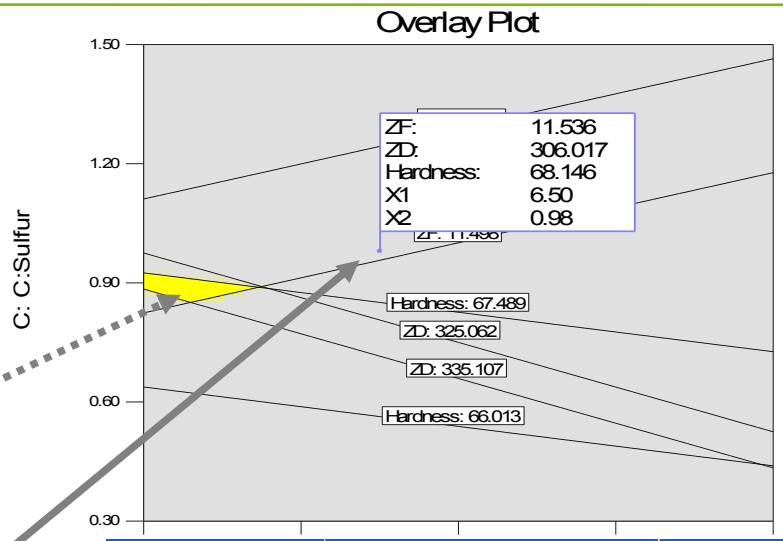
**ZF-MPa : 11.5-12.0**

**ZD-% : 325-335**

**H-° ShA : 65-67**

**The Design Expert optimization graph shows the location of the result as a yellow area, but**

**GrafCompounder result is tagged with a flag.**




| Ingredients | GrafCompounder | Design Expert® |
|---|---|---|
| ENB | 6.5 | 5.45 |
| C:Sulfur | 0.93 | 0.88 |
| B:DTDC | 0.98 | 0.98 |
| D:MBT | 1 | 1 |
| E:TiBTD | 1.51 | 1.51 |
| F:ZDiBC | 1.33 | 1.33 |
| G:DTP | 1.45 | 1.44 |
| ZF | 11.5 | 11.5 |
| ZD | 325 | 330 |
| Hardness | 67 | 67.5 |


25

3.

# Simulation of a DoE

- Experiments made in the Laboratory
  - NR based Compound — LL — UL
    - Filler 1: CB 336 — 30 phr — 70 phr
    - Filler 2: CB 550 — 0 phr — 20 phr
    - Naphtenic Oil: — 5 phr — 45 phr
  - Type of DoE: fractonal factorial
  - Software: Design Expert®
- Calculation made with GrafCompounder
  - Database: NR Formula index from MRPRA

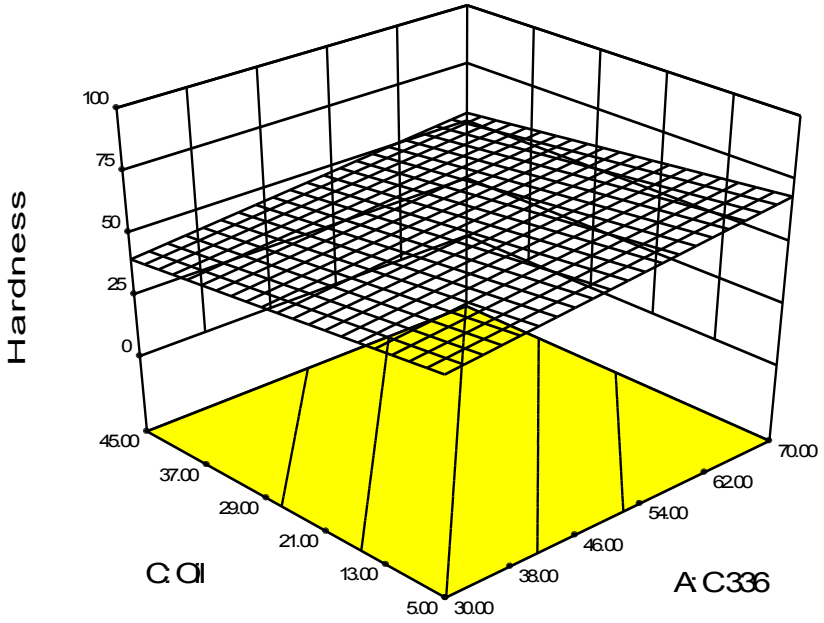
★ For comparison: Hardness, Tensile - / Elongation at break

# Hardness:

**X1 – A: CB 336**

**X2 = C: Napht oil**

**B: CB 550 = 10.00 phr**

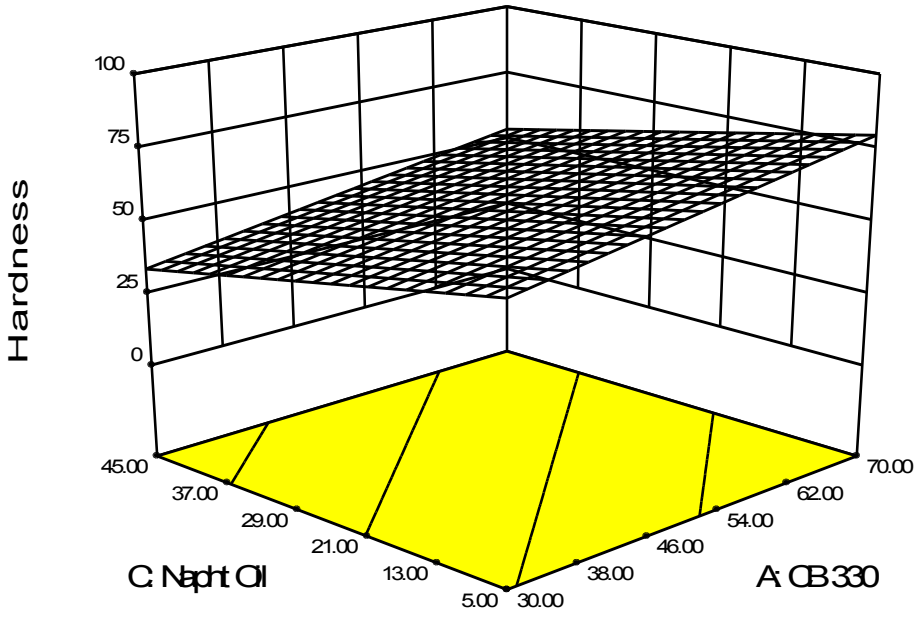



# Hardness Simulation

X1 – A: CB 330

X2 = C: Napht oil

B: CB 550 = 10.00 phr

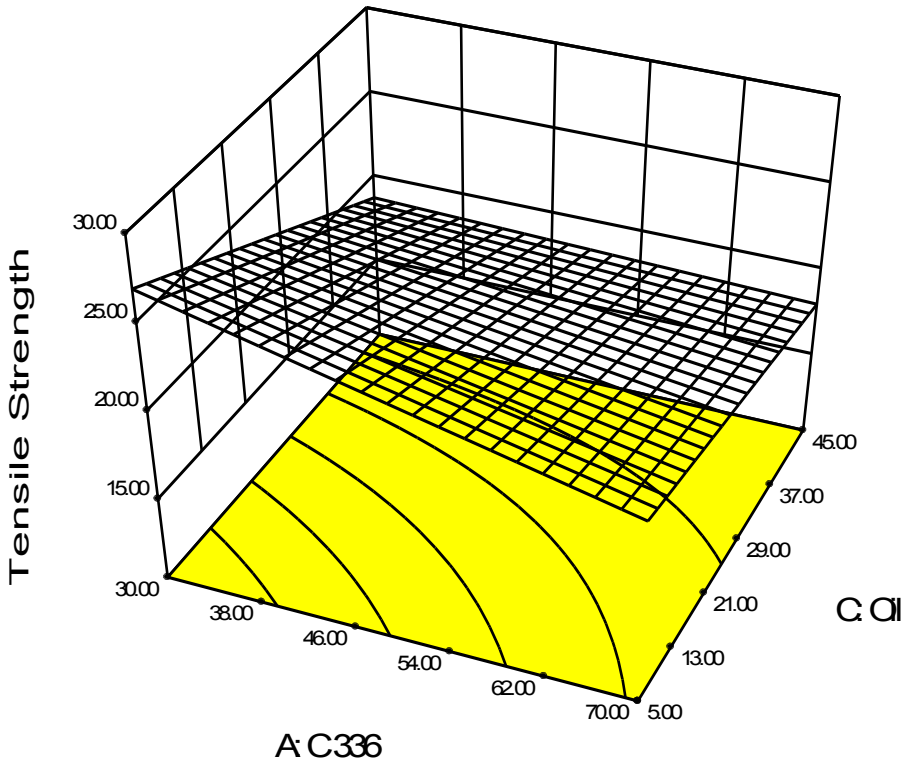


# Tensile at break:

**X1 – A: CB 336**

**X2 = C: Napht oil**

**B: CB 550 = 10.00 phr**

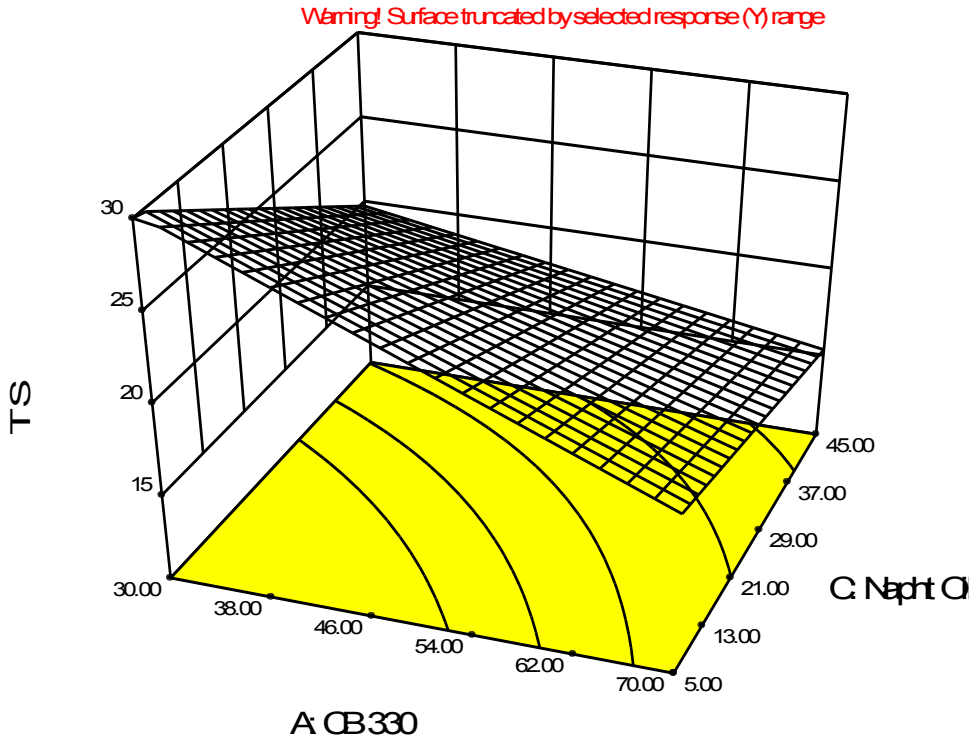



# Tensile at break Simulation

X1 – A: CB 330

X2 = C: Napht oil

B: CB 550 = 10.00 phr

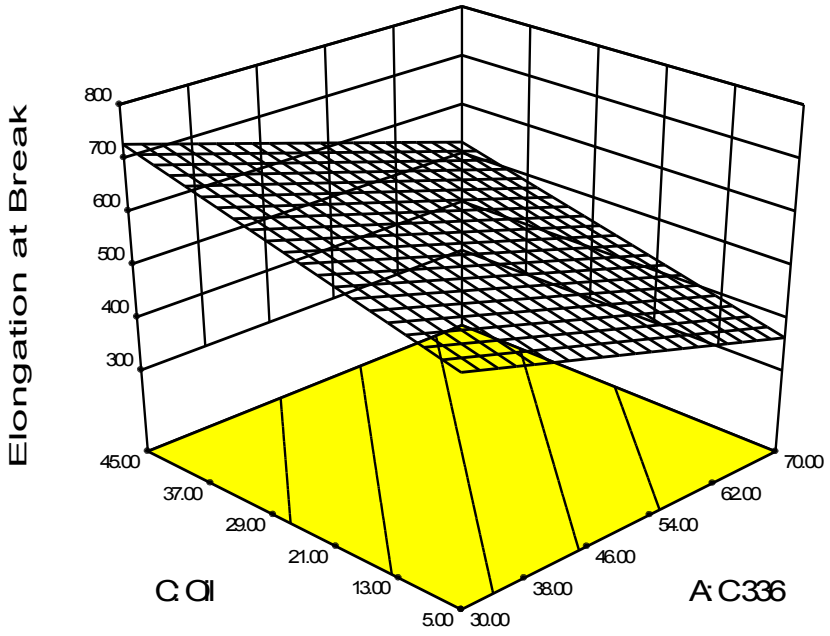


# Elongation at break:

**X1 – A: CB 336**

**X2 = C: Napht oil**

**B: CB 550 = 10.00 phr**

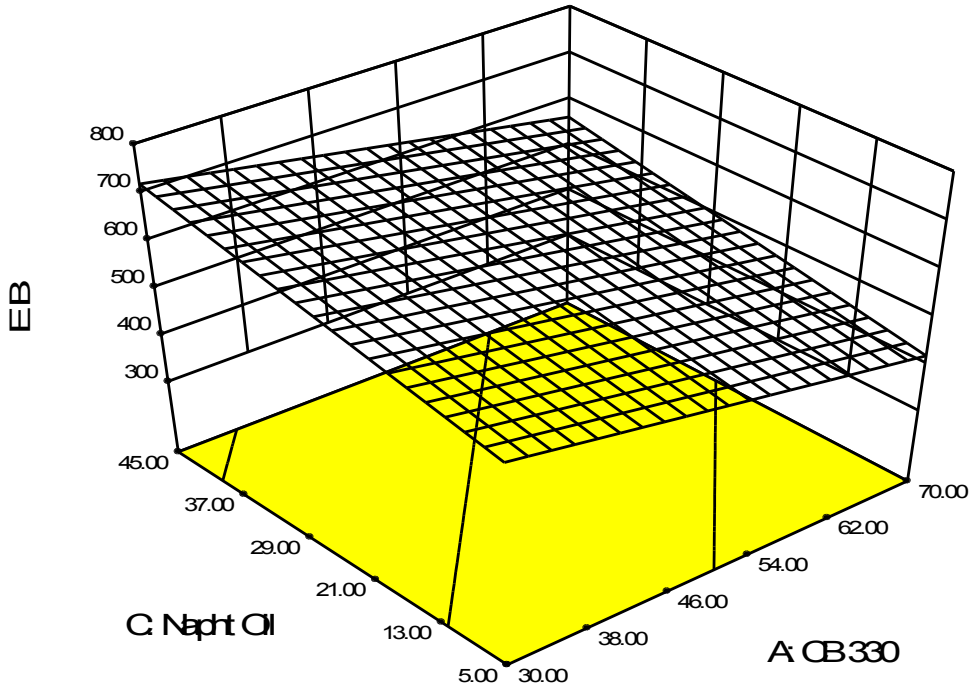



# Elongation at break Simulation

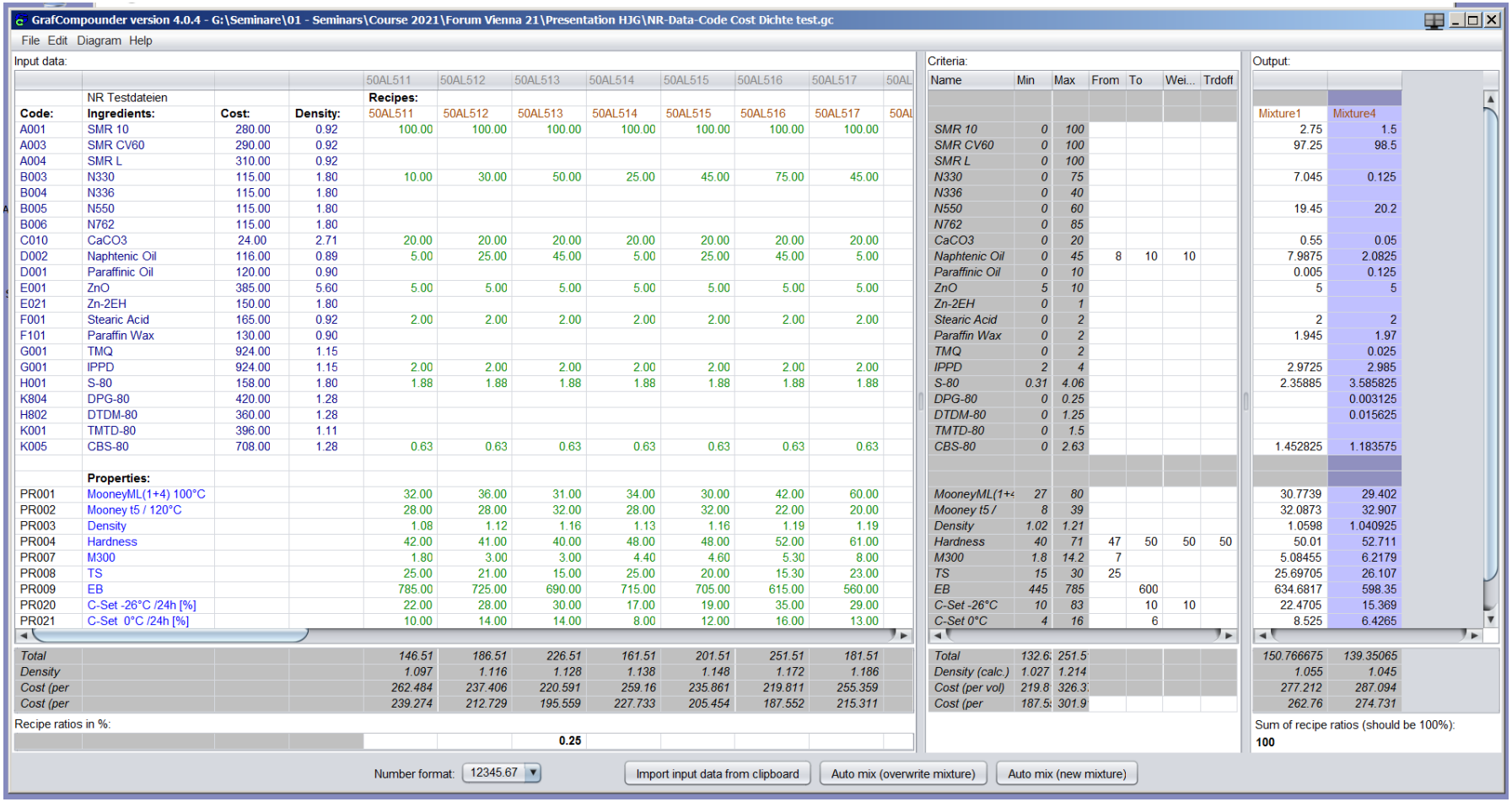
X1 – A: CB 330

X2 = C: Napht oil

B: CB 550 = 10.00 phr



## ➔ Screenshot of GrafCompounder with demo data, targets and a calculated compound



GrafCompounder version 4.0.4 - G:\Seminare\01 - Seminars\Course 2021\Forum Vienna 21\Presentation HJG\NR-Data-Code Cost Dichte test.gc

File Edit Diagram Help

Input data:

| | | | | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | NR Testdateien | | | **Recipes:** | | | | | | | |
| **Code:** | **Ingredients:** | **Cost:** | **Density:** | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL |
| A001 | SMR 10 | 280.00 | 0.92 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | |
| A003 | SMR CV60 | 290.00 | 0.92 | | | | | | | | |
| A004 | SMR L | 310.00 | 0.92 | | | | | | | | |
| B003 | N330 | 115.00 | 1.80 | 10.00 | 30.00 | 50.00 | 25.00 | 45.00 | 75.00 | 45.00 | |
| B004 | N336 | 115.00 | 1.80 | | | | | | | | |
| B005 | N550 | 115.00 | 1.80 | | | | | | | | |
| B006 | N762 | 115.00 | 1.80 | | | | | | | | |
| C010 | CaCO3 | 24.00 | 2.71 | 20.00 | 20.00 | 20.00 | 20.00 | 20.00 | 20.00 | 20.00 | |
| D002 | Naphtenic Oil | 116.00 | 0.89 | 5.00 | 25.00 | 45.00 | 5.00 | 25.00 | 45.00 | 5.00 | |
| D001 | Paraffinic Oil | 120.00 | 0.90 | | | | | | | | |
| E001 | ZnO | 385.00 | 5.60 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | |
| E021 | Zn-2EH | 150.00 | 1.80 | | | | | | | | |
| F001 | Stearic Acid | 165.00 | 0.92 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | |
| F101 | Paraffin Wax | 130.00 | 0.90 | | | | | | | | |
| G001 | TMQ | 924.00 | 1.15 | | | | | | | | |
| G001 | IPPD | 924.00 | 1.15 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | 2.00 | |
| H001 | S-80 | 158.00 | 1.80 | 1.88 | 1.88 | 1.88 | 1.88 | 1.88 | 1.88 | 1.88 | |
| K804 | DPG-80 | 420.00 | 1.28 | | | | | | | | |
| H802 | DTDM-80 | 360.00 | 1.28 | | | | | | | | |
| K001 | TMTD-80 | 396.00 | 1.11 | | | | | | | | |
| K005 | CBS-80 | 708.00 | 1.28 | 0.63 | 0.63 | 0.63 | 0.63 | 0.63 | 0.63 | 0.63 | |
| | | | | | | | | | | | |
| | **Properties:** | | | | | | | | | | |
| PR001 | MooneyML(1+4) 100°C | | | 32.00 | 36.00 | 31.00 | 34.00 | 30.00 | 42.00 | 60.00 | |
| PR002 | Mooney t5 / 120°C | | | 28.00 | 28.00 | 32.00 | 28.00 | 32.00 | 22.00 | 20.00 | |
| PR003 | Density | | | 1.08 | 1.12 | 1.16 | 1.13 | 1.16 | 1.19 | 1.19 | |
| PR004 | Hardness | | | 42.00 | 41.00 | 40.00 | 48.00 | 48.00 | 52.00 | 61.00 | |
| PR007 | M300 | | | 1.80 | 3.00 | 3.00 | 4.40 | 4.60 | 5.30 | 8.00 | |
| PR008 | TS | | | 25.00 | 21.00 | 15.00 | 25.00 | 20.00 | 15.30 | 23.00 | |
| PR009 | EB | | | 785.00 | 725.00 | 690.00 | 715.00 | 705.00 | 615.00 | 560.00 | |
| PR020 | C-Set -26°C /24h [%] | | | 22.00 | 28.00 | 30.00 | 17.00 | 19.00 | 35.00 | 29.00 | |
| PR021 | C-Set 0°C /24h [%] | | | 10.00 | 14.00 | 14.00 | 8.00 | 12.00 | 16.00 | 13.00 | |
| *Total* | | | | *146.51* | *186.51* | *226.51* | *161.51* | *201.51* | *251.51* | *181.51* | |
| *Density* | | | | *1.097* | *1.116* | *1.128* | *1.138* | *1.148* | *1.172* | *1.186* | |
| *Cost (per* | | | | *262.484* | *237.406* | *220.591* | *259.16* | *235.861* | *219.811* | *255.359* | |
| *Cost (per* | | | | *239.274* | *212.729* | *195.559* | *227.733* | *205.454* | *187.552* | *215.311* | |

Recipe ratios in %:

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | **0.25** | | | | | |

Criteria:

| Name | Min | Max | From | To | Wei... | Trdoff |
|---|---|---|---|---|---|---|
| *SMR 10* | *0* | *100* | | | | |
| *SMR CV60* | *0* | *100* | | | | |
| *SMR L* | *0* | *100* | | | | |
| *N330* | *0* | *75* | | | | |
| *N336* | *0* | *40* | | | | |
| *N550* | *0* | *60* | | | | |
| *N762* | *0* | *85* | | | | |
| *CaCO3* | *0* | *20* | | | | |
| *Naphtenic Oil* | *0* | *45* | 8 | 10 | 10 | |
| *Paraffinic Oil* | *0* | *10* | | | | |
| *ZnO* | *5* | *10* | | | | |
| *Zn-2EH* | *0* | *1* | | | | |
| *Stearic Acid* | *0* | *2* | | | | |
| *Paraffin Wax* | *0* | *2* | | | | |
| *TMQ* | *0* | *2* | | | | |
| *IPPD* | *2* | *4* | | | | |
| *S-80* | *0.31* | *4.06* | | | | |
| *DPG-80* | *0* | *0.25* | | | | |
| *DTDM-80* | *0* | *1.25* | | | | |
| *TMTD-80* | *0* | *1.5* | | | | |
| *CBS-80* | *0* | *2.63* | | | | |
| *MooneyML(1+* | *27* | *80* | | | | |
| *Mooney t5 /* | *8* | *39* | | | | |
| *Density* | *1.02* | *1.21* | | | | |
| *Hardness* | *40* | *71* | 47 | 50 | 50 | 50 |
| *M300* | *1.8* | *14.2* | 7 | | | |
| *TS* | *15* | *30* | 25 | | | |
| *EB* | *445* | *785* | | 600 | | |
| *C-Set -26°C* | *10* | *83* | | 10 | 10 | |
| *C-Set 0°C* | *4* | *16* | | 6 | | |
| *Total* | *132.6* | *251.5* | | | | |
| *Density (calc.)* | *1.027* | *1.214* | | | | |
| *Cost (per vol)* | *219.8* | *326.3* | | | | |
| *Cost (per* | *187.5* | *301.9* | | | | |

Output:

| Mixture1 | Mixture4 |
|---|---|
| 2.75 | 1.5 |
| 97.25 | 98.5 |
| | |
| 7.045 | 0.125 |
| | |
| 19.45 | 20.2 |
| | |
| 0.55 | 0.05 |
| 7.9875 | 2.0825 |
| 0.005 | 0.125 |
| 5 | 5 |
| | |
| 2 | 2 |
| 1.945 | 1.97 |
| | 0.025 |
| 2.9725 | 2.985 |
| 2.35885 | 3.585825 |
| | 0.003125 |
| | 0.015625 |
| | |
| 1.452825 | 1.183575 |
| | |
| 30.7739 | 29.402 |
| 32.0873 | 32.907 |
| 1.0598 | 1.040925 |
| 50.01 | 52.711 |
| 5.08455 | 6.2179 |
| 25.69705 | 26.107 |
| 634.6817 | 598.35 |
| 22.4705 | 15.369 |
| 8.525 | 6.4265 |
| *150.766675* | *139.35065* |
| *1.055* | *1.045* |
| *277.212* | *287.094* |
| *262.76* | *274.731* |

Sum of recipe ratios (should be 100%):
**100**

Number format: 12345.67 | Import input data from clipboard | Auto mix (overwrite mixture) | Auto mix (new mixture)

## Compound Simulation with GrafCompounder

- Creation of a formula with multiple criteria query including
  - Ingredients
  - Properties
- Traceability back to formulas used in calculation
  - Analysis of outliers and their correction or elimination in the database is possible.
  - Integration of results from statistical experimental designs to improve database
  - Merger of databases of different origin
    - either with copy / import
    - Merger of data.gc files

## Result of simulation MUST be confirmed by an experiment.

- Probability of a match between calculation and confirmation experiment result is about 90-5% according first experience

## Summary:

- **The resulting formulas calculated are inline with general rules of compounding**
  - **Differences with calculations based on regression is marginal**
- **Only one confirmation experiment would be needed as opposed to multiple trials in case of development targets.**
- **Area of use / advantage**
  - **Compound Cost estimation**
  - **Starting Formula for Compound Development**
  - **Simulation of Recipe for Specification Adjustments**
  - **Historic Data usage and improved Data storage**

- **New materials have to be evaluated with Statistic Experimental Design**

*More information under:* www.grafcompounder.com

➔ **Release of the „GrafCompounder“ Version 4.04 June 2021**

➔ **Upgrades for Owners of Version 3.211 provided for a special price**
**Free upgrade if purchased 2nd half 2020 / 1st half 2021**

**Thank you for joining this presentation.**

➔ **Any question, comment?**

***More information under:*** **www.grafcompounder.com**