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# **GrafCompounder 2.004**

**Working with the  
“GrafCompounder”  
Program**

**September 2014**

[www.grafcompounder.com](http://www.grafcompounder.com)

# GrafCompounder

- **The “GrafCompounder” is a software program that enables you to create recipes using your own recipe database for rubber, TPE, TP and other compounds, (it must contain ingredients, proportions and measured properties).**

**This software helps you save time and effort in recipe development by:**

- **Allowing for faster and more accurate decisions on starting formulas**

**Contributing to better ideas about further compound development**

**Allowing for use of historic data in compound development**

# GrafCompounder

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**The GrafCompounder uses the Multiple Linear Iteration method [MLI] to calculate a new recipe according to properties targeted.**

**The GrafCompounder enables you to analyze your database and identify faulty compound data.**

**It allows you to identify the ratio of contribution of each compound recipe on the final formulation. This possibility is helpful, if your confirmation test results do not match the results of the calculated compound.**



# GrafCompounder

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**This is a tutorial to familiarize you with the best way to use the “GrafCompounder 2.004” and to show you the program features.**

# Data preparation

The screenshot shows a spreadsheet with the following data:

|                     | 50AL511       | 50AL512       | 50AL513       | 50AL514       | 50AL515       | 50AL516       | 50AL517       | 50AL518       | 50AL542       |
|---------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| <b>Ingredients:</b> |               |               |               |               |               |               |               |               |               |
| NR (SMR - 10)       | 100.00        | 100.00        | 100.00        | 100.00        | 100.00        | 100.00        | 100.00        | 100.00        | 100.00        |
| N330                | 10.00         | 30.00         | 50.00         | 25.00         | 45.00         | 75.00         | 45.00         | 65.00         | 50.00         |
| CaCO <sub>3</sub>   | 20.00         | 20.00         | 20.00         | 20.00         | 20.00         | 20.00         | 20.00         | 20.00         |               |
| Naphtenic Oil       | 5.00          | 25.00         | 45.00         | 5.00          | 25.00         | 45.00         | 5.00          | 25.00         | 10.00         |
| ZnO                 | 5.00          | 5.00          | 5.00          | 5.00          | 5.00          | 5.00          | 5.00          | 5.00          | 5.00          |
| Stearic Acid        | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          |
| IPPD                | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          | 2.00          |
| S                   | 1.50          | 1.50          | 1.50          | 1.50          | 1.50          | 1.50          | 1.50          | 1.50          | 0.25          |
| TMTD - 80           |               |               |               |               |               |               |               |               | 1.00          |
| CBS - 80            | 0.65          | 0.65          | 0.65          | 0.65          | 0.65          | 0.65          | 0.65          | 0.65          | 2.10          |
| <b>Total</b>        | <b>146.15</b> | <b>186.15</b> | <b>226.15</b> | <b>161.15</b> | <b>201.15</b> | <b>251.15</b> | <b>181.15</b> | <b>221.15</b> | <b>172.35</b> |
| <b>Properties:</b>  |               |               |               |               |               |               |               |               |               |
| MooneyML(1+4) 1*    | 32.00         | 36.00         | 31.00         | 34.00         | 30.00         | 42.00         | 60.00         | 39.00         | 41.00         |
| Mooney t5 / 120°C   | 28.00         | 28.00         | 32.00         | 28.00         | 32.00         | 22.00         | 20.00         | 25.00         | 11.00         |
| Density             | 1.08          | 1.12          | 1.16          | 1.13          | 1.16          | 1.19          | 1.19          | 1.20          | 1.11          |
| Hardness            | 42.00         | 41.00         | 40.00         | 48.00         | 48.00         | 52.00         | 61.00         | 61.00         | 59.00         |
| M300                | 1.80          | 3.00          | 3.00          | 4.40          | 4.60          | 5.30          | 8.00          | 7.60          | 9.40          |
| TS                  | 25.00         | 21.00         | 15.00         | 25.00         | 20.00         | 15.30         | 23.00         | 18.00         | 23.00         |
| EB                  | 785.00        | 725.00        | 690.00        | 715.00        | 705.00        | 615.00        | 560.00        | 590.00        | 540.00        |
| DVR -26°C /24h      | 22.00         | 28.00         | 30.00         | 17.00         | 19.00         | 35.00         | 29.00         | 27.00         | 77.00         |
| DVR 0°C /24h        | 10.00         | 14.00         | 14.00         | 8.00          | 12.00         | 16.00         | 13.00         | 12.00         | 16.00         |
| DVR 23°C /72h       | 8.00          | 10.00         | 14.00         | 9.00          | 13.00         | 16.00         | 10.00         | 17.00         | 18.00         |
| DVR 70°C /24h       | 39.00         | 50.00         | 61.00         | 44.00         | 50.00         | 54.00         | 44.00         | 50.00         | 17.00         |

- In any calculation spreadsheet program such as Excel, prepare a data sheet that contains at least 3 formulas with their properties.

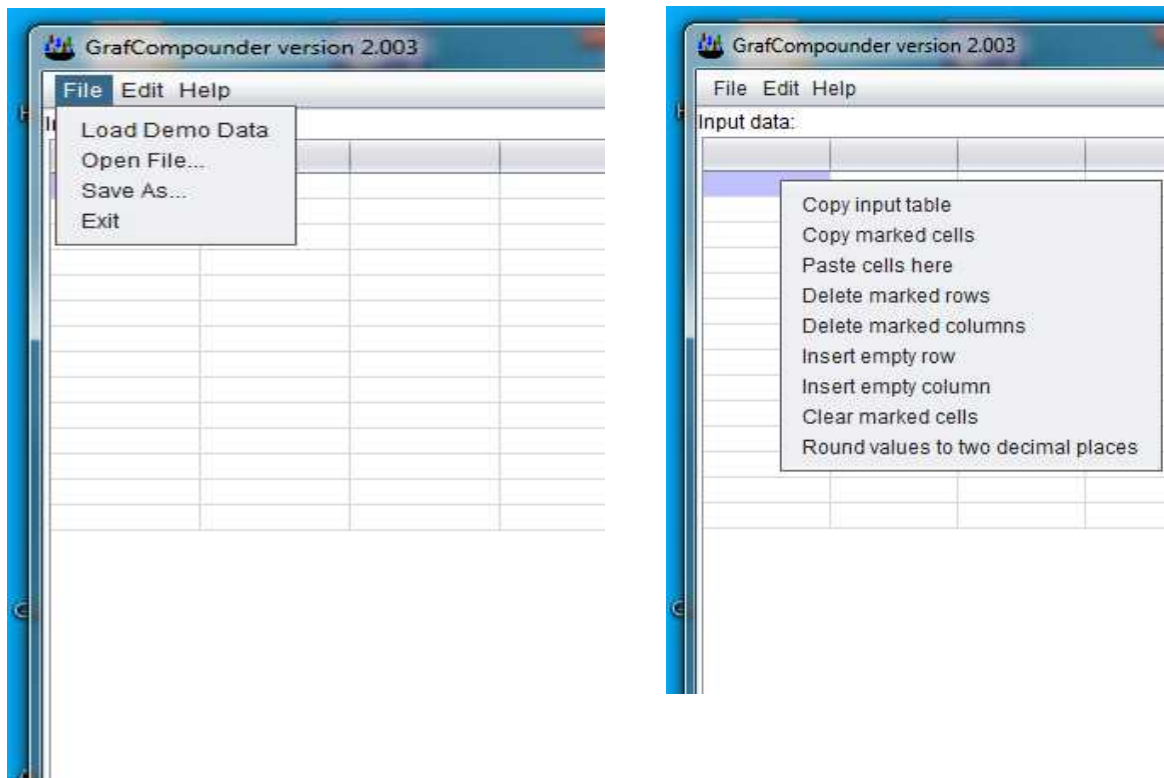
The first column has one cell named “Ingredients:” and one named “Properties:”.

The next column has one cell named “Recipes:” Please insert the required information exactly .

The above example shows how and where to enter formulas and properties.

It is important that the cells highlighted in yellow contains all necessary information. Otherwise, the program will not work.

# Data Transfer



**At this point you need to transfer the data into the GrafCompounder program. There are three options to assign the data:**

- 1) Paste the information from the previous Excel sheet by right clicking to get the short-cut menu or by clicking "Paste Input Data From Clipboard"**
- 2) As an alternative you can "Load test data" in same pull down menu.**
- 3) Open a file previously stored in .gc format. This is a new feature.**

# Data Transfer

The screenshot shows a spreadsheet with the following data:

|                     | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 |
|---------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| <b>Ingredients:</b> |         |         |         |         |         |         |         |         |         |
| NR (SMR - 10)       | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  |
| N330                | 10,00   | 30,00   | 50,00   | 25,00   | 45,00   | 75,00   | 45,00   | 65,00   | 50,00   |
| CaCO3               | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   |         |
| Naphtenic Oil       | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 10,00   |
| ZnO                 | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    |
| Stearic Acid        | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    |
| IPPD                | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    |
| S                   | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 0,25    |
| TMTD - 80           |         |         |         |         |         |         |         |         | 1,00    |
| CBS - 80            | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 2,10    |
| Total               | 146,15  | 186,15  | 226,15  | 161,15  | 201,15  | 251,15  | 181,15  | 221,15  | 172,35  |
| <b>Properties:</b>  |         |         |         |         |         |         |         |         |         |
| MooneyML(1+4) 1*    | 32,00   | 36,00   | 31,00   | 34,00   | 30,00   | 42,00   | 60,00   | 39,00   | 41,00   |
| Mooney t5 / 120°C   | 28,00   | 28,00   | 32,00   | 28,00   | 32,00   | 22,00   | 20,00   | 25,00   | 11,00   |
| Density             | 1,08    | 1,12    | 1,16    | 1,13    | 1,16    | 1,19    | 1,19    | 1,20    | 1,11    |
| Hardness            | 42,00   | 41,00   | 40,00   | 48,00   | 48,00   | 52,00   | 61,00   | 61,00   | 59,00   |
| M300                | 1,80    | 3,00    | 3,00    | 4,40    | 4,60    | 5,30    | 8,00    | 7,60    | 9,40    |
| TS                  | 25,00   | 21,00   | 15,00   | 25,00   | 20,00   | 15,30   | 23,00   | 18,00   | 23,00   |
| EB                  | 785,00  | 725,00  | 690,00  | 715,00  | 705,00  | 615,00  | 560,00  | 590,00  | 540,00  |
| DVR -26°C /24h      | 22,00   | 28,00   | 30,00   | 17,00   | 19,00   | 35,00   | 29,00   | 27,00   | 77,00   |
| DVR 0°C /24h        | 10,00   | 14,00   | 14,00   | 8,00    | 12,00   | 16,00   | 13,00   | 12,00   | 16,00   |
| DVR 23°C /72h       | 8,00    | 10,00   | 14,00   | 9,00    | 13,00   | 16,00   | 10,00   | 17,00   | 18,00   |
| DVR 70°C /24h       | 39,00   | 50,00   | 61,00   | 44,00   | 50,00   | 54,00   | 44,00   | 50,00   | 17,00   |

To use option one: Highlight the compound formula table

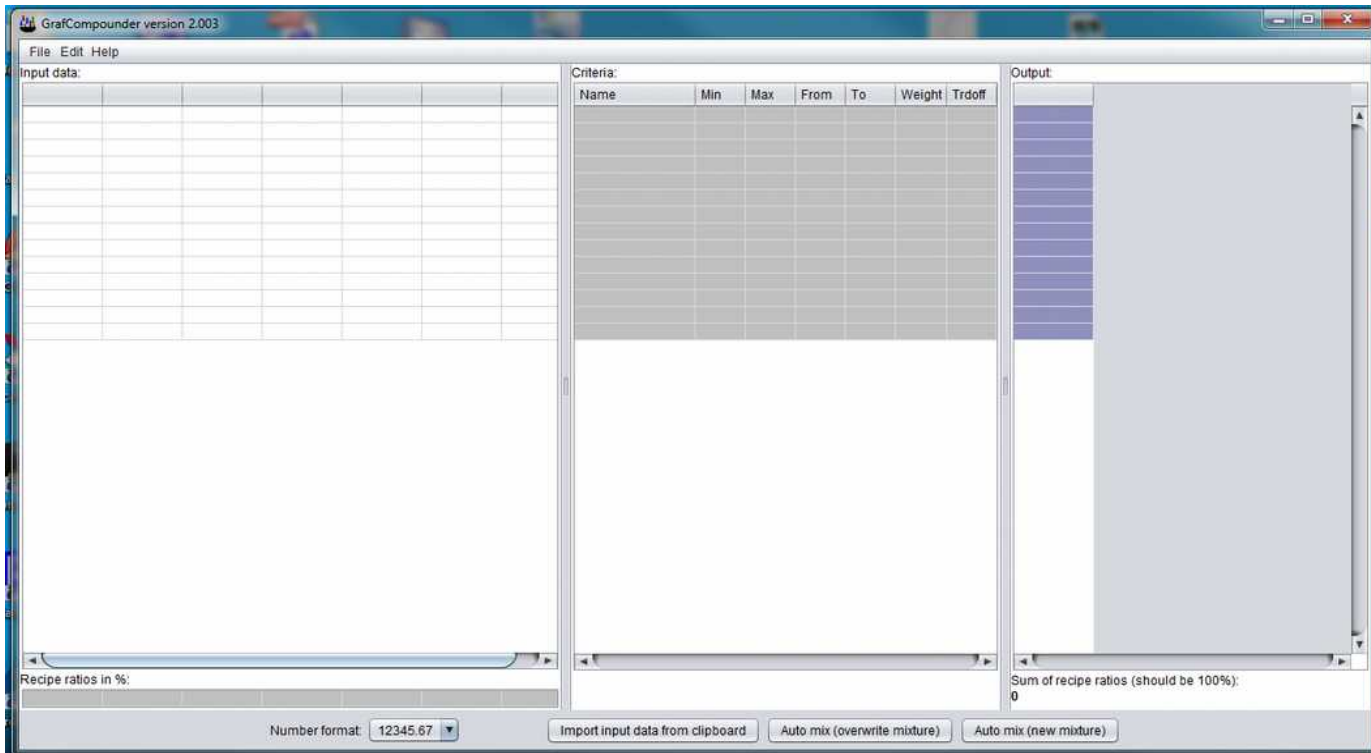
Copy the formula / property table:

Insert the license Dongle into a USB port on your PC/Laptop computer

Once the dongle is in place, open the GrafCompounder program.

- If you try to do this in the reverse order an error message will be displayed.

# Data Transfer



**After insertion of the dongle and start of the GrafCompounder program the screen should appear as shown**



# Data Transfer

The screenshot displays the GrafCompounder software interface. The main window is titled 'GrafCompounder version 2.003' and contains several panels:

- Input data:** A grid showing ingredients and their quantities across various recipes (50AL511 to 50AL542). The data cells are highlighted in yellow.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdoff. The 'Min' and 'Max' columns are empty.
- Output:** A list of ingredients with 'Mixture1' selected.
- Number format:** A dropdown menu at the bottom left is set to '1234,67'.
- Sum of recipe ratios:** A field at the bottom right shows '0', indicating that the ratios are not yet calculated.

**Click Paste and the data is copied into the program**  
**The example above shows the Formula data now inserted into the GrafCompounder.**

**However - the cells are highlighted in yellow. This signifies that no values are currently recognized and can not be used for any calculation.**

**- Min and Max rows are empty!**

**To fix this, the number format needs to be adjusted in the bottom left corner to take into account the fact the data have been input using a comma for the decimal place.**

# Data Transfer

The screenshot shows the GrafCompounder version 2.003 software interface. The main window is titled "GrafCompounder version 2.003" and has a menu bar with "File", "Edit", and "Help". The interface is divided into several sections:

- Input data:** A table with columns for ingredients and rows for various materials. The table is color-coded: ingredients are in red, and properties are in green.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdoff. It lists various materials and their minimum and maximum values.
- Output:** A vertical list of materials, with "Mixture 1" highlighted in blue.
- Recipe ratios in %:** A section at the bottom left with a dropdown menu set to "12345,67".
- Buttons:** "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

The "Input data" table shows the following data (ingredients in red, properties in green):

|                     | 50AL511       | 50AL512       | 50AL513       | 50AL514       | 50AL515       | 50AL516       | 50AL517       | 50AL518       | 50AL542       |
|---------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| <b>Ingredients:</b> |               |               |               |               |               |               |               |               |               |
| NR (SMR - 10)       | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        |
| N330                | 10,00         | 30,00         | 50,00         | 25,00         | 45,00         | 75,00         | 45,00         | 85,00         | 50,00         |
| CaCO3               | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         |
| Naphtenic Oil       | 5,00          | 25,00         | 45,00         | 5,00          | 25,00         | 45,00         | 5,00          | 25,00         | 10,00         |
| ZnO                 | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          |
| Stearic Acid        | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          |
| IPPD                | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          |
| S                   | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 0,25          |
| TMTD - 80           |               |               |               |               |               |               |               |               | 1,00          |
| CBS - 80            | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 2,10          |
| <b>Total</b>        | <b>146,15</b> | <b>186,15</b> | <b>226,15</b> | <b>161,15</b> | <b>201,15</b> | <b>251,15</b> | <b>181,15</b> | <b>221,15</b> | <b>172,35</b> |
| <b>Properties:</b>  |               |               |               |               |               |               |               |               |               |
| MooneyML(1+4) 100°C | 32,00         | 36,00         | 31,00         | 34,00         | 30,00         | 42,00         | 60,00         | 39,00         | 41,00         |
| Mooney t5 / 120°C   | 28,00         | 28,00         | 32,00         | 28,00         | 32,00         | 22,00         | 20,00         | 25,00         | 11,00         |
| Density             | 1,08          | 1,12          | 1,16          | 1,13          | 1,18          | 1,19          | 1,19          | 1,20          | 1,11          |
| Hardness            | 42,00         | 41,00         | 40,00         | 48,00         | 48,00         | 52,00         | 61,00         | 61,00         | 59,00         |
| M300                | 1,80          | 3,00          | 3,00          | 4,40          | 4,60          | 5,30          | 8,00          | 7,60          | 9,40          |
| TS                  | 25,00         | 21,00         | 15,00         | 25,00         | 20,00         | 15,30         | 23,00         | 18,00         | 23,00         |
| EB                  | 785,00        | 725,00        | 690,00        | 715,00        | 705,00        | 615,00        | 560,00        | 590,00        | 540,00        |
| DVR -26°C /24h      | 22,00         | 28,00         | 30,00         | 17,00         | 19,00         | 35,00         | 29,00         | 27,00         | 77,00         |
| DVR 0°C /24h        | 10,00         | 14,00         | 14,00         | 8,00          | 12,00         | 16,00         | 13,00         | 12,00         | 16,00         |
| DVR 23°C /72h       | 8,00          | 10,00         | 14,00         | 9,00          | 13,00         | 16,00         | 10,00         | 17,00         | 18,00         |
| DVR 70°C /24h       | 39,00         | 50,00         | 61,00         | 44,00         | 50,00         | 54,00         | 44,00         | 50,00         | 17,00         |

Once the "Number format" is adjusted to accommodate the comma:

- The recipes now appear red and the properties show as green
- The Min and Max columns show the highest and lowest numbers of the related row.

*Now you are ready for the first calculation if you choose this option*

# Data Transfer

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## Other options for adding data:

- 2) As a second option you can open the GrafCompounder program and hit "Load test data" in the pull down menu.
- 3) A third option is to open the GrafCompounder program and open a file previously stored in .gc format. This is a new feature.

***Now you are ready for the first calculation if you choose these options***

# Data analysis

GrafCompounder version 2.003

File Edit Help

Input data:

|                     | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 |
|---------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| Testdateien         |         |         |         |         |         |         |         |         |         |
| Ingredients:        |         |         |         |         |         |         |         |         |         |
| NR (SMR - 10)       | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  |
| N330                | 10,00   | 30,00   | 50,00   | 25,00   | 45,00   | 75,00   | 45,00   | 65,00   | 50,00   |
| CaCO3               | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   |
| Naphtenic Oil       | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 10,00   |
| ZnO                 | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    |
| Stearic Acid        | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    |
| IPPD                | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    |
| S                   | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 0,25    |
| TMTD - 80           |         |         |         |         |         |         |         |         | 1,00    |
| CBS - 80            | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 2,10    |
| Total               | 146,15  | 186,15  | 226,15  | 161,15  | 201,15  | 251,15  | 181,15  | 221,15  | 172,35  |
| Properties:         |         |         |         |         |         |         |         |         |         |
| MooneyML(1+4) 100°C | 32,00   | 36,00   | 31,00   | 34,00   | 30,00   | 42,00   | 60,00   | 39,00   | 41,00   |
| Mooney I5 / 120°C   | 28,00   | 28,00   | 32,00   | 28,00   | 32,00   | 22,00   | 20,00   | 25,00   | 11,00   |
| Density             | 1,08    | 1,12    | 1,16    | 1,13    | 1,16    | 1,19    | 1,19    | 1,20    | 1,11    |
| Hardness            | 42,00   | 41,00   | 40,00   | 48,00   | 48,00   | 52,00   | 61,00   | 61,00   | 59,00   |
| M300                | 1,80    | 3,00    | 3,00    | 4,40    | 4,60    | 5,30    | 8,00    | 7,60    | 9,40    |
| TS                  | 25,00   | 21,00   | 15,00   | 25,00   | 20,00   | 15,30   | 23,00   | 18,00   | 23,00   |
| EB                  | 785,00  | 725,00  | 690,00  | 715,00  | 705,00  | 615,00  | 560,00  | 590,00  | 540,00  |
| DVR -26°C /24h      | 22,00   | 28,00   | 30,00   | 17,00   | 19,00   | 35,00   | 29,00   | 27,00   | 77,00   |
| DVR 0°C /24h        | 10,00   | 14,00   | 14,00   | 8,00    | 12,00   | 16,00   | 13,00   | 12,00   | 16,00   |
| DVR 23°C /72h       | 8,00    | 10,00   | 14,00   | 9,00    | 13,00   | 16,00   | 10,00   | 17,00   | 18,00   |
| DVR 70°C /24h       | 39,00   | 50,00   | 61,00   | 44,00   | 50,00   | 54,00   | 44,00   | 50,00   | 17,00   |

Criteria:

| Name              | Min    | Max    | From | To | Wel... | Trdoff |
|-------------------|--------|--------|------|----|--------|--------|
| NR (SMR - 10)     | 100    | 100    |      |    |        |        |
| N330              | 10     | 75     | 48   | 52 |        |        |
| CaCO3             | 0      | 20     |      |    |        |        |
| Naphtenic Oil     | 5      | 45     |      |    |        |        |
| ZnO               | 5      | 5      |      |    |        |        |
| Stearic Acid      | 2      | 2      |      |    |        |        |
| IPPD              | 2      | 2      |      |    |        |        |
| S                 | 0,25   | 1,5    |      |    |        |        |
| TMTD - 80         | 0      | 1      |      |    |        |        |
| CBS - 80          | 0,65   | 2,1    |      |    |        |        |
| Total             | 146,15 | 251,15 |      |    |        |        |
| MooneyML(1+4)     | 30     | 60     |      |    |        |        |
| Mooney I5 / 120°C | 11     | 32     |      |    |        |        |
| Density           | 1,08   | 1,2    |      |    |        |        |
| Hardness          | 40     | 61     | 40   | 45 |        |        |
| M300              | 1,8    | 9,4    |      |    |        |        |
| TS                | 15     | 25     |      |    |        |        |
| EB                | 540    | 785    |      |    |        |        |
| DVR -26°C /24h    | 17     | 77     |      |    |        |        |
| DVR 0°C /24h      | 8      | 16     |      |    |        |        |
| DVR 23°C /72h     | 8      | 18     |      |    |        |        |
| DVR 70°C /24h     | 17     | 61     |      |    |        |        |

Output:

Mixture1

Sum of recipe ratios (should be 100%)  
0

Number format: 12345,67

Import input data from clipboard    Auto mix (overwrite mixture)    Auto mix (new mixture)

To begin the analysis, enter a range of values under criteria in the "Ingredients" or "Properties" rows that you wish to match.

The example shows the following criteria:

- Carbon black N 330 from 48 to 52
- Hardness from 40 to 45 Shore A

# Data analysis

The screenshot displays the GrafCompounder version 2.003 software interface. The main window is divided into several sections:

- Input data:** A table with columns for Testdateien (50AL511 to 50AL542) and rows for Ingredients (NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, JPPD, S, TMTD - 80, CBS - 80, Total) and Properties (MooneyML(1+4) 100°C, Mooney 15 / 120°C, Density, Hardness, M300, TS, EB, DVR -26°C /24h, DVR 0°C /24h, DVR 23°C /72h, DVR 70°C /24h).
- Criteria:** A table with columns for Name, Min, Max, From, To, Wel..., and Trdoff. It lists criteria such as NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, JPPD, S, TMTD - 80, and TS.
- Output:** A vertical list on the right side showing 'Mixture 1'.
- Dialog Box:** A central dialog box titled 'Automatic mixing finished, result matches all criteria' with a progress bar and the text 'Score of best mixture so far (lower is better): 0,0000'. It has 'Take this mixture' and 'Cancel' buttons.
- Bottom Panel:** Includes 'Recipe ratios in %', 'Number format: 12345,67', and buttons for 'Import input data from clipboard', 'Auto mix (overwrite mixture)', and 'Auto mix (new mixture)'.

## Click on “auto mix (overwrite mixture)”

- This tells the program to mix and where to place your results in the compounder form.

## The mixture is created

In this example a mixture is found, which satisfies the chosen criteria:

- If all criteria are met the “Score of best mixture so far (lower is better)” will equal 0
- Otherwise the score will be a number greater than 0.

# Data analysis

The screenshot displays the GrafCompounder version 2.003 software interface. It is divided into several sections:

- Input data:** A table with columns for various recipes (50AL511 to 50AL542) and rows for ingredients like NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, and Total.
- Properties:** A table with columns for various properties (MooneyML(1+4) 100°C, Mooney 15 / 120°C, Density, Hardness, M300, TS, EB, DVR -26°C /24h, DVR 0°C /24h, DVR 23°C /72h, DVR 70°C /24h) and rows for the same recipes as in the input data table.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdooff. It lists various criteria like NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, Total, MooneyML(1+4), Mooney 15 / 120°C, Density, Hardness, M300, TS, EB, DVR -26°C /24h, DVR 0°C /24h, DVR 23°C /72h, and DVR 70°C /24h.
- Output:** A table showing the results of the mixture, including Mixture1, Total, and Sum of recipe ratios (should be 100%).
- Recipe ratios in %:** A row at the bottom showing the percentage ratios for each recipe: 5,25, 11, 45,25, 6, 11, 13,5, 0,00, 8, 0,00.

Click on "take this mixture"

Because we chose "Auto mix (overwrite mixture)", the application has placed it in the first column and automatically assigned the name "Mixture1" to it.

This mixture is a combination of several of the compounds in the database. The ratios the formula is made of can be seen from the line at the bottom of the page: "Recipe ratios in %"

The horizontal sum should always equal 100%

# Naming the mixture

The screenshot shows the GrafCompounder version 2.003 software interface. It is divided into several sections:

- Input data:** A table with columns for ingredients (50ALS11 to 50ALS42) and rows for various components like NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, and Total. It also includes a section for Properties such as MooneyML, Density, Hardness, M300, TS, EB, and DVR values at different temperatures and times.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdoff. It lists the same ingredients and properties as the input data, with numerical values for Min and Max.
- Output:** A table with columns for Name and values. The first row is highlighted in blue and contains the text "50AL45Test" in the Name column and "100" in the values column. Other rows show numerical values for various properties.
- Recipe ratios in %:** A row of values: 5,25, 11, 45,25, 6, 11, 13,5, 0,00, 8, 0,00.
- Number format:** A dropdown menu set to "12345,67".
- Buttons:** "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

You can double-click the cell “Mixture 1“ to rename it

In the example above, the cell is being renamed to "50 AL45Test"

# Naming the mixture

The screenshot shows the GrafCompounder version 2.003 software interface. It is divided into several sections:

- Input data:** A table with columns for ingredients (Testdateien, Ingredients) and recipes (50AL511 to 50AL542). The ingredients list includes NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, MooneyML(1+4) 100°C, Mooney15 / 120°C, Density, Hardness, M300, TS, EB, DVR -26°C /24h, DVR 0°C /24h, DVR 23°C /72h, and DVR 70°C /24h.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdoff. It lists the same ingredients as the input data table.
- Output:** A table with columns for Name, Min, Max, From, To, Wei..., and Trdoff. It lists the same ingredients as the input data table, with a new column labeled "50AL45Test1" added at the end.
- Recipe ratios in %:** A row of values: 5,25, 11, 45,25, 6, 11, 13,5, 0,00, 8, 0,00.
- Number format:** 12345,67
- Buttons:** Import input data from clipboard, Auto mix (overwrite mixture), Auto mix (new mixture).

There are two options for analysis:

- 1) Copy "50 AL45Test" column information and insert in a separate spreadsheet.
- 2) Copy "50 AL45Test" column and append in last column in next column after 50AL542



# Data analysis – Option 1

|    | A                 | B        | C       | D       | E       | F       | G       | H       | I       | J       | K          | L      |
|----|-------------------|----------|---------|---------|---------|---------|---------|---------|---------|---------|------------|--------|
| 1  | Testdateien       |          |         |         |         |         |         |         |         |         |            |        |
| 2  |                   | Recipes: |         |         |         |         |         |         |         |         |            |        |
| 3  | Ingredients:      | 50AL511  | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45Test |        |
| 4  | NR (SMR - 10)     | 100,00   | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00     | 100,00 |
| 5  | N330              | 10,00    | 30,00   | 50,00   | 25,00   | 45,00   | 75,00   | 45,00   | 65,00   | 50,00   | 48,23      |        |
| 6  | CaCO3             | 20,00    | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   |         | 20,00      |        |
| 7  | Naphtenic Oil     | 5,00     | 25,00   | 45,00   | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 10,00   | 34,50      |        |
| 8  | ZnO               | 5,00     | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00       |        |
| 9  | Stearic Acid      | 2,00     | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00       |        |
| 10 | IPPD              | 2,00     | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00       |        |
| 11 | S                 | 1,50     | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 0,25    | 1,50       |        |
| 12 | TMTD - 80         |          |         |         |         |         |         |         |         | 1,00    |            |        |
| 13 | CBS - 80          | 0,65     | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 2,10    | 0,65       |        |
| 14 | Total             | 146,15   | 186,15  | 226,15  | 161,15  | 201,15  | 251,15  | 181,15  | 221,15  | 172,35  | 213,88     |        |
| 15 |                   |          |         |         |         |         |         |         |         |         |            |        |
| 16 | Properties:       |          |         |         |         |         |         |         |         |         |            |        |
| 17 | MooneyML(1+4) 1*  | 32,00    | 36,00   | 31,00   | 34,00   | 30,00   | 42,00   | 60,00   | 39,00   | 41,00   | 33,80      |        |
| 18 | Mooney t5 / 120°C | 28,00    | 28,00   | 32,00   | 28,00   | 32,00   | 22,00   | 20,00   | 25,00   | 11,00   | 29,20      |        |
| 19 | Density           | 1,08     | 1,12    | 1,16    | 1,13    | 1,16    | 1,19    | 1,19    | 1,20    | 1,11    | 1,16       |        |
| 20 | Hardness          | 42,00    | 41,00   | 40,00   | 48,00   | 48,00   | 52,00   | 61,00   | 61,00   | 59,00   | 44,88      |        |
| 21 | M300              | 1,80     | 3,00    | 3,00    | 4,40    | 4,60    | 5,30    | 8,00    | 7,60    | 9,40    | 3,88       |        |
| 22 | TS                | 25,00    | 21,00   | 15,00   | 25,00   | 20,00   | 15,30   | 23,00   | 18,00   | 23,00   | 17,62      |        |
| 23 | EB                | 785,00   | 725,00  | 690,00  | 715,00  | 705,00  | 615,00  | 560,00  | 590,00  | 540,00  | 683,86     |        |
| 24 | DVR -26°C /24h    | 22,00    | 28,00   | 30,00   | 17,00   | 19,00   | 35,00   | 29,00   | 27,00   | 77,00   | 27,81      |        |
| 25 | DVR 0°C /24h      | 10,00    | 14,00   | 14,00   | 8,00    | 12,00   | 16,00   | 13,00   | 12,00   | 16,00   | 13,32      |        |
| 26 | DVR 23°C /72h     | 8,00     | 10,00   | 14,00   | 9,00    | 13,00   | 16,00   | 10,00   | 17,00   | 18,00   | 13,35      |        |
| 27 | DVR 70°C /24h     | 39,00    | 50,00   | 61,00   | 44,00   | 50,00   | 54,00   | 44,00   | 50,00   | 17,00   | 54,58      |        |
| 28 |                   |          |         |         |         |         |         |         |         |         |            |        |

**Option 1: Right click on the "50 AL501test" column and open the short cut menu**

**Choose "copy this mixture to clipboard"**

# Creating the Formula – Option 1

|    | A                 | B        | C       | D       | E       | F       | G       | H       | I       | J       | K          | L      |
|----|-------------------|----------|---------|---------|---------|---------|---------|---------|---------|---------|------------|--------|
| 1  | Testdateien       |          |         |         |         |         |         |         |         |         |            |        |
| 2  |                   | Recipes: |         |         |         |         |         |         |         |         |            |        |
| 3  | Ingredients:      | 50AL511  | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45Test |        |
| 4  | NR (SMR - 10)     | 100,00   | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00     | 100,00 |
| 5  | N330              | 10,00    | 30,00   | 50,00   | 25,00   | 45,00   | 75,00   | 45,00   | 65,00   | 50,00   | 48,23      |        |
| 6  | CaCO3             | 20,00    | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00      |        |
| 7  | Naphtenic Oil     | 5,00     | 25,00   | 45,00   | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 10,00   | 34,50      |        |
| 8  | ZnO               | 5,00     | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00       |        |
| 9  | Stearic Acid      | 2,00     | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00       |        |
| 10 | IPPD              | 2,00     | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00       |        |
| 11 | S                 | 1,50     | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 0,25    | 1,50       |        |
| 12 | TMTD - 80         |          |         |         |         |         |         |         |         |         | 1,00       |        |
| 13 | CBS - 80          | 0,65     | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 2,10    | 0,65       |        |
| 14 | Total             | 146,15   | 186,15  | 226,15  | 161,15  | 201,15  | 251,15  | 181,15  | 221,15  | 172,35  | 213,88     |        |
| 15 |                   |          |         |         |         |         |         |         |         |         |            |        |
| 16 | Properties:       |          |         |         |         |         |         |         |         |         |            |        |
| 17 | MooneyML(1+4) 1P  | 32,00    | 36,00   | 31,00   | 34,00   | 30,00   | 42,00   | 60,00   | 39,00   | 41,00   | 33,80      |        |
| 18 | Mooney t5 / 120°C | 28,00    | 28,00   | 32,00   | 28,00   | 32,00   | 22,00   | 20,00   | 25,00   | 11,00   | 29,20      |        |
| 19 | Density           | 1,08     | 1,12    | 1,16    | 1,13    | 1,16    | 1,19    | 1,19    | 1,20    | 1,11    | 1,16       |        |
| 20 | Hardness          | 42,00    | 41,00   | 40,00   | 48,00   | 48,00   | 52,00   | 61,00   | 61,00   | 59,00   | 44,88      |        |
| 21 | M300              | 1,80     | 3,00    | 3,00    | 4,40    | 4,60    | 5,30    | 8,00    | 7,60    | 9,40    | 3,88       |        |
| 22 | TS                | 25,00    | 21,00   | 15,00   | 25,00   | 20,00   | 15,30   | 23,00   | 18,00   | 23,00   | 17,62      |        |
| 23 | EB                | 785,00   | 725,00  | 690,00  | 715,00  | 705,00  | 615,00  | 560,00  | 590,00  | 540,00  | 683,86     |        |
| 24 | DVR -26°C /24h    | 22,00    | 28,00   | 30,00   | 17,00   | 19,00   | 35,00   | 29,00   | 27,00   | 77,00   | 27,81      |        |
| 25 | DVR 0°C /24h      | 10,00    | 14,00   | 14,00   | 8,00    | 12,00   | 16,00   | 13,00   | 12,00   | 16,00   | 13,32      |        |
| 26 | DVR 23°C /72h     | 8,00     | 10,00   | 14,00   | 9,00    | 13,00   | 16,00   | 10,00   | 17,00   | 18,00   | 13,35      |        |
| 27 | DVR 70°C /24h     | 39,00    | 50,00   | 61,00   | 44,00   | 50,00   | 54,00   | 44,00   | 50,00   | 17,00   | 54,58      |        |
| 28 |                   |          |         |         |         |         |         |         |         |         |            |        |

Switch to the calculation program sheet with the formulas in it.

Insert the copied cells after the last formula column.

- Adjust any minute amounts or eliminate them
- Select number format you want.

Review the formula by comparing it with the formulas it was compounded from.

# Review the Formula - Option 1

The screenshot shows a spreadsheet with the following data:

|    | A                 | B        | C       | D       | E       | F       | G       | H       | I       | J       | K          | L |
|----|-------------------|----------|---------|---------|---------|---------|---------|---------|---------|---------|------------|---|
| 1  | Testdateien       |          |         |         |         |         |         |         |         |         |            |   |
| 2  |                   | Recipes: |         |         |         |         |         |         |         |         |            |   |
| 3  | Ingredients:      | 50AL511  | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45Test |   |
| 4  | NR (SMR - 10)     | 100,00   | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00  | 100,00     |   |
| 5  | N330              | 10,00    | 30,00   | 50,00   | 25,00   | 45,00   | 75,00   | 45,00   | 65,00   | 50,00   | 48,23      |   |
| 6  | CaCO3             | 20,00    | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   | 20,00   |         | 20,00      |   |
| 7  | Naphtenic Oil     | 5,00     | 25,00   | 45,00   | 5,00    | 25,00   | 45,00   | 5,00    | 25,00   | 10,00   | 34,50      |   |
| 8  | ZnO               | 5,00     | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00    | 5,00       |   |
| 9  | Stearic Acid      | 2,00     | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00       |   |
| 10 | IPPD              | 2,00     | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00    | 2,00       |   |
| 11 | S                 | 1,50     | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 1,50    | 0,25    | 1,50       |   |
| 12 | TMTD - 80         |          |         |         |         |         |         |         |         |         | 1,00       |   |
| 13 | CBS - 80          | 0,65     | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 0,65    | 2,10    | 0,65       |   |
| 14 | Total             | 146,15   | 186,15  | 226,15  | 161,15  | 201,15  | 251,15  | 181,15  | 221,15  | 172,35  | 213,88     |   |
| 15 |                   |          |         |         |         |         |         |         |         |         |            |   |
| 16 | Properties:       |          |         |         |         |         |         |         |         |         |            |   |
| 17 | MooneyML(1+4) 1*  | 32,00    | 36,00   | 31,00   | 34,00   | 30,00   | 42,00   | 60,00   | 39,00   | 41,00   | 33,80      |   |
| 18 | Mooney t5 / 120°C | 28,00    | 28,00   | 32,00   | 28,00   | 32,00   | 22,00   | 20,00   | 25,00   | 11,00   | 29,20      |   |
| 19 | Density           | 1,08     | 1,12    | 1,16    | 1,13    | 1,16    | 1,19    | 1,19    | 1,20    | 1,11    | 1,16       |   |
| 20 | Hardness          | 42,00    | 41,00   | 40,00   | 48,00   | 48,00   | 52,00   | 61,00   | 61,00   | 59,00   | 44,88      |   |
| 21 | M300              | 1,80     | 3,00    | 3,00    | 4,40    | 4,60    | 5,30    | 8,00    | 7,60    | 9,40    | 3,88       |   |
| 22 | TS                | 25,00    | 21,00   | 15,00   | 25,00   | 20,00   | 15,30   | 23,00   | 18,00   | 23,00   | 17,62      |   |
| 23 | EB                | 785,00   | 725,00  | 690,00  | 715,00  | 705,00  | 615,00  | 560,00  | 590,00  | 540,00  | 683,86     |   |
| 24 | DVR -26°C /24h    | 22,00    | 28,00   | 30,00   | 17,00   | 19,00   | 35,00   | 29,00   | 27,00   | 77,00   | 27,81      |   |
| 25 | DVR 0°C /24h      | 10,00    | 14,00   | 14,00   | 8,00    | 12,00   | 16,00   | 13,00   | 12,00   | 16,00   | 13,32      |   |
| 26 | DVR 23°C /72h     | 8,00     | 10,00   | 14,00   | 9,00    | 13,00   | 16,00   | 10,00   | 17,00   | 18,00   | 13,35      |   |
| 27 | DVR 70°C /24h     | 39,00    | 50,00   | 61,00   | 44,00   | 50,00   | 54,00   | 44,00   | 50,00   | 17,00   | 54,58      |   |
| 28 |                   |          |         |         |         |         |         |         |         |         |            |   |

You have now created your first formula using the GrafCompounder.

Analyse the "Properties"

Are they within the expected range?

Carry out a confirming experiment!

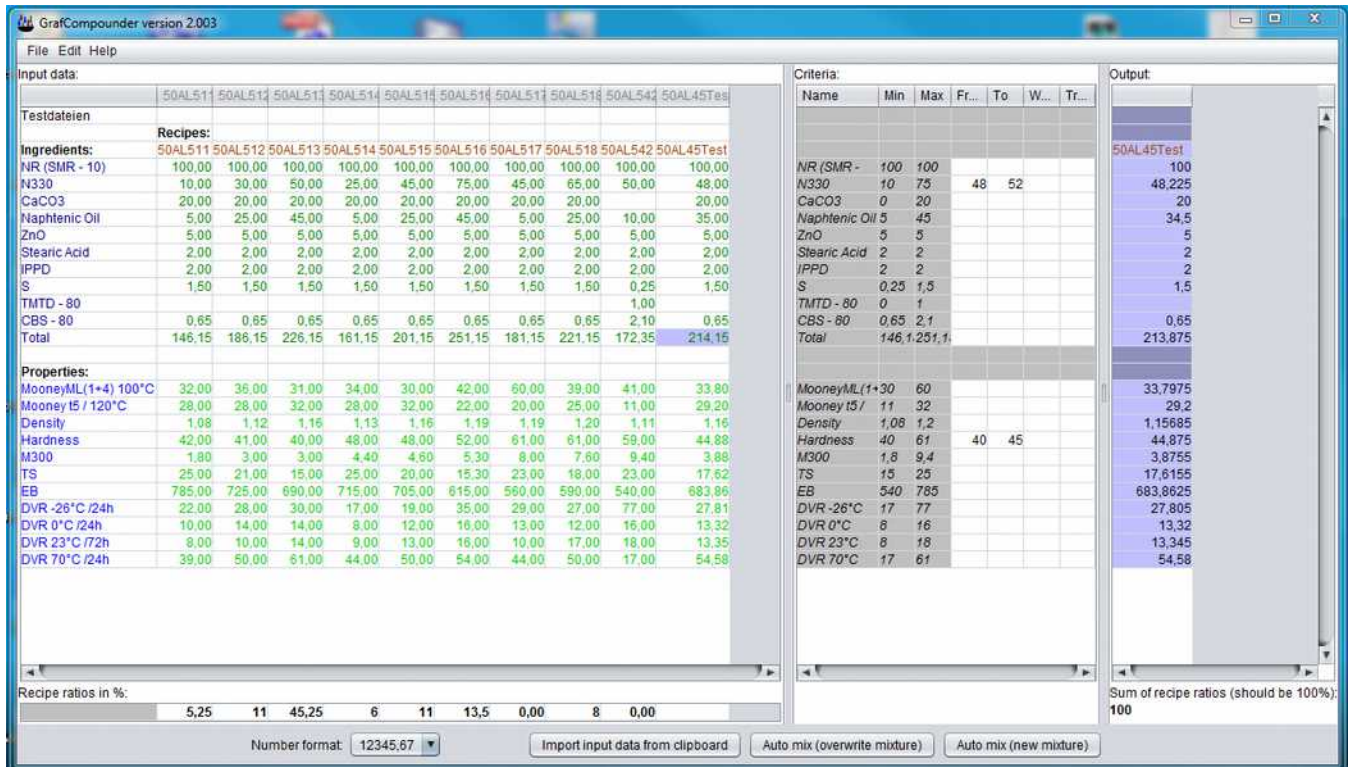
# Data Analysis – Option 2

The screenshot displays the GrafCompunder version 2.003 interface. The main window is a spreadsheet with columns for different test dates (50AL511 to 50AL45Test) and rows for ingredients and properties. A right-click context menu is open over a cell in the 'MooneyML(1+4) 100°C' row, showing various actions. The 'Round values to two decimal places' option is highlighted. The 'Criteria' and 'Output' panels are visible on the right side of the window.

**Option 2: You can paste this formula into the Grafcompunder spreadsheet**

- Round the values to two decimal places with a right click to get the pull down menu

# Data analysis – Option 2



The screenshot displays the GrafCompounder version 2.003 software interface. It is divided into several sections:

- Input data:** A table with columns for different recipe variants (50AL511 to 50AL45Test) and rows for ingredients and properties.
- Criteria:** A table with columns for Name, Min, Max, Fr..., To, W..., and Tr... It lists various material properties and their values.
- Output:** A table showing the calculated values for each recipe variant based on the input data and criteria.
- Recipe ratios in %:** A row at the bottom showing the percentage contribution of each recipe variant to the total.

| Input data:         | 50AL511       | 50AL512       | 50AL513       | 50AL514       | 50AL515       | 50AL516       | 50AL517       | 50AL518       | 50AL542       | 50AL45Test    |
|---------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| <b>Ingredients:</b> |               |               |               |               |               |               |               |               |               |               |
| NR (SMR - 10)       | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        |
| N330                | 10,00         | 30,00         | 50,00         | 25,00         | 45,00         | 75,00         | 45,00         | 65,00         | 50,00         | 48,00         |
| CaCO3               | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         |
| Naphtenic Oil       | 5,00          | 25,00         | 45,00         | 5,00          | 25,00         | 45,00         | 5,00          | 25,00         | 10,00         | 35,00         |
| ZnO                 | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          |
| Stearic Acid        | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          |
| IPPD                | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          |
| S                   | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 0,25          | 1,50          |
| TMTD - 80           |               |               |               |               |               |               |               |               |               | 1,00          |
| CBS - 80            | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 2,10          | 0,65          |
| <b>Total</b>        | <b>146,15</b> | <b>186,15</b> | <b>226,15</b> | <b>161,15</b> | <b>201,15</b> | <b>251,15</b> | <b>181,15</b> | <b>221,15</b> | <b>172,35</b> | <b>214,15</b> |
| <b>Properties:</b>  |               |               |               |               |               |               |               |               |               |               |
| MooneyML(1+4) 100°C | 32,00         | 36,00         | 31,00         | 34,00         | 30,00         | 42,00         | 60,00         | 39,00         | 41,00         | 33,80         |
| MooneyIS / 120°C    | 28,00         | 28,00         | 32,00         | 28,00         | 32,00         | 22,00         | 20,00         | 25,00         | 11,00         | 29,20         |
| Density             | 1,08          | 1,12          | 1,16          | 1,13          | 1,16          | 1,19          | 1,19          | 1,20          | 1,11          | 1,16          |
| Hardness            | 42,00         | 41,00         | 40,00         | 48,00         | 48,00         | 52,00         | 61,00         | 61,00         | 59,00         | 44,88         |
| M300                | 1,80          | 3,00          | 3,00          | 4,40          | 4,60          | 5,30          | 8,00          | 7,60          | 9,40          | 3,88          |
| TS                  | 25,00         | 21,00         | 15,00         | 25,00         | 20,00         | 15,30         | 23,00         | 18,00         | 23,00         | 17,62         |
| EB                  | 785,00        | 725,00        | 690,00        | 715,00        | 705,00        | 615,00        | 560,00        | 590,00        | 540,00        | 683,86        |
| DVR -26°C /24h      | 22,00         | 28,00         | 30,00         | 17,00         | 19,00         | 35,00         | 29,00         | 27,00         | 77,00         | 27,81         |
| DVR 0°C /24h        | 10,00         | 14,00         | 14,00         | 8,00          | 12,00         | 16,00         | 13,00         | 12,00         | 16,00         | 13,32         |
| DVR 23°C /72h       | 8,00          | 10,00         | 14,00         | 9,00          | 13,00         | 16,00         | 10,00         | 17,00         | 18,00         | 13,35         |
| DVR 70°C /24h       | 39,00         | 50,00         | 61,00         | 44,00         | 50,00         | 54,00         | 44,00         | 50,00         | 17,00         | 54,58         |

You may want to manipulate the ingredient data in the formula

- i.e. - take out odd or small numbers
- You need to recalculate the total if you do this

# Data Analysis – Option 2

**Input data:**

|                     | 50AL511       | 50AL512       | 50AL513       | 50AL514       | 50AL515       | 50AL516       | 50AL517       | 50AL518       | 50AL542       | 50AL45Test    |
|---------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| <b>Ingredients:</b> |               |               |               |               |               |               |               |               |               |               |
| NR (SMR - 10)       | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        | 100,00        |
| N330                | 10,00         | 30,00         | 50,00         | 25,00         | 45,00         | 75,00         | 45,00         | 65,00         | 50,00         | 48,00         |
| CaCO3               | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         | 20,00         |
| Naphthenic Oil      | 5,00          | 25,00         | 45,00         | 5,00          | 25,00         | 45,00         | 5,00          | 25,00         | 10,00         | 35,00         |
| ZnO                 | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          | 5,00          |
| Stearic Acid        | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          |
| IPPD                | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          | 2,00          |
| S                   | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 1,50          | 0,25          | 1,50          |
| TMTD - 80           |               |               |               |               |               |               |               |               |               | 1,00          |
| CBS - 80            | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 0,65          | 2,10          | 0,65          |
| <b>Total</b>        | <b>146,15</b> | <b>186,15</b> | <b>226,15</b> | <b>161,15</b> | <b>201,15</b> | <b>251,15</b> | <b>181,15</b> | <b>221,15</b> | <b>172,35</b> | <b>214,15</b> |

**Properties:**

|                     | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45Test |
|---------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|------------|
| MooneyML(1+4) 100°C | 32,00   | 36,00   | 31,00   | 34,00   | 30,00   | 42,00   | 60,00   | 39,00   | 41,00   | 33,80      |
| Mooney 15 / 120°C   | 28,00   | 28,00   | 32,00   | 28,00   | 32,00   | 22,00   | 20,00   | 25,00   | 11,00   | 29,20      |
| Density             | 1,08    | 1,12    | 1,15    | 1,13    | 1,16    | 1,19    | 1,19    | 1,20    | 1,11    | 1,16       |
| Hardness            | 42,00   | 41,00   | 40,00   | 48,00   | 48,00   | 52,00   | 61,00   | 61,00   | 59,00   | 44,88      |
| M300                | 1,80    | 3,00    | 3,00    | 4,40    | 4,80    | 5,30    | 8,00    | 7,60    | 9,40    | 3,88       |
| TS                  | 25,00   | 21,00   | 15,00   | 25,00   | 20,00   | 15,30   | 23,00   | 16,00   | 23,00   | 17,62      |
| EB                  | 785,00  | 725,00  | 690,00  | 715,00  | 705,00  | 615,00  | 560,00  | 590,00  | 540,00  | 683,86     |
| DVR -26°C /24h      | 22,00   | 28,00   | 30,00   | 17,00   | 19,00   | 35,00   | 29,00   | 27,00   | 77,00   | 27,81      |
| DVR 0°C /24h        | 10,00   | 14,00   | 14,00   | 8,00    | 12,00   | 16,00   | 13,00   | 12,00   | 16,00   | 13,32      |
| DVR 23°C /72h       | 8,00    | 10,00   | 14,00   | 9,00    | 13,00   | 16,00   | 10,00   | 17,00   | 18,00   | 13,35      |
| DVR 70°C /24h       | 39,00   | 50,00   | 61,00   | 44,00   | 50,00   | 54,00   | 44,00   | 50,00   | 17,00   | 54,58      |

**Criteria:**

| Name           | Min          | Max          | Fr... | To | W... | Tr... |
|----------------|--------------|--------------|-------|----|------|-------|
| NR (SMR - 10)  | 100          | 100          |       |    |      |       |
| N330           | 10           | 75           | 48    | 52 |      |       |
| CaCO3          | 0            | 20           |       |    |      |       |
| Naphthenic Oil | 5            | 45           |       |    |      |       |
| ZnO            | 5            | 5            |       |    |      |       |
| Stearic Acid   | 2            | 2            |       |    |      |       |
| IPPD           | 2            | 2            |       |    |      |       |
| S              | 0,25         | 1,5          |       |    |      |       |
| TMTD - 80      | 0            | 1            |       |    |      |       |
| CBS - 80       | 0,65         | 2,1          |       |    |      |       |
| <b>Total</b>   | <b>146,1</b> | <b>251,1</b> |       |    |      |       |

**Output:**

| Name           | Value          |
|----------------|----------------|
| 50AL45Test     | 100            |
| NR (SMR - 10)  | 48,225         |
| N330           | 20             |
| CaCO3          | 34,5           |
| Naphthenic Oil | 5              |
| ZnO            | 2              |
| Stearic Acid   | 2              |
| IPPD           | 2              |
| S              | 1,5            |
| TMTD - 80      | 0,65           |
| CBS - 80       | 213,875        |
| <b>Total</b>   | <b>213,875</b> |

**Recipe ratios in %:**

| Recipe  | Ratio (%) |
|---------|-----------|
| 50AL511 | 5,25      |
| 50AL512 | 11        |
| 50AL513 | 45,25     |
| 50AL514 | 6         |
| 50AL515 | 11        |
| 50AL516 | 13,5      |
| 50AL517 | 0,00      |
| 50AL518 | 8         |
| 50AL542 | 0,00      |

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

The formula is now added to your database and will be used in further calculations.

**It is strongly recommended that you:**

- Perform a confirmation experiment
- Make necessary corrections of properties, if there is any differences seen from calculated and confirmation experiment values
- You need to recalculate the total

# Creating a 2<sup>nd</sup> Formula

Input data:

|                     | 50AL51 | 50AL52 | 50AL53 | 50AL54 | 50AL55 | 50AL56 | 50AL57 | 50AL58 | 50AL542 | 50AL45T |
|---------------------|--------|--------|--------|--------|--------|--------|--------|--------|---------|---------|
| <b>Ingredients:</b> |        |        |        |        |        |        |        |        |         |         |
| NR (SMR - 10)       | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00  | 100.00  |
| N330                | 10.00  | 30.00  | 50.00  | 25.00  | 45.00  | 75.00  | 45.00  | 65.00  | 50.00   | 48.23   |
| CaCO3               | 20.00  | 20.00  | 20.00  | 20.00  | 20.00  | 20.00  | 20.00  | 20.00  |         | 20.00   |
| Naphtenic Oil       | 5.00   | 25.00  | 45.00  | 5.00   | 25.00  | 45.00  | 5.00   | 25.00  | 10.00   | 34.50   |
| ZnO                 | 5.00   | 5.00   | 5.00   | 5.00   | 5.00   | 5.00   | 5.00   | 5.00   | 5.00    | 5.00    |
| Stearic Acid        | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00    | 2.00    |
| IPPD                | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00   | 2.00    | 2.00    |
| S                   | 1.50   | 1.50   | 1.50   | 1.50   | 1.50   | 1.50   | 1.50   | 1.50   | 0.25    | 1.50    |
| TMTD - 80           |        |        |        |        |        |        |        |        |         | 1.00    |
| CBS - 80            | 0.65   | 0.65   | 0.65   | 0.65   | 0.65   | 0.65   | 0.65   | 0.65   | 2.10    | 0.65    |
| Total               | 146.15 | 186.15 | 226.15 | 161.15 | 201.15 | 251.15 | 181.15 | 221.15 | 172.35  | 213.88  |
| <b>Properties:</b>  |        |        |        |        |        |        |        |        |         |         |
| MooneyML(1+4) 100°C | 32.00  | 36.00  | 31.00  | 34.00  | 30.00  | 42.00  | 60.00  | 39.00  | 41.00   | 33.80   |
| Mooney I5 / 120°C   | 28.00  | 28.00  | 32.00  | 28.00  | 32.00  | 22.00  | 20.00  | 25.00  | 11.00   | 29.20   |
| Density             | 1.08   | 1.12   | 1.18   | 1.13   | 1.16   | 1.19   | 1.19   | 1.20   | 1.11    | 1.16    |
| Hardness            | 42.00  | 41.00  | 40.00  | 48.00  | 48.00  | 52.00  | 61.00  | 59.00  | 44.88   | 44.88   |
| M300                | 1.80   | 3.00   | 3.00   | 4.40   | 4.60   | 5.30   | 8.00   | 7.60   | 9.40    | 3.88    |
| TS                  | 25.00  | 21.00  | 15.00  | 25.00  | 20.00  | 15.30  | 23.00  | 18.00  | 23.00   | 17.62   |
| EB                  | 785.00 | 725.00 | 690.00 | 715.00 | 705.00 | 615.00 | 560.00 | 590.00 | 540.00  | 683.86  |
| DVR -26°C /24h      | 22.00  | 28.00  | 30.00  | 17.00  | 19.00  | 35.00  | 29.00  | 27.00  | 77.00   | 27.81   |
| DVR 0°C /24h        | 10.00  | 14.00  | 14.00  | 8.00   | 12.00  | 16.00  | 13.00  | 12.00  | 16.00   | 13.32   |
| DVR 23°C /72h       | 8.00   | 10.00  | 14.00  | 9.00   | 13.00  | 16.00  | 10.00  | 17.00  | 18.00   | 13.35   |
| DVR 70°C /24h       | 39.00  | 50.00  | 61.00  | 44.00  | 50.00  | 54.00  | 44.00  | 50.00  | 17.00   | 54.58   |

Recipe ratios in %:

|      |    |       |   |    |      |   |
|------|----|-------|---|----|------|---|
| 5.25 | 11 | 45.25 | 6 | 11 | 13.5 | 8 |
|------|----|-------|---|----|------|---|

Criteria:

| Name           | Min    | Max    | From | To | Wel... | Trd... |
|----------------|--------|--------|------|----|--------|--------|
| NR (SMR - 10)  | 100    | 100    |      |    |        |        |
| N330           | 10     | 75     | 48   | 52 |        |        |
| CaCO3          | 0      | 20     |      |    |        |        |
| Naphtenic Oil  | 5      | 45     |      |    |        |        |
| ZnO            | 5      | 5      |      |    |        |        |
| Stearic Acid   | 2      | 2      |      |    |        |        |
| IPPD           | 2      | 2      |      |    |        |        |
| S              | 0.25   | 1.3    |      |    |        |        |
| TMTD - 80      | 0      | 1      |      |    |        |        |
| CBS - 80       | 0.65   | 2.1    |      |    |        |        |
| Total          | 146.15 | 251.15 |      |    |        |        |
| MooneyML(1+4)  | 30     | 60     |      |    |        |        |
| Mooney I5 /    | 11     | 32     |      |    |        |        |
| Density        | 1.08   | 1.2    |      |    |        |        |
| Hardness       | 40     | 61     | 40   | 45 |        |        |
| M300           | 1.8    | 9.4    |      |    |        |        |
| TS             | 15     | 25     | 20   |    |        |        |
| EB             | 540    | 765    |      |    |        |        |
| DVR -26°C /24h | 17     | 77     |      |    |        |        |
| DVR 0°C /24h   | 8      | 16     |      |    |        |        |
| DVR 23°C /72h  | 8      | 18     |      |    |        |        |
| DVR 70°C /24h  | 17     | 61     |      |    |        |        |

Output:

| 50AL45Test     |          |
|----------------|----------|
| NR (SMR - 10)  | 100      |
| N330           | 48.225   |
| CaCO3          | 20       |
| Naphtenic Oil  | 34.5     |
| ZnO            | 5        |
| Stearic Acid   | 2        |
| IPPD           | 2        |
| S              | 1.5      |
| TMTD - 80      |          |
| CBS - 80       | 0.65     |
| Total          | 213.875  |
| MooneyML(1+4)  | 33.7975  |
| Mooney I5 /    | 29.2     |
| Density        | 1.15685  |
| Hardness       | 44.875   |
| M300           | 3.8755   |
| TS             | 17.6155  |
| EB             | 683.8625 |
| DVR -26°C /24h | 27.805   |
| DVR 0°C /24h   | 13.32    |
| DVR 23°C /72h  | 13.345   |
| DVR 70°C /24h  | 54.58    |

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

## To create a 2nd formula:

- Change the chosen criteria or introduce a new criterion
- We have added “Tensile Strength (TS) greater than 20 MPa” to the list of criteria in the example above.
  - *We disable 50AL45Test, because no confirmation experiment has been done yet.*

# Creating a 2<sup>nd</sup> Formula

Automatic mixing in process ...

Score of best mixture so far (lower is better): 103.9664

Take best mixture so far    Cancel

Because we do not want the first formula to be overwritten, and because we will use the 2nd formula for comparison,

- click on: “Auto mix (new mixture)”
- Since no mixture is found which exactly fulfils all criteria in this case, the new compound has a score of 100.2232.
- Click on " Take best mixture so far "



# Creating a 2nd formula

The screenshot shows the GrafCompounder version 2.003 software interface. It is divided into three main sections: Input data, Criteria, and Output.

**Input data:** A table with columns for ingredients (50AL511 to 50AL45Test) and rows for various components like NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, and Total. It also includes a Properties section with values for MooneyML, Mooney t5, Density, Hardness, M300, TS, EB, and DVR at different temperatures and times.

**Criteria:** A table with columns for Name, Min, Max, Fr..., To, W..., and Tr... It lists criteria such as NR (SMR - 100), N330 (48 to 52), CaCO3, Naphtenic Oil (5 to 45), ZnO (5 to 5), Stearic Acid (2 to 2), IPPD (2 to 2), S (0.25 to 1.5), TMTD - 80 (0 to 1), CBS - 80 (0.65 to 2.1), MooneyML (1+30) (60), Mooney t5 (11 to 32), Density (1.08 to 1.2), Hardness (40 to 61), M300 (1.8 to 9.4), TS (15 to 25), EB (540 to 785), DVR -26°C (17 to 77), DVR 0°C (8 to 16), DVR 23°C (8 to 18), and DVR 70°C (17 to 61).

**Output:** A table showing the results for the recipe, including values for 50AL45Test and Mixture2. The total output is 213,875 and 199,623.

At the bottom, there is a 'Recipe ratios in %' section with values: 0,00, 63, 0,00, 8,25, 0,00, 24,75, 0,00, 0,00, 4. There are also buttons for 'Import input data from clipboard', 'Auto mix (overwrite mixture)', and 'Auto mix (new mixture)'.

The 2nd formula will be inserted into the next available column and named automatically **Mixture2**.

- The reason that the new mixture does not have a perfect score of 0 is because the CB N330 ingredient of the new compound missed the limits of 48 to 52 phr.
- Further mixtures with additional criteria can be produced, renamed and transferred in your calculation program in the same manner.

# Creating Formulas

## Using “Weight” and “Trdoff”

The screenshot shows the GrafCompounder software interface with three main tables: Input data, Criteria, and Output.

**Input data (Recipes):**

|               | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45T4 |
|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|----------|
| NR (SMR - 10) | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00   |
| N330          | 10.00   | 30.00   | 50.00   | 25.00   | 45.00   | 75.00   | 45.00   | 65.00   | 50.00   | 48.23    |
| CaCO3         | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00    |
| Naphtenic Oil | 5.00    | 25.00   | 45.00   | 5.00    | 25.00   | 45.00   | 5.00    | 25.00   | 10.00   | 34.50    |
| ZnO           | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00     |
| Stearic Acid  | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00     |
| IPPD          | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00     |
| S             | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 0.25    | 1.50     |
| TMTD - 80     |         |         |         |         |         |         |         |         |         | 1.00     |
| CBS - 80      | 0.85    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 2.10    | 0.65     |
| Total         | 146.15  | 186.15  | 226.15  | 161.15  | 201.15  | 251.15  | 181.15  | 221.15  | 172.35  | 213.88   |

**Criteria:**

| Name              | Min    | Max    | From | To | Wei... | Trd... |
|-------------------|--------|--------|------|----|--------|--------|
| NR (SMR - 10)     | 100    | 100    |      |    |        |        |
| N330              | 10     | 75     |      |    |        |        |
| CaCO3             | 0      | 20     |      |    |        |        |
| Naphtenic Oil     | 5      | 45     |      |    |        |        |
| ZnO               | 5      | 5      |      |    |        |        |
| Stearic Acid      | 2      | 2      |      |    |        |        |
| IPPD              | 2      | 2      |      |    |        |        |
| S                 | 0.25   | 1.5    |      |    |        |        |
| TMTD - 80         | 0      | 1      |      |    |        |        |
| CBS - 80          | 0.65   | 2.1    |      |    |        |        |
| Total             | 146.15 | 251.15 |      |    |        |        |
| MooneyML(1+4)     | 30     | 60     |      |    |        |        |
| Mooney 15 / 120°C | 11     | 32     |      |    |        |        |
| Density           | 1.08   | 1.2    |      |    |        |        |
| Hardness          | 40     | 61     | 40   | 45 |        |        |
| M300              | 1.8    | 9.4    |      |    |        |        |
| TS                | 15     | 25     | 20   |    |        |        |
| EB                | 540    | 785    |      |    |        |        |
| DVR -26°C/24h     | 17     | 77     |      |    |        |        |
| DVR 0°C/24h       | 8      | 16     |      |    |        |        |
| DVR 23°C/72h      | 8      | 18     |      |    |        |        |
| DVR 70°C/24h      | 17     | 61     |      |    |        |        |

**Output:**

|                   | 50AL45Test | Mixture3 |
|-------------------|------------|----------|
| NR (SMR - 10)     | 100        | 100      |
| N330              | 48.225     | 48       |
| CaCO3             | 20         | 20       |
| Naphtenic Oil     | 34.5       | 33       |
| ZnO               | 5          | 5        |
| Stearic Acid      | 2          | 2        |
| IPPD              | 2          | 2        |
| S                 | 1.5        | 1.5      |
| TMTD - 80         |            |          |
| CBS - 80          | 0.65       | 0.65     |
| Total             | 213.875    | 212.15   |
| MooneyML(1+4)     | 33.7975    | 38.4     |
| Mooney 15 / 120°C | 29.2       | 25.6     |
| Density           | 1.15685    | 1.148    |
| Hardness          | 44.875     | 45.4     |
| M300              | 3.8755     | 3.92     |
| TS                | 17.5155    | 18.72    |
| EB                | 683.8625   | 681      |
| DVR -26°C/24h     | 27.805     | 30.8     |
| DVR 0°C/24h       | 13.32      | 14.8     |
| DVR 23°C/72h      | 13.345     | 12.4     |
| DVR 70°C/24h      | 54.58      | 51.6     |

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

### "Mixture 2" – Choices:

- In the previous example CB N 330 has dropped, but we want it to stay at that level.
- Put a weight (5 in our example) on that property. This will lift the importance of the selected property above other selections.
- With “Auto mix (new mixture) ” you can see the result of the weight in Mixture 3 now. Notice, that differences between Mixture1 and Mixture2 are small.
- In such cases you may chose “Auto mix (overwrite mixture) to save mixture column space on your screen.

# Creating Formulas

## Using “Weight” and “Trdoff”

The screenshot shows the GrafCompounder software interface with three main panels:

- Input data:** A table with columns for various materials (50AL511 to 50AL518, 50AL54, 50AL45T) and rows for ingredients (NR, N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD-80, CBS-80) and properties (MooneyML, Density, Hardness, M300, TS, EB, DVR at different temperatures).
- Criteria:** A table defining constraints for each material, including Min, Max, From, To, Wel., and Trd. values.
- Output:** A table showing the results for three mixtures (50AL45Test, Mixture3, Mixture4), including values for ingredients and properties.

At the bottom, there are buttons for "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

In our example we noticed the high Elongation (EB) and high C-Set Values (DVR) at the same time.

- By changing the criteria the formulas can be improved: if we set EB to 550 max, this should improve the DVR as well
- When we select “Auto mix (new Mixture)” and accept the formula at score 513,27 this formula becomes new “Mixture 4”.
- The result shows shorter EB – still far from 550%, with improved DVR; but now Hardness has increased

# Creating Formulas

## Using “Weight” and “Trdoff”

The screenshot shows the GrafCompounder 2.004 software interface. The main window is divided into several sections:

- Input data:** A table with columns for ingredients and rows for different recipes (50AL51 to 50AL54).
- Recipes:** A table listing ingredients and their weights for various recipes.
- Criteria:** A table with columns: Name, Min, Max, From, To, Wei..., Trd... It lists properties like NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, JPPD, S, TMTD - 80, CBS - 80, and DVR properties.
- Output:** A table showing the results of the automatic mixing process, including the score of the best mixture (4392.5886) and the recipe ratios.

A dialog box titled "Automatic mixing in process ..." is open over the Criteria table. It displays the "Score of best mixture so far (lower is better): 4392.5886" and has buttons for "Take best mixture so far" and "Cancel".

**In case of a conflict: we have a conflicting target between elongation (EB) and Hardness so we proceed using “Weight” and “Trdoff”:**

- On Hardness we change the weight to 10
- Elongation stays with the same weight of 10
- For CB N 330 we stay with 5 to stay close to the value at least.

***Run with Auto mix (new mixture)***

# Creating Formulas

## Using “Weight” and “Trdoff”

The screenshot displays the GrafCompunder version 2.004 software interface. It is divided into several sections:

- Input data:** A table with columns for ingredients (50AL51 to 50AL54) and rows for various components like NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, and Total. It also includes a 'Properties' section with values for MooneyML, Density, Hardness, M300, TS, EB, and DVR at different temperatures and times.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trd... It lists criteria such as NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, and Total, along with their respective values and 'Trdoff' values.
- Output:** A table showing results for 'Mixture4' and 'Mixture5' across various properties like MooneyML, Density, Hardness, M300, TS, EB, and DVR.

At the bottom of the interface, there are buttons for 'Import input data from clipboard', 'Auto mix (overwrite mixture)', and 'Auto mix (new mixture)'. A status bar at the very bottom shows 'Number format: 12345.67' and 'Sum of recipe ratios (should be 100%): 100'.

The result shows

- Hardness is in target
- ICB N 330 has a minor increase
- However, Elongation is much too high, and DVR (C-Set) has increased again.

**To solve the conflict, we set “Trdoff” to 10 on Elongation again and run Auto Mix**

# Creating Formulas

## Using “Weight” and “Trdoff”

The screenshot shows the GrafCompoander version 2.004 software interface. It features a main window with several panes:

- Input data:** A table with columns for ingredients (NR, N330, CaCO3, Naphthenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD-80, CBS-80) and recipe ratios (50AL51, 50AL52, 50AL53, 50AL54, 50AL55, 50AL56, 50AL57, 50AL58, 50AL542, 50AL45T).
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trd... It lists ingredients like NR (SMR - 10), N330, CaCO3, Naphthenic Oil, ZnO, Stearic Acid, IPPD, S, and TMTD-80 with their respective values.
- Output:** A table showing results for Mixture4 and Mixture5, including values for various ingredients and properties.
- Properties:** A table listing properties like MooneyML(1+4) 100°C, Mooney 15 / 120°C, Density, Hardness, M300, TS, EB, and DVR at different temperatures and times.

In the center, a dialog box titled "Automatic mixing in process ..." is displayed. It contains a progress bar and the text "Score of best mixture so far (lower is better): 4988.0526". Below the text are two buttons: "Take best mixture so far" and "Cancel".

The score at 4988 shows, that the conflict can not be solved (at least with this small example database).

- We removed 50AL45Test column from the output to allow the comparison of only Mixture 4 and Mixture 5 with the next one.

# Creating Formulas

## Using “Weight” and “Trdoff”

The screenshot shows the GrafCompoander version 2.004 software interface. It is divided into three main sections: Input data, Criteria, and Output.

**Input data:** A table with columns for recipes (50AL511 to 50AL45T) and rows for ingredients and properties. The ingredients include NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, JPPD, S, TMTD - 80, CBS - 80, and Total. Properties include Mooney/ML(1+4) at 100°C and 120°C, Density, Hardness, M300, TS, EB, and DVR at -26°C/24h, 0°C/24h, 23°C/72h, and 70°C/24h.

**Criteria:** A table with columns for Name, Min, Max, From, To, Wel..., and Trd... It lists the same ingredients and properties as the input data, with numerical values and 'Trdoff' values. For example, Hardness has a 'Trdoff' of 10.

**Output:** A table showing the results for three mixtures (Mixture4, Mixture5, Mixture6). It lists the same ingredients and properties as the input data, with numerical values. The sum of recipe ratios is 100.

At the bottom of the interface, there are buttons for "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

The analysis of the result is:

- Hardness at 55ShA again
- Elongation at 570% now close to target and DVR 70C is improved
- CB N330 is at 50 phr, which is in target

**We then set “Trdoff” to 10 on hardness again and run Auto Mix, overwriting Mixture 6**

# Creating formulas

## Using “Weight” and “Trdoff”

The screenshot shows the GrafCompoinder version 2.004 software interface. It is divided into several sections:

- Input data:** A table with columns for ingredients (NR (SMR - 10), N330, CaCO3, Naphtenic Oil, ZnO, Stearic Acid, IPPD, S, TMTD - 80, CBS - 80, Total) and rows for different recipes (50AL511 to 50AL45T).
- Properties:** A table showing various properties (MooneyML(1+4) 100°C, Mooney I5 / 120°C, Density, Hardness, M300, TS, EB, DVR -26°C /24h, DVR 0°C /24h, DVR 23°C /72h, DVR 70°C /24h) for each recipe.
- Criteria:** A table with columns for Name, Min, Max, From, To, Wei..., and Trd... It lists the same ingredients as the input data table.
- Output:** A table showing results for Mixture4, Mixture5, and Mixture7, with values for various properties.

At the bottom of the interface, there are buttons for "Import input data from clipboard", "Auto mix (overwrite mixture)", and "Auto mix (new mixture)".

The analysis of this result is:

- Hardness is at 45ShA again
- Elongation is at 640%, now far from target again, and DVR 70C much higher as before
- CB N330 with 50 phr is in target

**Conclusion:**

- Weight and Trdoff are tools for optimization in case of conflicting targets



# Mixing Manually

GrafCompounder version 2.004

File Edit Help

Input data:

|                     | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51     | 50AL45test |
|---------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|------------|------------|
| Demo Data           |         |         |         |         |         |         |         |         |         |            |            |
| Ingredients:        | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45T... |            |
| NR (SMR - 10)       | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00     |            |
| N330                | 10.00   | 30.00   | 50.00   | 25.00   | 45.00   | 75.00   | 45.00   | 65.00   | 50.00   | 48.23      |            |
| CaCO3               | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00      |            |
| Naphtenic Oil       | 5.00    | 25.00   | 45.00   | 5.00    | 25.00   | 45.00   | 5.00    | 25.00   | 10.00   | 34.50      |            |
| ZnO                 | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00       |            |
| Stearic Acid        | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00       |            |
| IPPD                | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00       |            |
| S                   | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 0.25    | 1.50       |            |
| TMTD - 80           |         |         |         |         |         |         |         |         |         | 1.00       |            |
| CBS - 80            | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 2.10    | 0.65       |            |
| Total               | 146.15  | 186.15  | 226.15  | 161.15  | 201.15  | 251.15  | 181.15  | 221.15  | 172.35  | 213.88     |            |
| Properties:         |         |         |         |         |         |         |         |         |         |            |            |
| MooneyML(1+4) 100°C | 32.00   | 36.00   | 31.00   | 34.00   | 30.00   | 42.00   | 60.00   | 39.00   | 41.00   | 33.80      |            |
| Mooney t5 / 120°C   | 28.00   | 28.00   | 32.00   | 28.00   | 32.00   | 22.00   | 20.00   | 25.00   | 11.00   | 29.20      |            |
| Density             | 1.08    | 1.12    | 1.16    | 1.13    | 1.16    | 1.19    | 1.19    | 1.20    | 1.11    | 1.16       |            |
| Hardness            | 42.00   | 41.00   | 40.00   | 48.00   | 48.00   | 52.00   | 61.00   | 61.00   | 59.00   | 44.88      |            |
| M300                | 1.80    | 3.00    | 3.00    | 4.40    | 4.60    | 5.30    | 8.00    | 7.60    | 9.40    | 3.88       |            |
| TS                  | 25.00   | 21.00   | 15.00   | 25.00   | 20.00   | 15.30   | 23.00   | 18.00   | 23.00   | 17.62      |            |
| EB                  | 785.00  | 725.00  | 690.00  | 715.00  | 705.00  | 615.00  | 560.00  | 590.00  | 540.00  | 683.86     |            |
| DVR -26°C /24h      | 22.00   | 28.00   | 30.00   | 17.00   | 19.00   | 35.00   | 29.00   | 27.00   | 77.00   | 27.81      |            |
| DVR 0°C /24h        | 10.00   | 14.00   | 14.00   | 8.00    | 12.00   | 16.00   | 13.00   | 12.00   | 16.00   | 13.32      |            |
| DVR 23°C /72h       | 8.00    | 10.00   | 14.00   | 9.00    | 13.00   | 16.00   | 10.00   | 17.00   | 18.00   | 13.35      |            |
| DVR 70°C /24h       | 39.00   | 50.00   | 61.00   | 44.00   | 50.00   | 54.00   | 44.00   | 50.00   | 17.00   | 54.58      |            |

Recipe ratios in %:

|   |    |    |   |    |    |   |
|---|----|----|---|----|----|---|
| 4 | 12 | 45 | 7 | 11 | 13 | 8 |
|---|----|----|---|----|----|---|

Number format: 12345.67

Import input data from clipboard

Auto mix (overwrite mixture)

Auto mix (new mixture)

Criteria:

| Name           | Min    | Max    | From | To | Wel... | Trd... |
|----------------|--------|--------|------|----|--------|--------|
| NR (SMR - 10)  | 100    | 100    |      |    |        |        |
| N330           | 10     | 75     | 48   | 52 |        |        |
| CaCO3          | 0      | 20     |      |    |        |        |
| Naphtenic Oil  | 5      | 45     |      |    |        |        |
| ZnO            | 5      | 5      |      |    |        |        |
| Stearic Acid   | 2      | 2      |      |    |        |        |
| IPPD           | 2      | 2      |      |    |        |        |
| S              | 0.25   | 1.5    |      |    |        |        |
| TMTD - 80      | 0      | 1      |      |    |        |        |
| CBS - 80       | 0.65   | 2.1    |      |    |        |        |
| Total          | 146.15 | 251.15 |      |    |        |        |
| MooneyML(1+4)  | 30     | 60     |      |    |        |        |
| Mooney t5 /    | 11     | 32     |      |    |        |        |
| Density        | 1.08   | 1.2    |      |    |        |        |
| Hardness       | 40     | 61     | 40   | 45 |        |        |
| M300           | 1.8    | 9.4    |      |    |        |        |
| TS             | 15     | 25     |      |    |        |        |
| EB             | 340    | 785    |      |    |        |        |
| DVR -26°C /24h | 17     | 77     |      |    |        |        |
| DVR 0°C /24h   | 8      | 16     |      |    |        |        |
| DVR 23°C /72h  | 8      | 18     |      |    |        |        |
| DVR 70°C /24h  | 17     | 61     |      |    |        |        |

Output:

|                | 50AL54Test |
|----------------|------------|
| NR (SMR - 10)  | 100        |
| N330           | 48.15      |
| CaCO3          | 20         |
| Naphtenic Oil  | 34.4       |
| ZnO            | 5          |
| Stearic Acid   | 2          |
| IPPD           | 2          |
| S              | 1.5        |
| TMTD - 80      |            |
| CBS - 80       | 0.65       |
| Total          | 213.7      |
| MooneyML(1+4)  | 33.81      |
| Mooney t5 /    | 29.22      |
| Density        | 1.157      |
| Hardness       | 44.88      |
| M300           | 3.893      |
| TS             | 17.649     |
| EB             | 683.65     |
| DVR -26°C /24h | 27.73      |
| DVR 0°C /24h   | 13.3       |
| DVR 23°C /72h  | 13.32      |
| DVR 70°C /24h  | 54.61      |

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

**Note that the mixture 50AL45test is composed of different formulas in differing ratios, shown in the row at the bottom**

- Some recipes are very similar and you may want to eliminate all the recipes with a percentage smaller than 10
- Or, you may want to see the effect on the final test mixture by changing those ratios manually

# Mixing Manually

The screenshot shows the GrafCompunder version 2.004 software interface. The main window displays a table with columns for various recipes (50AL51 to 50AL45) and rows for ingredients and properties. The 'Recipe ratios in %' section at the bottom is highlighted in yellow, showing values 16, 45, 19, and 20. The 'Criteria' table on the right shows values for various materials, and the 'Output' table shows the resulting values for the selected recipe (50AL45Test).

| Input data:         | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51  | 50AL51     | 50AL45T... |
|---------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|------------|------------|
| Demo Data           |         |         |         |         |         |         |         |         |         |            |            |
| Ingredients:        | 50AL511 | 50AL512 | 50AL513 | 50AL514 | 50AL515 | 50AL516 | 50AL517 | 50AL518 | 50AL542 | 50AL45T... |            |
| NR (SMR - 10)       | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00  | 100.00     |            |
| N330                | 10.00   | 30.00   | 50.00   | 25.00   | 45.00   | 75.00   | 45.00   | 65.00   | 50.00   | 48.23      |            |
| CaCO3               | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00   | 20.00      |            |
| Naphtenic Oil       | 5.00    | 25.00   | 45.00   | 5.00    | 25.00   | 45.00   | 5.00    | 25.00   | 10.00   | 34.50      |            |
| ZnO                 | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00    | 5.00       |            |
| Stearic Acid        | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00       |            |
| IPPD                | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00    | 2.00       |            |
| S                   | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 1.50    | 0.25    | 1.50       |            |
| TMTD - 80           |         |         |         |         |         |         |         |         | 1.00    |            |            |
| CBS - 80            | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 0.65    | 2.10    | 0.65       |            |
| Total               | 146.15  | 186.15  | 226.15  | 161.15  | 201.15  | 251.15  | 181.15  | 221.15  | 172.35  | 213.88     |            |
| Properties:         |         |         |         |         |         |         |         |         |         |            |            |
| MooneyML(1+4) 100°C | 32.00   | 36.00   | 31.00   | 34.00   | 30.00   | 42.00   | 60.00   | 39.00   | 41.00   | 33.80      |            |
| Mooney I5 / 120°C   | 28.00   | 28.00   | 32.00   | 28.00   | 32.00   | 22.00   | 20.00   | 25.00   | 11.00   | 29.20      |            |
| Density             | 1.08    | 1.12    | 1.16    | 1.13    | 1.16    | 1.19    | 1.19    | 1.20    | 1.11    | 1.16       |            |
| Hardness            | 42.00   | 41.00   | 40.00   | 48.00   | 48.00   | 52.00   | 61.00   | 61.00   | 59.00   | 44.88      |            |
| M300                | 1.80    | 3.00    | 3.00    | 4.40    | 4.80    | 5.30    | 8.00    | 7.60    | 9.40    | 3.88       |            |
| TS                  | 25.00   | 21.00   | 15.00   | 25.00   | 20.00   | 15.30   | 23.00   | 18.00   | 23.00   | 17.62      |            |
| EB                  | 785.00  | 725.00  | 690.00  | 715.00  | 705.00  | 615.00  | 560.00  | 590.00  | 540.00  | 683.86     |            |
| DVR -26°C /24h      | 22.00   | 28.00   | 30.00   | 17.00   | 19.00   | 35.00   | 29.00   | 27.00   | 77.00   | 27.81      |            |
| DVR 0°C /24h        | 10.00   | 14.00   | 14.00   | 8.00    | 12.00   | 16.00   | 13.00   | 12.00   | 16.00   | 13.32      |            |
| DVR 23°C /72h       | 8.00    | 10.00   | 14.00   | 9.00    | 13.00   | 16.00   | 10.00   | 17.00   | 18.00   | 13.35      |            |
| DVR 70°C /24h       | 39.00   | 50.00   | 61.00   | 44.00   | 50.00   | 54.00   | 44.00   | 50.00   | 17.00   | 54.58      |            |

| Criteria: | Name          | Min    | Max    | From | To | Wei... | Trd... |
|-----------|---------------|--------|--------|------|----|--------|--------|
|           | NR (SMR - 10) | 100    | 100    |      |    |        |        |
|           | N330          | 10     | 75     | 48   | 52 |        |        |
|           | CaCO3         | 0      | 20     |      |    |        |        |
|           | Naphtenic Oil | 5      | 45     |      |    |        |        |
|           | ZnO           | 5      | 5      |      |    |        |        |
|           | Stearic Acid  | 2      | 2      |      |    |        |        |
|           | IPPD          | 2      | 2      |      |    |        |        |
|           | S             | 0.25   | 1.5    |      |    |        |        |
|           | TMTD - 80     | 0      | 1      |      |    |        |        |
|           | CBS - 80      | 0.65   | 2.1    |      |    |        |        |
|           | Total         | 146.15 | 251.15 |      |    |        |        |

| Output         | 50AL54Test |
|----------------|------------|
| NR (SMR - 10)  | 100        |
| N330           | 50.85      |
| CaCO3          | 20         |
| Naphtenic Oil  | 38         |
| ZnO            | 5          |
| Stearic Acid   | 2          |
| IPPD           | 2          |
| S              | 1.5        |
| TMTD - 80      |            |
| CBS - 80       | 0.65       |
| Total          | 220        |
| MooneyML(1+4)  | 33.81      |
| Mooney I5 /    | 29.36      |
| Density        | 1.1596     |
| Hardness       | 44.08      |
| M300           | 3.764      |
| TS             | 16.97      |
| EB             | 683.45     |
| DVR -26°C /24h | 28.59      |
| DVR 0°C /24h   | 14.02      |
| DVR 23°C /72h  | 13.57      |
| DVR 70°C /24h  | 55.75      |

Recipe ratios in %: 16 45 19 20

Number format: 12345.67

Import input data from clipboard Auto mix (overwrite mixture) Auto mix (new mixture)

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

- Just double click and set the values to whatever percentage you want
- While doing that, you will see the changes in the 50AL45Test column!
- Take care that the total adds up always to 100%

# Creating a Formula

## Excluding a Compound

The screenshot shows the GrafCompounder version 2.004 interface. It is divided into three main sections: Input data, Criteria, and Output.

**Input data:** A table with columns for various formula IDs (50AL51, 50AL52, 50AL53, 50AL54, 50AL513, 50AL514, 50AL515, 50AL516, 50AL517, 50AL518, 50AL542, 50AL45T) and rows for ingredients and properties. The 'Total' row shows values for each column, with 50AL513 having a value of 19.0476.

**Criteria:** A table with columns for Name, Min, Max, From, To, Wel..., and Trd... It lists various ingredients and their minimum and maximum values.

**Output:** A table with columns for formula IDs and values. It shows the results of the calculations, with 50AL513 having a value of 19.0476.

At the bottom, there is a 'Recipe ratios in %' section with a 'Number format' dropdown set to '12345.67' and buttons for 'Import input data from clipboard', 'Auto mix (overwrite mixture)', and 'Auto mix (new mixture)'.

Say we make an assumption that the data of 50AL513 formula is in question and should be excluded from all calculations

-Deactivation is done with a right click of the cell with the compound name 50AL513 and the name is crossed out

-In the recipes ratio % row we now see a blank cell  
 -The score is still unequal to zero, but now goes to 19.0476

# GrafCompounder

## Data Storage

The screenshot shows the GrafCompounder version 2.004 interface. It features a main data table with columns for various recipes (50AL51 to 50AL45T) and rows for ingredients and properties. An 'Exit Confirmation' dialog box is overlaid on the screen, asking 'Have you saved your data?' with 'Yes, Exit' and 'No, Cancel' buttons. To the right, there is a 'Criteria' table and an 'Output' table. The 'Criteria' table lists materials like NR (SMR-10), N330, CaCO3, etc., with their respective minimum and maximum values. The 'Output' table shows the results for a specific recipe, '50AL54Test Mixture8', with values for each ingredient and property.

| Criteria      | Name | Min    | Max    | From | To | Wei... | Trd... |
|---------------|------|--------|--------|------|----|--------|--------|
| NR (SMR- 10)  |      | 100    | 100    |      |    |        |        |
| N330          |      | 10     | 75     | 48   | 52 |        |        |
| CaCO3         |      | 0      | 20     |      |    |        |        |
| Naphtenic Oil |      | 5      | 45     |      |    |        |        |
| ZnO           |      | 5      | 5      |      |    |        |        |
| Stearic Acid  |      | 2      | 2      |      |    |        |        |
| IPPD          |      | 2      | 2      |      |    |        |        |
| S             |      | 0.25   | 1.5    |      |    |        |        |
|               |      | 0      | 1      |      |    |        |        |
|               |      | 0.65   | 2.1    |      |    |        |        |
|               |      | 146.15 | 251.15 |      |    |        |        |
|               |      | 30     | 60     |      |    |        |        |
|               |      | 11     | 32     |      |    |        |        |
|               |      | 1.08   | 1.2    |      |    |        |        |
|               |      | 41     | 61     | 40   | 45 |        |        |
|               |      | 1.8    | 9.4    |      |    |        |        |
|               |      | 15.3   | 25     |      |    |        |        |
|               |      | 540    | 765    |      |    |        |        |
|               |      | 17     | 77     |      |    |        |        |
|               |      | 8      | 16     |      |    |        |        |
|               |      | 8      | 18     |      |    |        |        |
|               |      | 17     | 54     |      |    |        |        |

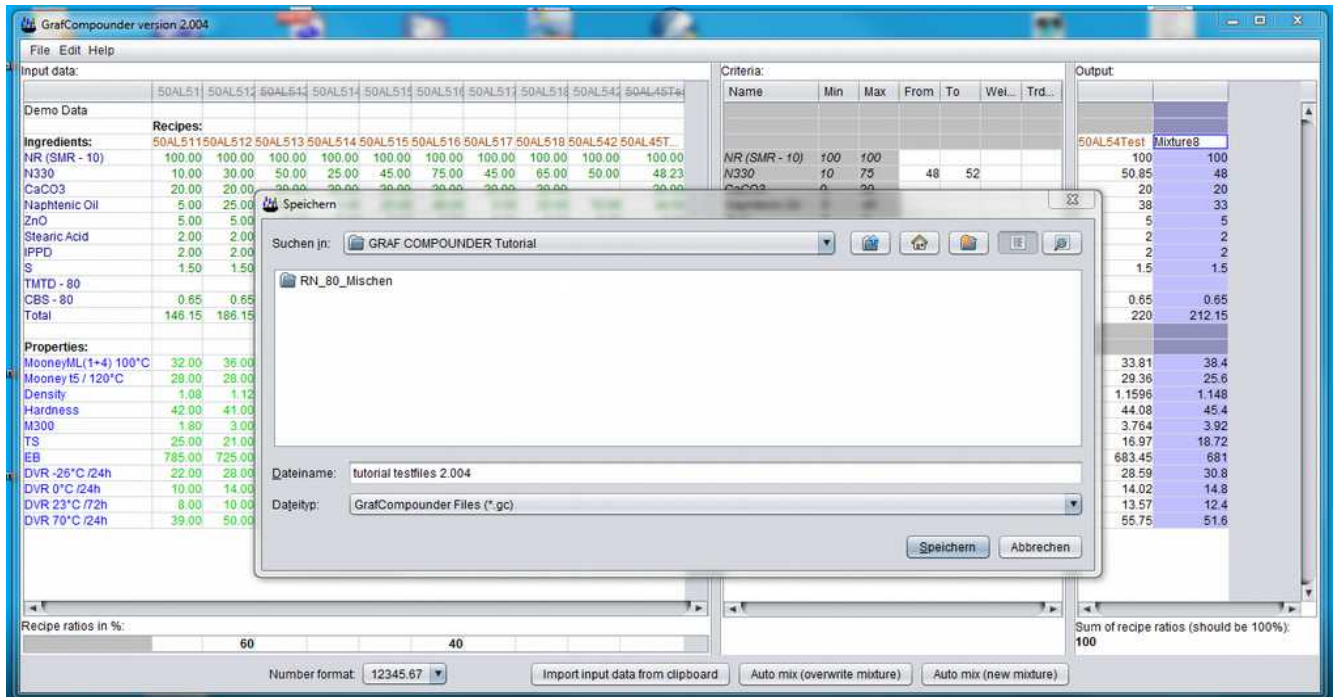
You need to store your results before closing the program

- There are two options:

1) Copy the data table and paste it into your Excel spread sheet

# GrafCompounder

## Data Storage



- The 2<sup>nd</sup> option is:
  - 2) Give the file a new name and store the data in .gc format.

*Note that this format can be opened by the GrafCompounder only*

# Summary

- **With the GrafCompounder you have a newly created tool, which allows you to analyse a compound database using:**
  - **Limits,**
  - **Weight's and**
  - **Trade off's**

**Similar to a simulation tool.**

**You can see the influence of each compound on the result.**

**You can influence this result manually via changing the ratio of the compounds used.**

**Quick analysis of the compounds, which are the result of different criteria and formulation inputs, enables you to make fast and accurate decisions, saving you time and money**

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**The formulas produced due to the selection criteria correspond to the general rules of compounding.**

**These formulas will show property scores larger than the 90% confidence interval compared to those seen in the confirmation experiment.**