Tipps&Tricks with G[raf]Compounder

No. 1
Accelerator Study

Introduction:
Pretend you have a data set (in this case 20 compounds with property data) and you want to test the accuracy of prediction with G[raf]Compounder Tool.
You would select the classical test procedure: You chose one compound data set, eliminate it form the file but use its property data for prediction. In othere words, you use the reamining data to predict a compound, which is not a member of your data sets anymore.

Procedure:
First step is to find out, how measurement errors and outliers will influence the result. You can use graphs to analyse correlations beetween properties with a regression line fit and / or the correlation coeffcient. Your choice is a plot Vulcameter Fmax-min (170°C) over M100, which is shown inn **Figure 1**. The original data shown in Fig.1, the correlation coefficient 0,77.
Second step is to inactivate Compound D, select other compounds for discharge, which are a bit far from regression line. With this measures you have improved the correlation coeffcient to 0,93 (**Figure 2**).
Third step, type all the property data of compound D into the criteria window and use the same values in both columns ("From" and "To"), but without tolerance band. The result is a compound "Mixture 1", which has same / similar properties as Compound D. All property deviations between "Compound D" and "Mixture1" should be inside the measurement error at least.
Fourth step: We click the button "Auto mix (overwrite mixture)" and compare properties of predicted compound with the target "Compound D". In the table below (**Table 1**) you may analyze the data. I have formated all numbers to two digits.
Of course you want to see the predicted "Mixture 1" in the 2D Diagram, which is done with "Refresh recipes" button, as well as the position of Compound D – the target compound (**Figure 3**). Arrow points to a darker yellow spot.
Fifth Step: Finally you need to confirm the result. It means, you will mix the compound using the same procedure of preparation as you did for target "Compound D". Even better, you would repeat mixing

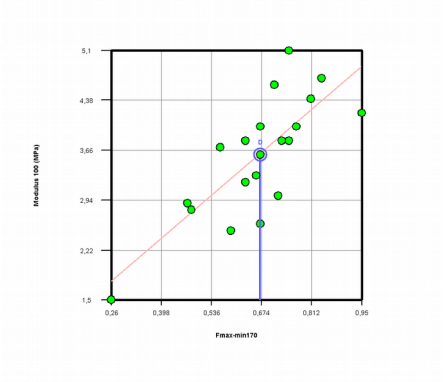

Figure 1: M100 (MPa) over Fmax-min (170°C): Indicated compound D

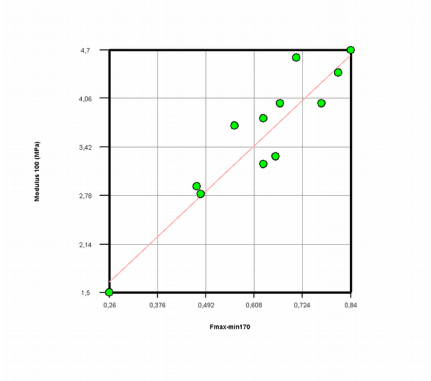

Figure 2: M100 (MPa) over Fmax-min (170°C): Data sets eliminated; correlation coefficient 0,93

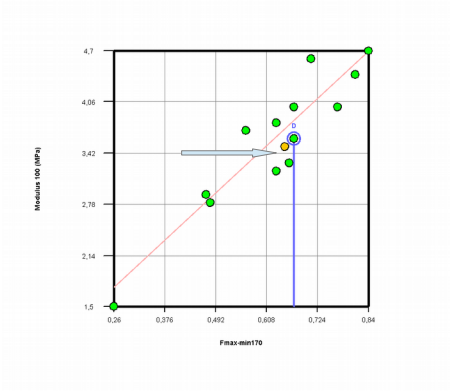

Figure 3: M100 (MPa) over Fmax-Fmin ((170°C): Indicated target Compound D, and predicted compound "Mixture1" with arrow

"Compound D" and the compound "Mixture1". It would enable to learn about tolerances of preparation and raw material changes under consideration, that Compound D was mixed some time ago.

Further Analysis: Most likely you want to see the positon of both compound in other correlation diagrams. For visualization I have selected a graph of CSet (24h 90°C) % M100 (MPa) (**Figure 4**) and Tesnsile Strength (MPa) over Elongation (%) (see Figure 5)
Data taken from test sheets vulcanized at 150°C.

Conclusion: In this experiment it is shown, that using a compound as a target, which is manufactured at the same time with the other compound of the data sets, is helpful to demonstrate the ability and accuracy of the prediction with G[raf]Compounder Software.
Including all properties of the target compound as prediction criteria is helpful to investigate the result in detail but not necessary in practice.

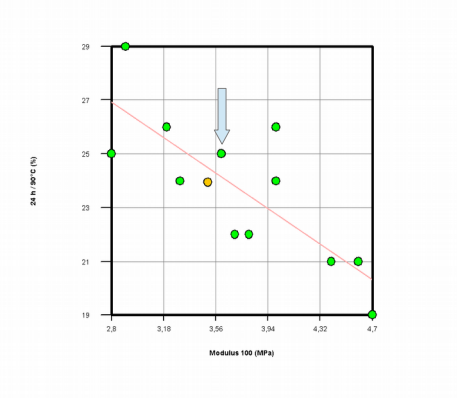

Figure 4: CSet (24h 90°C) % over M100 (Mpa) – correlation coeffcient = - 0,79

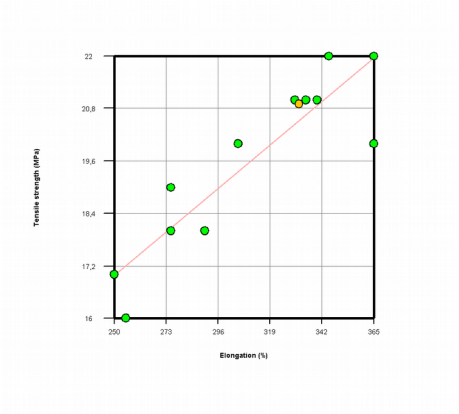

Figure 5: Tensile strength (MPa) over Elongation (%): Target "Compound D" and resulting compound "Mixture1"indicated with arrow.

Table 1: *Recipe and Property Data of Target "Compound D" and Predicted Compound "Mixture1"*

	Recipes:	
Ingredients:	*D*	Mixture1
SMR 50CV	100,00	100,00
Ruß N 550	45,00	45,00
Naphtolen ZD	3,00	3,00
Stearinsäure	2,00	2,00
Vulkanox HS/LG	1,50	1,50
ZnO spez.	3,00	3,00
S-80	0,50	0,40
SDT+ZDT(02)	6,00	6,46
MBTS-80	1,00	0,97
Properties:		
Mooney Scorch 120 °C		
t5/120	9,30	9,73
t35/120	16,40	18,11
Vulcameter 150 °C		
t02/150	0,70	0,86
t90/150	12,50	12,50
Fmax-min150	0,67	0,67
Vulcameter 170 °C		
t02/170	0,60	0,60
t90/170	3,70	4,00
Fmax-min170	0,67	0,65
Vulcameter 190 °C		
t02/190	0,36	0,30
t90/190	1,04	1,16
Fmax-min	0,48	0,51
Vulcanization: 150 °C		
Density (g/mm3)		
Hardness (°ShA)	59,00	58,92
Elasticity (%)	59,00	59,40
Tear strength (N/mm)	33,00	31,09
Modulus 100 (MPa)	3,60	3,50
Modulus 300 (MPa)	18,40	17,42
Tensile strength (MPa)	21,00	20,90
Elongation (%)	330,00	331,84
C - Set acc. DIN 53517		
24 h / 90°C (%)	25,00	23,95
24 h /100°C (%)	29,00	29,49
24 h /125°C (%)	42,00	38,92
72 h /125°C (%)	40,00	37,44
Vulcanization: 180 °C		
Hardness (°ShA)	59,00	58,42
Elasticity (%)	57,00	57
Tear strength (N/mm)	30,00	27,38
Modulus 100 (MPa)	3,20	3,2
Modulus 300 (MPa)	15,70	14,9
Tensile strength (MPa)	21,00	20,01
Elongation (%)	360,00	340,73
C - Set acc. DIN 53517		
24 h / 90°C (%)	21,00	16,06
24 h /100°C (%)	24,00	24,76
24 h /125°C (%)	38,00	36,86
72 h / 90°C (%)	33,00	32,94
Hot air ageing: 7 d / 70 °C	(Vulkanization at 150 °C)	
Hardness (°ShA)	61,00	63,8
Tear strength (N/mm)	25,00	29,52
Modulus 100 (MPa)	4,20	4,25
Tensile strength (MPa)	21,00	19,2
Elongation (%)	300,00	290,19

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