Tipps&Tricks with G[raf]Compounder

No. III
Comparison of Predicition with DoE software 2nd Order Regression

This communication has two aspects:

1. Data sets of rubber compounds may contain physical properties with second order effects, like dynamic properties. Accuracy of prediction using original data in AI (Artificial Intelligence) software is same as prediciton of compounds based on regression.
2. Predicition of Compounds using given values of ingredients yield same result with DoE (Design of Experiments) Software in comparison with AI (G[raf]Compounder).

Introduction:

A Filler / Oil loading study was made to evaluate performance of an NBR compound for a bushing. ANOVA (Analysis of Variance) gave linear correlation of the basic physicals, but the dynamic properties needed an addition of 2FI terms (Two Factor Interaction) to improve the fit on the regression equation for significance.
The none linear correlation between two properties in a x/y diagram (see *Figure 1*) is visualized.

In this communication I want to demonstrate, that AI based software like G[raf]Compounder and Point Prediction with the DoE software get same result, even the **properties are NOT linear correlated**.

In the **first experiment** data taken from this DoE had the following Factors and Limits:

1. CB N550: 27 phr – 67 phr
2. Silica treated: 20 phr – 60 phr
3. Oil (Mesmoll) 5 phr – 19 phr

Compound was based on NBR 28 ACN / 30 M.
All other ingredients are at constant level.

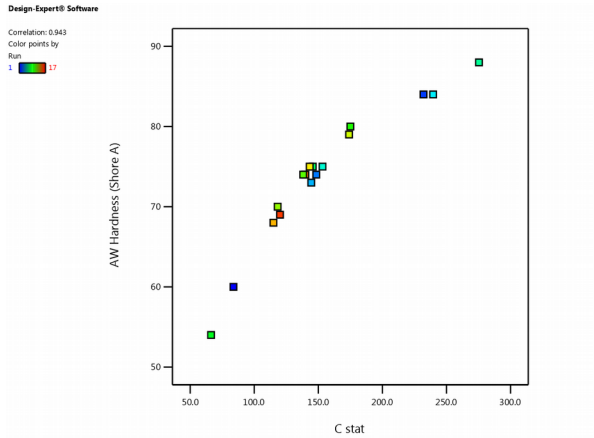


Figure 1: Hardness over C-Static. Correlation 0.94

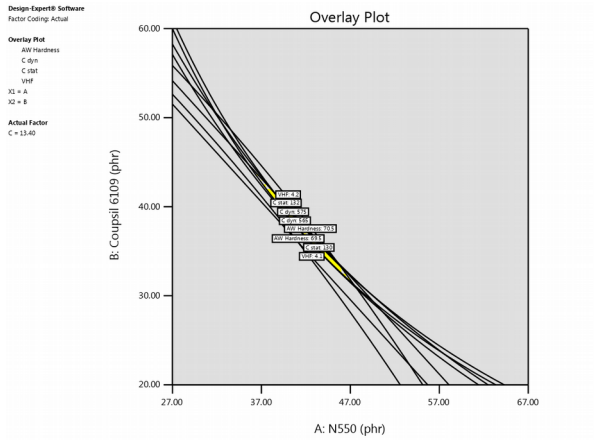


Figure 2: Overlay plot of c-dyn, c-stat, VHF and hardness with x-axis CB N550 and y-axis silica at Oil 13,4 phr.

The dependency of c-dyn, c-stat, dyn-hardening (VHF) and Hardness on Ingredients is shown in an overlay plot with the graphic optimization tool (*Figure 2*).

Setting the values for the factors as followed

1. CB N550: 40 phr
2. Silica treated: 40 phr
3. Oil (Mesmoll) 12 phr

we get a table with all predicted values from all 21 properties measured (*Table 1*).

Exactly these prediciton will be copied into the G[raf]Compounder in the criteria window, but with out upper and lower limits. Then we calculate. The fitness function shows a value of 283, which is quite low, but not zero. Therefore some deviation must be expected. For the evaluation of the results *see table 1*.

Regarding the factors G[raf]Compounder results are:

1. CB N550: 43 phr
2. Silica treated: 39 phr
3. Oil (Mesmoll) 12 phr

The calculated ingredient values are very close to the values used for prediction with the DoE software, while the property values have less than 1% deviation.
The estimated change of the ingredients of +/- 1 phr based on the minor deviation of the properties, but I like to point out: All are inside the measurement tolerances.

The position of the result in the x/y diagram [VHF over Hardness] is indicated by an arrow (F*igure 3*).

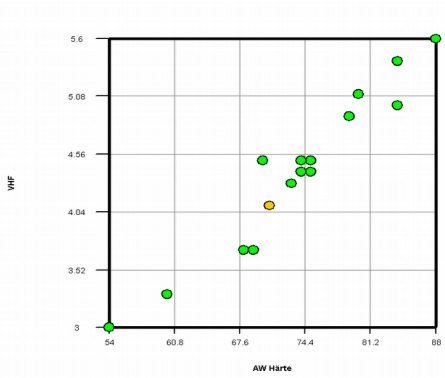
In t**he second experiment** the ingredients are set at the same values like it is done in the DoE software (see above) in the first experiment.

Exactly same values are put in the criteria window of the G[raf]Compounder again without any tolerances (*see factors in table 2*). The results reported underneath in *table 2 (*see responses*),* but without any comment for your own evaluation.

			DoE Prediction tool	G[raf]Compounder
Factor 1	A:CB N550	phr	*40.00*	42.30
Factor 2	B:Silical 6109	phr	*40.00*	38.60
Factor 3	C:Mesamoll	phr	*12.00*	13.44
Response 1	AW Hardness	Shore A	*71.00*	70.69
Response 2	AW TS	MPa	*16.60*	16.46
Response 3	AW EB	%	*350.00*	351.95
Response 4	AW Modul100	MPa	*5.10*	4.80
Response 5	Tear 53507B	N/m	*8.90*	9.10
Response 6	C-Set DIN 22h/100C	%	*30.20*	30.80
Response 7	C-Set VW 94h/100C	%	*79.50*	80.00
Response 8	Ozone VW	Stufe	*0.00*	0.00
Response 9	Density	g/cm³	*1.22*	1.22
Response 10	Aged Hardness	Shore A	*79.00*	78.41
Response 11	Aged TS	MPa	*17.30*	16.91
Response 12	Aged EB	%	*234.00*	235.83
Response 13	Aged Modul100	MPa	*7.90*	7.59
Response 14	C dyn	N	*595.20*	540.44
Response 15	C stat	N	*136.00*	129.04
Response 16	VHF	No	*4.20*	4.10
Response 17	Loss Angle	Grad	*14.80*	15.05
Response 18	F max 175°C	Nm	*6.30*	5.71
Response 19	F min 175°C	Nm	*0.70*	0.76
Response 20	F max-min 175°C	Nm	*5.60*	4.96
Response 21	T 10 175°C	sec	*39.00*	39.99
Response 22	T 90 175°C	sec	*94.00*	93.23

Table 1: Factors and Responses: Comparison of DoE Prediction with GrafCompounder Calculation

Figure 3: VHF (dynamic Hardening) over Hardness



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Factor 2	B:Silical 6109	phr	*40.00*	40.00
Factor 3	C:Mesamoll	phr	*12.00*	12.00
Response 1	AW Hardness	Shore A	*71.00*	69.38
Response 2	AW TS	MPa	*16.60*	17.02
Response 3	AW EB	%	*350.00*	343.30
Response 4	AW Modul100	MPa	*5.10*	5.32
Response 5	Tear 53507B	N/m	*8.90*	8.49
Response 6	C-Set DIN 22h/100C	%	*30.20*	29.36
Response 7	C-Set VW 94h/100C	%	*79.50*	80.63
Response 8	Ozone VW	Stufe	*0.00*	1.33
Response 9	Density	g/cm³	*1.22*	1.21
Response 10	Aged Hardness	Shore A	*79.00*	77.55
Response 11	Aged TS	MPa	*17.30*	16.57
Response 12	Aged EB	%	*234.00*	239.28
Response 13	Aged Modul100	MPa	*7.90*	7.60
Response 14	C dyn	N	*595.20*	603.32
Response 15	C stat	N	*136.00*	140.83
Response 16	VHF	No	*4.20*	3.92
Response 17	Loss Angle	Grad	*14.80*	14.11
Response 18	F max 175°C	Nm	*6.30*	5.97
Response 19	F min 175°C	Nm	*0.70*	1.06
Response 20	F max-min 175°C	Nm	*5.60*	4.91
Response 21	T 10 175°C	sec	*39.00*	42.58
Response 22	T 90 175°C	sec	*94.00*	94.32

Table 2: Ingredients / values specified and compound properties calculated

In the diagram: “VHF (dynamic Hardening) over Hardness” the result of this calculation is indicated by an darker arrow to distiguish from previous one (*Figure 4*).

Conclusion:

It is shown, that AI software can handle small data sets as well as larger ones, which is published on the website www.grafcompounder.com

The difference between data processing using regression analysis and data processing without any treatment using AI (Artificial Intelligence) software is far inside measurement error if a confirmation experiment would be performed.

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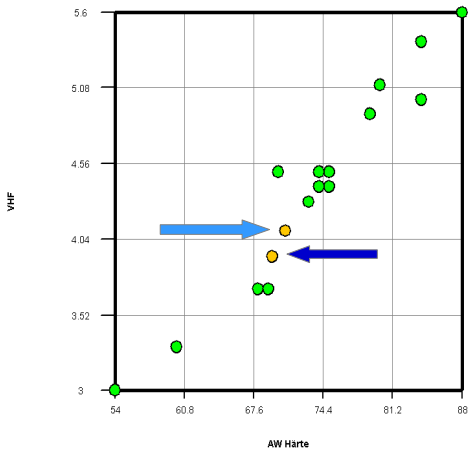

Figure 4: Hardness over VHF (dynamic hardening factor)
light arrow: experiment 1
dark arrow: experiment 2