No. 2
Finding optimum solution with conflicting targets

Introduction:

A conglomerate of recipes based on NR only is used for this demonstration. The data file contains 109 Recipes. They are from different projects containing recipes of some DoE's and few others trials. The frequency distribution of some bulk materials (N330, N550; Aromatic Oil) and sulphur is shown in *Figure 1*.

The distribution of the carbon blacks (CB) contents are more uneven as you would expect in historically grown data sets. Specifically, there are missing compression set values and hot air aging data, like you would usually see in similar selection. Few of the vulcanization systems based on sulfenamides (controls), the majority of the formulas are based on systems built with Dithiophospates.

First Step is defining targets:

*W*e take a look at the range of the property data (*Figure 2*). There is quite a wide spread. Please look at Modulus, Tensile, Elongation, Tear strength and C-Set 24h/70°C for example.

We start with checking some correlations to evaluate, if we have data sets with sufficient quality or if there is a necessity for cleaning.

If we take Modulus 300 over Hardness in a 2D diagram with the original data, we get quite a scatter plot (*Figure 3*).

93 of total 105 recipes included in this figure:
- Discarded one Recipe because no Hardness value
- Discarded eleven more recipes, because they have no values for Modulus 300
- Correlation coefficient is 0,77

To increase the correlation we can define a "correlation corridor" and discard recipes, which seem to be a bit farer from an estimated regression line. It is supposed, that the spread is caused by measurement errors, outliers and the like. Investigation of these recipes (*see Figure 4*) show,
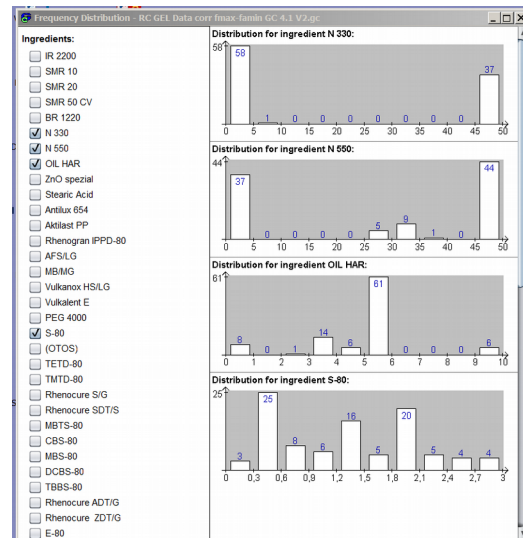
Figure 1: Frequency distribution of bulk material and sulphur in data file. Compound base on IR / NR.

Fmax - Fmin (Nm)	0,32	0,91
Vulcanization: 160		
Hardness (°ShA)	42	65
Elasticity (%)	20	75
Modulus 100	1,1	5,1
Modulus 300	5	16
M300 - M100	3,9	11,9
Modulus M 500	14,7	22,98
Tensile strength	10,5	26
Elongation (%)	235	640
Tear N/mm	10	84
C - Set acc. DIN		
24 h / 70°C (%)	11	25
24 h / 90°C (%)	14	51

Figure 2: Min-Max Property data of compounds in the data set.

1st column – properties
2nd column – min values
3rd column – max values

that they are from one DoE trial and all containing CB N330 in contrast with other recipes with CB N550. Other compounds in the file contain CB N330, but these compounds are closer to the estimated regression line (Figure 4) and there is no reason to discard them. It seems something odd with this specific DoE trial, perhaps a carbon black distribution problem.

The value of the correlation coeffcient is now up to 0,86, which is accepted for purpose of this demonstration (Figure 4).

Second step: Defining the targets

We need to **decide, what we want**. In this case I selected:

- Hardness 55 °SH A – medium,
- Elasticity 70% minimum, as high as possible,
- Modulus 300 14 - 16 MPa (on the higher side),
- Compression set
  24h/90°C 14% (as low as possible)
  C-set 24h/70°C (there are not enough data for sufficient calculation).

The possible conflict is between Hardness and Elasticity on one side and Modulus 300 on the other side.

Now we put data with its limits in the criteria window (table 1).

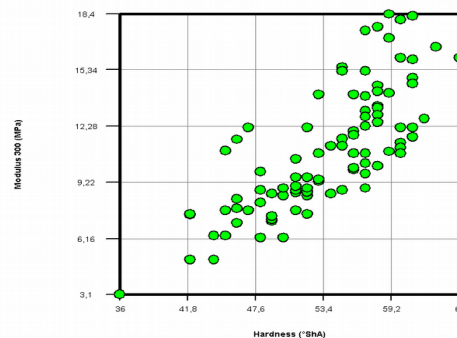We start a calculation with this criteria. The fitness function gives a value of 383, which we accept. The criteria and the result are shown in the t*able 1* below:

Figure 3: Modulus 300 over Hardness: Original data set

Figure 4: Modulus 300 over Hardness: Discarded 19 Recipes

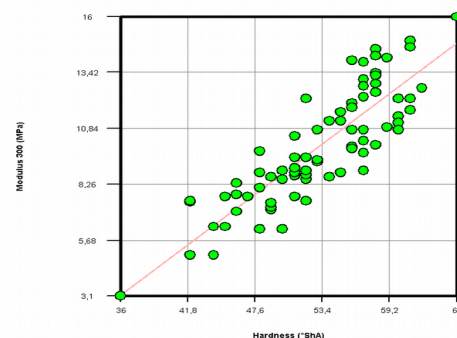| Name	Criteria:			Result
	From	To	Weight	
Hardness °SHA	55	55		55
Elaticity - %s	70	70		69
M300 - MPa	14	16		**10**
C-Set 24h/90°C - %		14		**17**

Table 1: Criteria and result of first calculation.

Hardness and Elasticity is a match, Modulus and C-Set fails.

Third step: Modification of Criteria with weight.

With the Modulus 10 MPa we are far from target. In this case we put a **weight of 100** in the criteria window. The calulation gives a fitness function value of 425, which is good enough. The results are listed in *Table 2* below.

Name	Criteria:			
	From	To	Weight	Result
Hardness °SHA	55	55		61
Elaticity - %s	70	70		66
M300 - MPa	14	16	100	14
C-Set 24h/90°C - %		14		**19**

Table 2: Criteria and result of second calculation.

Modulus lower limit is matched at the expense of Hardness and Elasticity mainly, and a slight increase of the compression set.
In the 2D graph both mixtures are indicated by an arrow in *Figure 5*.
What are the differences of the compound. See the results in table 3 for yoour inspection:

Ingredient	First calculation	Second calculation
CB N330 - phr	18,50	35,70
CB N550 - phr	26,50	9,25
Oil HAR	4,00	3,40

All other changes were marginal and are not reported here.

Conclusion:

- Hardness increase and Elasticity drop are the well known effect of CB changes to finer CB N330
- Modulus increase is related to increase of CB N330 as well.
- Compression set increase is caused by absorption of more accelerator on the CB surface, means less accelerators are available for crosslinking.
- It should be mentioned, that tensile remains same but Elongation at break changes from 420% to 305%, which is also in line with experience.
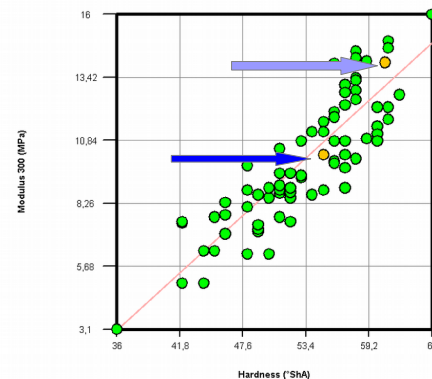
Figure 5: Modulus 300 over Hardness:
Dark blue arrow – first calculation,
Light blue arrow – second calculation

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