Simulation of a statistical experimental design with a new software tool

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Even nowadays rubber compound development is often performed using trial and error methods. Numerous approaches have been made to improve this situation and to draw conclusions from development work having been conducted in the past and to utilize former data and experiences for new formulation development projects. Databank searches, spreadsheet evaluations, linear regressions, statistic experimental design (DoE), or the software GrafCompounder may serve as typical examples for the efforts undertaken in this respect. In this publication, a comparison between the DoE approach and the GrafCompounder is discussed. This will show that the outputs predicted with the MLI software on a database that contains widely varying ingredients/compound recipes can produce similar results to actual compound data analysed with regression analysis (DoE model equations). It will be shown that there is little, if any, difference in correlation to property targets and that those distinctions can be explained in terms of the variances in ingredients. In addition, it will be shown that a historic database can be used regardless of where the compounds were mixed or what equipment was used to mix them and, as long as one understands the influences of the different ingredients used, accurate predictions of compound performance attributes can be made.

1 Introduction

For the most part, rubber compound development is still performed using trial and error methods. Iterations of compounds are made, trialled and then, as soon as the new compound is established, those recipes are stored away in a database. When the time comes to develop another compound, the laboratory work restarts instead of analysing and using the data already stored. This results in wasted time and knowledge. The question is how we can utilize the data in a more efficient manner [1 – 6].

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One solution is to analyse existing recipe data using common table calculation, or databank search tools. These tools sort the data in a certain order based on a compound's ingredients and/or properties, thus allowing the user to identify a suitable compound based on their search criteria. From there, if it does not completely fulfil all requirements, the identified compound can be used as a start for further development work.

Another possible solution is to utilize linear regression. Shortly after statistic experimental design was invented, certain ingredient suppliers (Cabot, Degussa, Bayer) [7] started supplying information on the influence of fillers and oil on compound properties mostly in the form of graphs like contour plots. A closer look at this data shows that most of the relationships between various ingredients and the physical properties of the compounds can be described using a linear regression equation. While these suppliers discovered that in some cases, nonlinear conditions existed, they made assumptions that fairly accurate approximations/conclusions could be made using a linear solution. This information was used to create base compounds in the past and in certain simple applications, can still be used today. Another method, called Design of Experiments (DoE) deals with planning, conducting, analysing and interpreting controlled tests to evaluate the factors that control the value of a parameter or group of parameters. A strategically planned and executed DoE can provide a great deal of information about the effect on a response variable due to one or more factors [8, 9].

Further efforts have been made recently to calculate the properties of compounds based on nonlinear regression equations and even on neuronal network mathematics as well. A couple of patents have been granted on this subject. The author tested one program over a period of two years with little success [10].

However, with advancements in knowledge with respect to ingredient properties as well as process-property relationships, it has become clearer that almost all dependencies can be described linearly as long as truly independent factors are chosen for the experiment. For factors that are dependent on each other such as temperature / time, the relationship can be best described by second order regression. If it does not follow an exponential equation the dependency can be best described via WLF (Williams, Landel, Ferry) or Arrhenius equations. The author has proven this linear correlation between the components of the material and their physical properties through multiple compounding trials.

Based on these relationships, a program named GrafCompounder has been developed, in which a compositional ratio of the multi-component material can be simulated with the use of a multiple linear iteration method (MLI) [11]. It should be considered as well, that even in those cases where there is no exact linear correlation, a linearization shows sufficient accuracy, if small intervals between ingredient changes are calculated in small steps. Therefore this software, in almost all cases, allows one to predict the properties of a compound using an already established compound database, which contains varied data inputs. The resulting calculated compound can be used directly or at least as a starting point for further development work.

The difference/advantage between this approach and the DoE is the fact that the compounder can use any existing database for his investigation, while a DoE requires the creation of specific formulations according to the statistic experimental design rules. Additionally, the GrafCompounder can predict what specific recipe will meet certain target requirements, while with the DoE, it can only infer certain dependencies from the input factors.

In this publication, a comparison between the DoE approach and the GrafCompounder is discussed. This will show that the outputs predicted with the MLI software on a database that contains widely varying ingredients/compound recipes can produce similar results to actual compound data analysed with regression analysis (DoE model equations). It will be shown that there is little, if any, difference in correlation to property targets and those distinctions can be explained in terms of the variances in ingredients.

Tab. 1: Compound recipes used in laboratory trial

Ingredient	Amount / phr
NR STR 20	100
CB N330	var
CB N550	var
Naphthenic oil	var
ZnO	5
Stearic acid	2
Paraffin wax	2
TMQ	1
IPPD	2
S	1.5
TMTD	0.5
CBS	1.3

Tab. 2: Ingredients used in formulation database

Ingredients	Lower limit LL in phr	Upper limit UL in phr
CB N330	0.00	75.00
CB N326	0.00	40.00
CB N550	0.00	60.00
$CaCO_3$	0.00	20.00
Naphthenic oil	0.00	45.00
Paraffinic oil	0.00	10.00
ZnO	0.00	10.00
Stearic acid	0.00	2.00
Paraffin wax	0.00	2.00
TMQ	0.00	2.00
IPPD	2.00	3.00
S	0.25	3.25
DPG	0.00	0.20
DTDM	0.00	1.00
TMTD	0.00	1.20
CBS	0.00	2.10

2 Experimental

2.1 Preparation of compounds

A fractional experimental design was performed in the laboratory of Mahidol University, Bangkok, Thailand. The compounds were based on the STR 20 natural rubber. The recipe is given in **table 1.**

As factors, two fillers and the oil were varied within the following limits:

Filler 1: CB N330 30 phr – 70 phr
Filler 2: CB N550 0 phr – 20 phr
Oil: Naphthenic oil 5 phr – 45 phr

All compounds were mixed in a 0.4 L laboratory mixer (Brabender OHG), and compression moulded in a laboratory press: 2 mm sheets were moulded at 160 °C/10 min and the 6 mm sheets were moulded at 160 °C/15 min.

The NR used was STR 20; all other ingredients used were standard materials taken as is from the market.

Physical properties were measured according to ISO standards.

The data were then processed with the statistic experimental design software Design Expert. A factorial design was chosen without centre point, giving eight data sets.

2.2 Simulation of compounds

For simulation purposes compound data were taken from "Natural Rubber Formulary and Property Index" [12].

The compounds were mixed on a laboratory scale mixer, but the size and type of the mixer was not disclosed.

The sheets were moulded and vulcanized in a laboratory platen press. The compounds were moulded with various times and temperatures, typically 14 min or 15 min/150 °C.

Physical properties were measured according to ISO standards.

The compounds were based on SMR 10 or SMR CV. As carbon black either CB N330 or CB N326 was used.

The list of ingredients used in this database and the spread of data, respective their lower (LL) and upper limits (UL) of ingredients used in all compounds are given in **table 2.**

2.3 Simulation conditions

NR compound data were processed with GrafCompounder software. CB N330 and/or CB N326 was used as the reinforcing carbon black in the database for simulation **(tab. 2),** instead CB 330 was used in the laboratory work because of its availability, but considered as exchangeable with CB N326 for the purpose of this project.

Naphthenic oil was the preferred oil in NR compounds. In some cases paraffinic oil was used for the recipes included in the database **(tab. 2)** although the solubility is less in NR. If the simulation resulted in a minor portion of paraffinic oil, the content was set to zero and the amount of naphthenic oil was adjusted accordingly.

For appropriate calculation some boundary conditions were used:

- CB N330 had a target value with a higher weight. If the resulting compound contained CB N326 the amount was added to the CB N330 amount, keeping in mind that CB N330 and CB N326 were seen as exchangeable.
- $CaCO_3$ was set to 5 phr max., but in the final compound it was eliminated under the assumption that such a low amount would not yield a measurable effect on any property.
- Sulfur was set to a maximum of 1.5 phr.
- CBS was set to a target between 1.0 phr and 1.3 phr.
- TMTD was set to a target between 0.3 phr and 0.5 phr with a higher weight.

The weight is a program feature, to give the selected targets a preference. The runs to calculate the experiment executed at the same time in the laboratory were done in two ways:

- In the first calculation the ingredients were set in between the targets with the boundary conditions as mentioned above.
- In the second run the ingredients and the hardness were used. The hardness in conjunction with the ingredients gave much closer recipes, which could be now processed with the DoE software. The DoE software allows the input of historical data. This is a possibility to calculate a design even without knowing its design layout.

The data were processed with the statistic experimental design software Design Expert.

A factorial design was chosen without a centre point, which gave eight sets of data points. Both, the executed design and the measured properties (see 2.1) and the simulated design with the calculated properties, were compared by statistics and 3D contour plots.

3 Results and discussion

3.1 Fractional experimental design

The results of the experimental DoE are shown in **table 3.** All factors have a significant influence on the responses. In the table the minimum and the maximum value for each response is given with its mean, the standard deviation, the ratio of the maximum and minimum value, the transformation and the model used. Only in a couple of responses a nonlinear model (R2FI or R3FI) is required to produce a statistically significant regression. The majority of the responses are best described with a linear regression equation. In case the ratio between the maximum and minimum value is close to, or greater than 10, a transformation of the response data is advantageous. It produces a correlation between the data measured and calculated with the regression equations, which is more accurate.

As expected, all factors have a significant effect on the responses. All ratios are larger than 1. Surprisingly the influence on compression set at 70 °C and 100 °C is smaller than the influence on compression set at 23 °C. The ratio of tensile with 1.6 is quite small, but in this case we are dealing with much larger numbers.

In this paper we will focus on the basic physicals like hardness, tensile and elongation, which are the most important responses when it comes to typical specifications.

Most of the responses are best described with main effects linear regression, but a few – like tensile and compression set – require at least one mixed term, nonlinear regression R2FI or R3FI, to achieve the best fit; however, the nonlinearity is quite small.

3.1.1 Hardness

The influence of the two carbon blacks – CB N330 and CB N550 – on hardness is larger than the influence of oil:

$$H = 42 + 0.36 \cdot (\text{CB N330}) + 0.40 \cdot (\text{CB N550}) - 0.35 \cdot (\text{Oil}) \quad (1)$$

Figure 1 of actual versus predicted hardness values demonstrates the accuracy of the measurement and the correlation and the

Tab. 3: Coefficient table of experiments performed

Ingredient	Unit	Type	Minimum	Maximum	Mean	Std. dev.			
CB N330	phr	Numeric	30.00	70.00	50.00	20.00			
CB N550	phr	Numeric	0.00	20.00	10.00	10.00			
Naphthenic oil	phr	Numeric	5.00	45.00	25.00	20.00			
Property	**Unit**	**Obs.**	**Minimum**	**Maximum**	**Mean**	**Std. dev.**	**Ratio**	**Trans**	**Model**
ML(1+4) 100 °C	MU	8	12.16	68.38	32.71	19.1588	5.62336	None	Main effects
Mooney t_5 120 °C	min	8	4.00	14.22	8.97125	3.3462	3,555	None	Main effects
F_{min}	dNm	8	0.23	3.35	1.2275	1.04498	14.5652	Natural log	Main effects
F_{max}	dNm	8	4.77	28.30	13.8425	7.91856	5.93291	None	Main effects
t_{s2} 165 °C	min	8	0.30	1.41	0.8175	0.421282	4.7	None	R3FI
t_{10} 165 °C	min	8	0.32	1.24	0.72125	0.360454	3,875	None	Main effects
t_{90} 165 °C	min	8	0.55	2.08	1.3	0.429119	3.78182	None	R3FI
Density	g/cm³	8	1,015	1,199	1.1055	0.0601712	1.18128	None	Mean
Hardness	Shore A	8	37	74	54,875	11,569	2.00272	None	Main effects
M100	MPa	8	0.70	6.98	2.53	2.04331	9.97143	Natural log	Main effects
M200	MPa	8	1.42	15.65	6.14	4.74414	11.0211	Natural log	Main effects
Tensile strength	MPa	8	17.33	28.21	21.2375	4.0434	1.62781	None	R2FI
Elongation at break	%	8	245	730	547,125	154,931	2.97959	Power	Main effects
Compression set 23 °C/24 h	%	8	4.60	11.42	8.3975	1.99843	2.48261	None	R3FI
Compression set 70 °C/72 h	%	8	26.41	38.02	30.6638	4.22769	1.43961	None	R2FI
Compression set 100 °C/24 h	%	8	38.54	50.19	42,945	4.26904	1.30228	None	Main effects
E´ at RT	MPa	8	2.03	45.91	15.5716	14.6972	22,597	Natural log	Main effects
E" at RT	MPa	8	0.08	5.17	1.52133	1.72362	64.5561	Natural log	Main effects
tan δ at RT	no	8	0.04	0.11	0.0788823	0.0292583	2.90352	None	Main effects

dependency of the hardness on CB N330 and oil at two different CB N550 levels (0 phr / 20 phr).

3.1.2 Tensile at break

The effect of the factors on tensile at break (TB) is significant only when mixed terms are introduced: AC represents the interaction between CB N330 and oil. The interaction factor BC (CB N550 and oil) is less important. We theorise the tensile measurement is less accurate perhaps because of its sensitivity to dispersion.

$$TB = 34 - 0.17 \cdot (CB\ N330) - 0.11 \cdot (CB\ N550) - 0.31 \cdot (Oil) + 3.33E^{-003} \cdot (CB\ N330)(Oil) \quad (2)$$

Figure 2 of the actual TB values versus predicted demonstrates the difference in accuracy of the measurement compared to hardness and the correlation and the dependency of the TB on CB N330 and oil at two different CB N550 levels (0 phr / 20 phr).

3.1.3 Elongation at break

Finally we look at the dependency of the elongation at break (EB) on the various factors. In contrast to the TB calculations the linear regression is a good fit. The influences of CB N330 and CB N550 are larger than the oil and no mixed term is required to fit the data.

$$EB = 750 - 5.0 \cdot (CB\ N330) - 5.36 \cdot (CB\ N550) + 4.10 \cdot (Oil) \quad (3)$$

Figure 3 demonstrates the accuracy of the measurement, which is in line with the TB. The link between both responses is the stress/strain curve. The effect of CB N330 on EB at low and high levels of CB N550 is also shown. The data for EB are in good agreement with the linear regression equation shown above.

3.2 GrafCompounder simulation of DoE

To perform the simulation, as mentioned, a compromise on some raw materials was necessary. SMR was used instead of STR. The carbon blacks CB N326 and CB N330 were taken as comparable. We used these assumptions as we are dealing with basic physicals only, but they may not hold true for more sophisticated compound properties. Additionally, if the calculations gave a very small number in phr of ingredients and the effect of these ingredients on compound properties was recognized as small then they were ignored/eliminated altogether. The content of ingredients was also rounded in case of odd numbers.

Fig. 1: Hardness plot – predicted versus actual data and 3D contour plots at two CB N550 levels

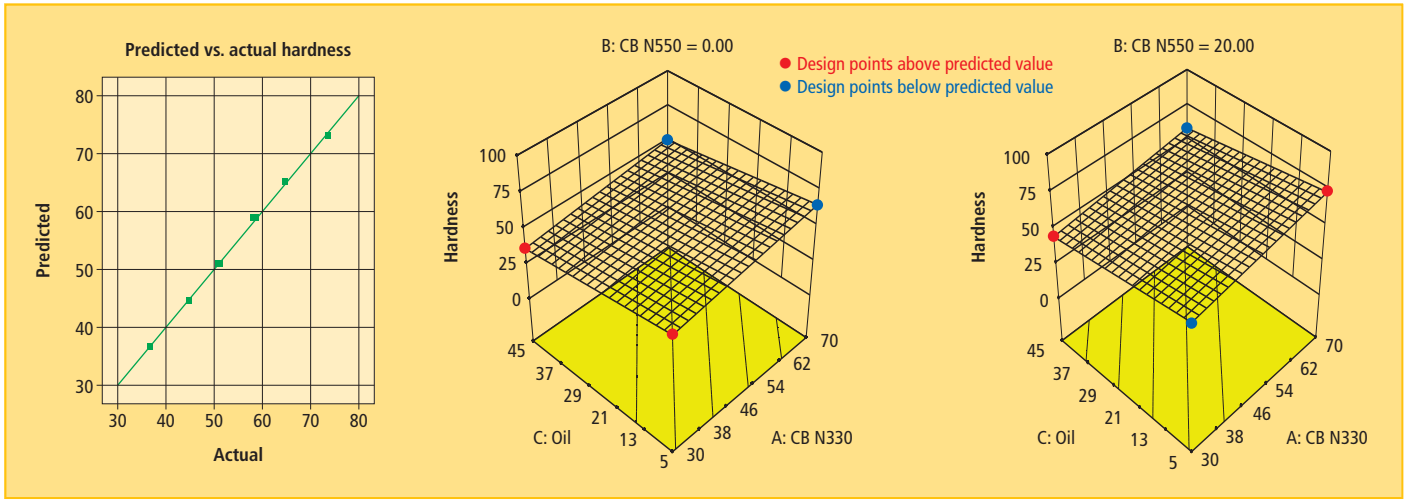
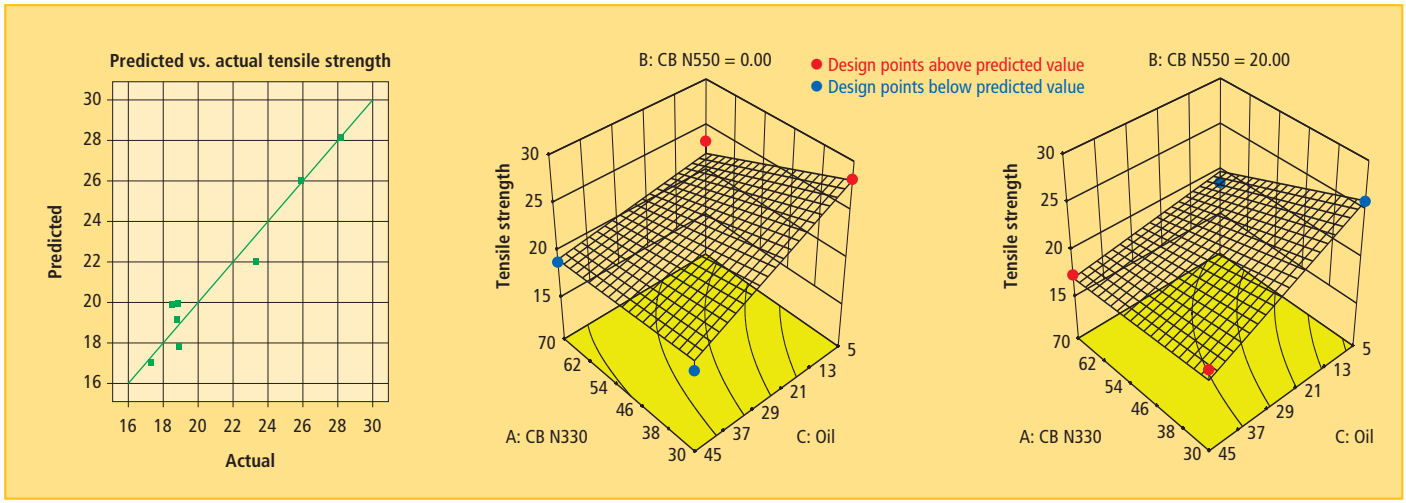


Fig. 2: Tensile plot – predicted versus actual data and 3D contour plots at two CB N550 levels



3.2.1 Simulation run with input of ingredients only

At first the database query was performed with CB N330 in target (intervall was ± 1 phr and a weight of 50), CB N550 in target with a weight of 10 and a Trdoff of 10, $CaCO_3$ instead was set to 0 with a Trdoff of 10. Trdoff is a program feature, which grants a preference in case of a conflict with another value. Other carbon blacks used in the database were set to zero. Sulfur was set in between 1.4 and 1.6 phr with a weight of 50 for all queries. This was done to force the compound calculation in the desired direction. Given these conditions, ten compounds were calculated and the data transferred into the DoE software and analyzed.

It turned out that the spread of data – irrespective of the standard deviation – was much smaller compared to the DoE laboratory results **(tab. 4).** In comparison with **table 3** the hardness has a ratio of 1.14 compared to 2.002, which is quite a large difference. The minimum value for hardness achieved was 59 Shore A and the highest value was 67.6 Shore A. Only the compression set 70 h/24 °C and 24 h/-26 °C has a ratio in the order of 1.8. Data with such a narrow spread means an insignificant correlation between factors and responses. The data were not processed further.

3.2.2 Consequences of the simulation run with input of ingredients only

One reason for this is obviously the size of the database. It would be helpful combining

Tab. 4: Coefficient table of simulated experimental design – first run

Name	Unit	Type	Minimum	Maximum	Coded	Values	Mean	Std. dev.	
CB N330	phr	Numeric	23.30	53.60					
CB N550	phr	Numeric	0.00	20.00					
Naphthenic oil	pht	Numeric	7.00	14.00					
Name	**Unit**	**Obs.**	**Minimum**	**Maximum**	**Mean**	**Std. dev.**	**Ratio**	**Trans**	**Model**
ML(1+4) 100 °C	MU	10	40.52	51.25	47,499	3.15473	1.26481	None	2FI
Mooney t_5 120 °C	min	10	14.36	21.74	17,327	1.95226	1.51393	None	Linear
Density	g/cm³	10	1.11	1.13	43,040	0.00674949	1.01802	None	Linear
Hardness	Shore A	10	59.24	67.64	61,794	2.34816	1.1418	None	Linear
M300	MPa	10	8.77	11.2	9.59	0.754836	1.27708	None	Linear
Tensile strength	MPa	10	21.8	24.75	23,623	0.879293	1.13532	None	Linear
Elongation at break	%	10	524.74	571.24	549.56	15.3184	1.08862	None	Linear
Compression set –26 °C/24 h	%	10	34.31	65	50,481	8.58112	1.89449	None	2FI
Compression set 0 °C/24 h	%	10	11.16	15.04	13,187	1.40904	1.34767	None	Linear
Compression set 23 °C/72 h	%	10	9.84	17.76	13,145	2.26318	1.80488	None	Linear
Compression set 70 °C/24 h	%	10	21.75	27.46	25,226	1.58228	1.26253	None	2FI

Tab. 5: Coefficient table of simulated experimental design – second run

Name	Unit	Type	Minimum	Maximum	Coded	Values	Mean	Std. dev.	
CB N330/26	phr	Numeric	0.00	67.50			26.92	20.99	
CB N550	phr	Numeric	0.00	56.00			20.45	18.86	
Oil	phr	Numeric	7.00	36.00			16.95	9.97	
Name	**Unit**	**Obs.**	**Minimum**	**Maximum**	**Mean**	**Std. dev.**	**Ratio**	**Trans**	**Model**
ML(1+4) 100 °C	MU	16	30.7	48.44	39.9775	6.32151	1.57785	None	Quadratic
Mooney t_5 120 °C	min	16	17.01	32.79	24.1144	5.06844	1.92769	None	Quadratic
Density	g/cm³	16	1.07	1.17	1.12375	0.0318067	1.09346	None	Linear
Hardness	Shore A	16	42	69	56,085	8,414	1.63173	None	Linear
M300	MPa	16	3.3	14.0	8.11375	3.49055	4.30368	None	Linear
Tensile strength	MPa	16	18	26	21.9213	2.63913	1.46735	None	R2FI
Elongation at break	%	16	453	686	575,873	74.1789	1.51602	None	Linear
Compression set –26 °C/24 h	%	16	22.4	55.5	34.5281	8.47521	2.47082	None	Quadratic
Compression set 0 °C/24 h	%	16	7.5	16.0	11.1738	2.70492	2.14477	None	Quadratic
Compression set 23 °C/72 h	%	16	7.8	17.3	11.4387	3.08663	2.21795	None	2FI
Compression set 70 °C/24 h	%	16	22.3	52.5	32.6637	9.02146	2.3618	None	Linear

the carbon blacks (CB N330 + CB N326) with their influence on the spread. Combining the carbon blacks means, we added the amount of CB N326 to CB N330 calculating further with the total, which gives a slight shift to the higher reinforcing CB; in **table 5** referred to as CB N330/26. The same procedure was done for the oils. In case paraffinic and naphthenic oil showed up in the calculated recipe, it was taken as exchangeable (referred to as oil in **table 5)** and further calculation was done with the total of paraffinic and naphthenic oil. Physical properties will not be largely affected, but some minor effects could be expected due to this consolidation.

3.3 Simulation run with input of ingredients and hardness

In the second run ingredient limits as shown above as well as hardness were taken as factors. Here, more recipes were calculated than needed for such a statistic experimental design with three factors, but the same weights and Trdoffs were used as before.

With this modified strategy the simulated compounds and values were processed with the DoE software and the results listed in **table 5** were achieved. The data in the table show clearly the similarity in the spread of data to the conducted DoE, if one looks specifically at the hardness and other values, for example, the modulus M300.

3.3.1 Hardness: simulated DoE

Hardness was evaluated to show the correlation to filler and oil. The analyses shown in **figure 4** are similar to the results of the conducted DoE. The normal probability plot is shown instead of the predicted versus actual plot. This plot shows nothing unusual with the linear regression model equation.

As expected, hardness decreases with increasing amount of oil and increases with increasing amount of filler. The magnitude of the slope of the plane is shown in the regression equation as onset and factors.

$$\text{Hardness} = 42 + 0.506 \cdot (\text{CB N330/26}) + 0.55 \cdot (\text{CB N550}) - 0.64 \cdot (\text{Oil}) \quad (4)$$

As already seen, the onset of 42 is comparable to the order of the hardness of unfilled NR, while the factors for the fillers and oil are slightly higher than those seen from actual results, but this is to be expected.

3.3.2 Tensile: simulated DoE

TB is dependent upon crosslink density and reinforcement, but as mentioned, is also sen-

Fig. 3: Elongation plot – predicted versus actual data and 3D contour plots at two CB N550 levels

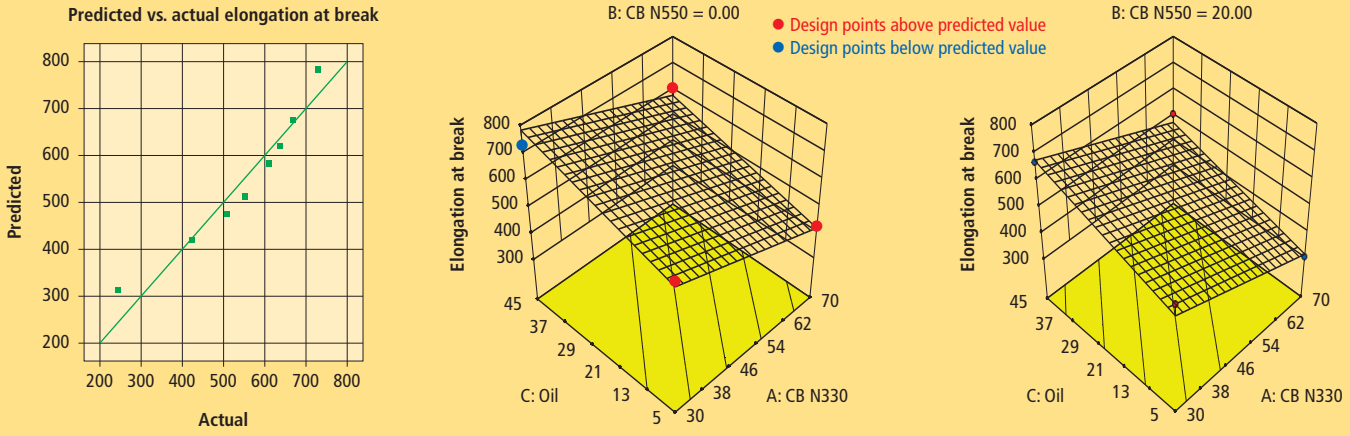
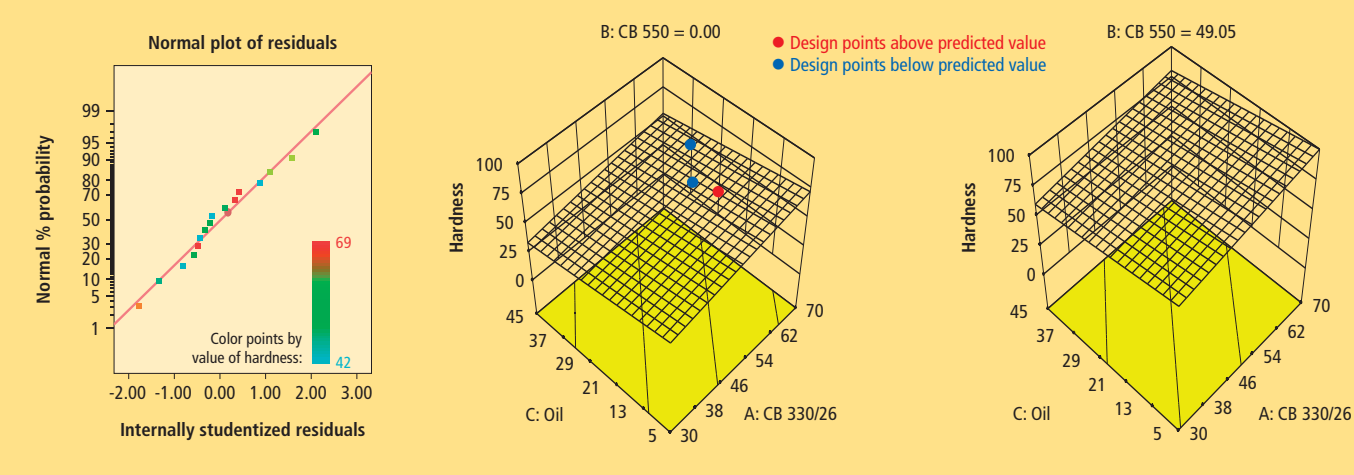


Fig. 4: Hardness – normal probability plot and 3D contour plots at two CB N550 levels (simulated design)



sitive to dispersion. Given this, it should be a very good measure of whether an accurate simulation of a DoE is possible. Based on the hardness results, one can expect a similar deviation between the TB of the conducted DoE and the TB of the simulated DoE. Also as mentioned, there is the assumption that the STR 20 used in the conducted DoE is comparable to SMR 10 or SMR 20. **Figure 5** shows the normal probability plot and the 3D surface plots with CB N330/26 on the x-axis and oil on the y-axis at two different CB N550 levels.

The regression equation has the following factors describing the onset and slope:

$$TB = 31.7 - 0.11 \cdot (CB\ N330/26) - 0.14 \cdot (CB\ N550) - 0.23 \cdot (Oil) \quad (5)$$

The factors show a minor difference of the onset, as well as a smaller influence of CB N330/26 and oil in comparison to the conducted DoE. For a more accurate result – even though there is no real need to do so as the statistic is only slightly improved – the mixed term is given in **equation 6:**

$$TB = 34.6 - 0.19 \cdot (CB\ N330/26) - 0.18 \cdot (CB\ N550) - 0.35 \cdot (Oil) + 3.35E^{-003} \cdot (CB\ N330/26)(Oil) \quad (6)$$

The mixed term shows the influence of the CB N330/26 and the oil with its effect on the slope of the plane in the 3D contour plot to be very small.

3.3.3 Elongation: simulated DoE

Dependency of EB on the fillers and oil is shown in **figure 6.** The normal probability plot and the 3D surface plots at two levels of CB N550 are shown. The regression **equation 7** shows a slightly lower onset and a larger influence of CB N330/26 than seen in the conducted trial. The CB N550 and the oil influences, however, are very similar.

$$EB = 727 - 3.9 \cdot (CB\ N330/26) - 5.3 \cdot (CB\ N550) + 0.36 \cdot (Oil) \quad (7)$$

4 General analysis of the results

Another way to look at the findings of this project is to compare all regression equations for the selected physicals and discuss them with respect to material behaviour **(tab. 6).**

The intercepts of the regression equations are almost the same no matter whether it is taken from the conducted or simulated results. The intercept of 42 for the hardness is close to the hardness of unfilled natural rubber. Surprisingly the contribution of the hardness increase of CB N550 is higher than for the CB N330 and CB N330/26. Again the reason for this may be the differing interactions of the CB N550 with the different natural rubbers as well as the processing conditions.

As far as hardness is influenced by the oil, the differences may be because of the dif-

Fig. 5: Tensile – normal probability plot and 3D contour plots at two CB N550 levels (simulated design)

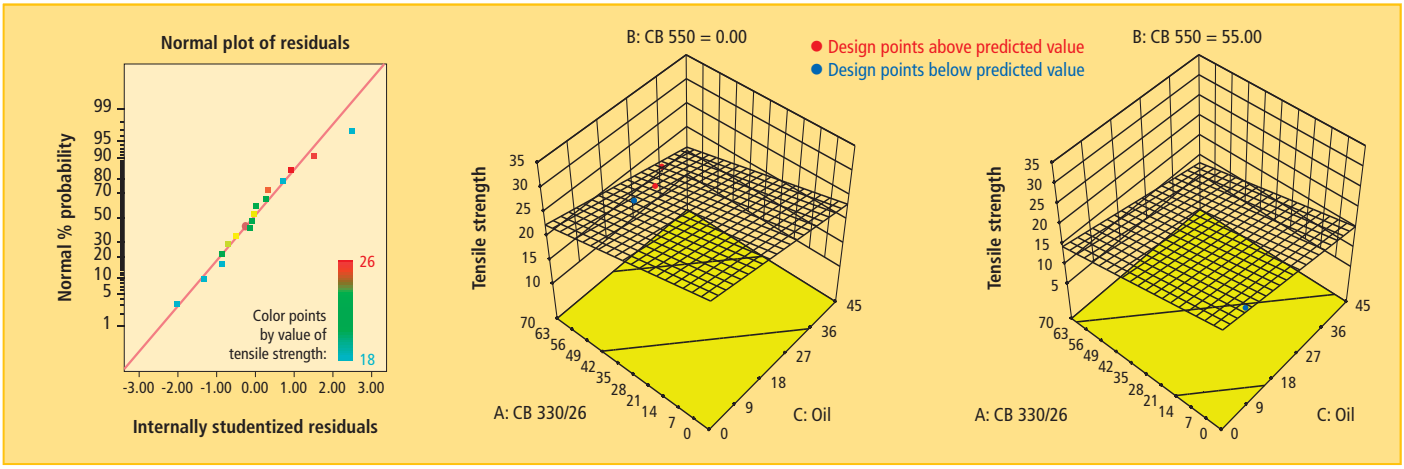
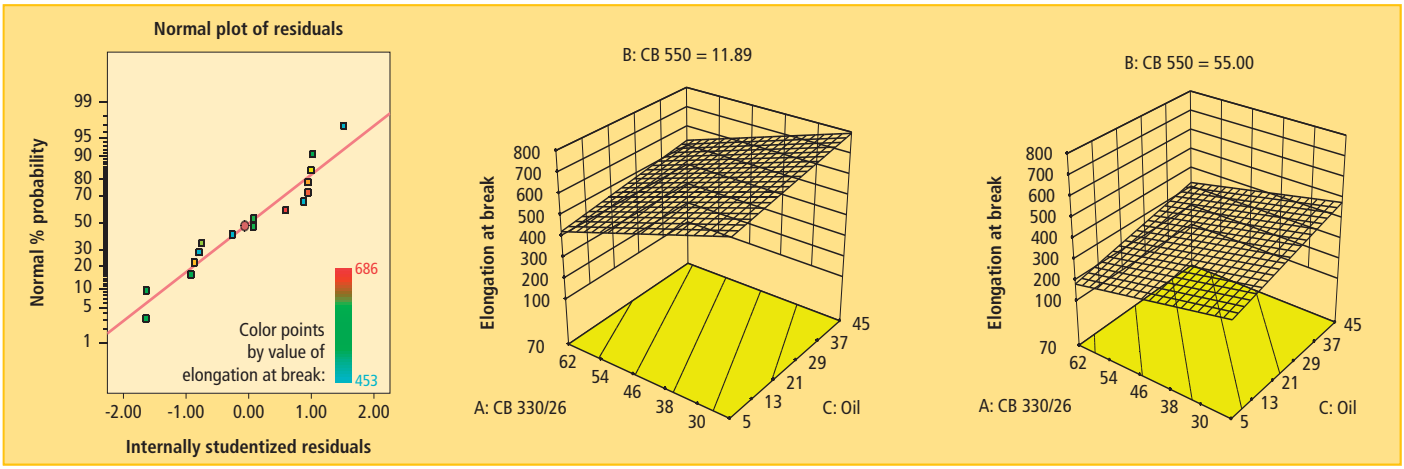


Fig. 6: Elongation – normal probability plot and 3D contour plots at two CB N550 levels (simulated design)



fering nature of the oils (naphthenic / paraffinic-naphthenic blend) and their solubility in the different rubbers.

The regression equations describing the TB are similar regardless which method is used. A small difference can be recognized only in the N550 influence. Again, one needs to keep in mind that such differences can occur due to dispersion or/and due to different preparation methods. In the evaluated case, TB is estimated to be on the higher side compared with the simulated case. In actuality, a confirmation experiment would fail with higher TB.

This is also true to some extent for the regression describing the EB. The factors for the influence of the CB N330 and CB N330/26 respectively might be because of their differing structures.

5 Conclusions

Typically, using very different sets of data and unknown processing conditions to make predictive conclusions is very risky. However, this paper has proven that even though the ingredients in the laboratory DoE vary significantly from those used for the simulations, all of the physicals have very similar trends. Any differences seen are quite small and they can be explained by the following:

- There is a difference in the molecular weight of the STR versus the SMR rubbers.
- Varying reinforcement levels exist between the CB N330 and CB N326. These carbon blacks are similar in absorption but dissimilar in surface activity.

With an intimate knowledge of the effects of raw materials in a compound, the risks mentioned above can be foreseen and therefore invalid conclusions can be avoided.

Therefore, in general, the results show that even with such extreme differences between the data generated for the conducted and simulated DoEs it is possible to achieve similar conclusions. This means that any historic database can be used regardless of where the compounds were mixed or what equipment was used to mix them and, as long as one understands the influences of the different ingredients used, accurate predictions of compound performance attributes can be made.

6 Acknowledgment

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Tab. 6: Factors of regression equations: performed versus simulated experimental design

Property:		Hardness		Tensile		Elongation	
Factor		Conducted	Simulated	Conducted	Simulated	Conducted	Simulated
Intercept		42.00	42.00	34.00	34.60	750.00	727.00
A	CB N330	0.36		–0.17		–5.00	
A	CB N330/26		0.50		–0.19		–3.90
B	CB N550	0.40	0.55	–0.11	–0.18	–5.36	–5.30
C	Oil		–0.64		–0.35		3.60
C	Naphtenic oil	–0.35		–0.31		4.10	
AC				0.00333	0.00335		

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