DKG SÜD / SÜD WEST

Vorausschauende Daten Analyse

und

Organisation von Daten

in der

Mischungsentwicklung

April 3-4, Würzburg, Germany

Dr. Hans-Joachim Graf

- **Introduction**
- **Predictive data analysis**
- **Organization of data**
- **Database**
- **Tools for analysis**
- **Conclusion**

Data Analysis

- **Statistics**
  - *Analysis of happenstance data, to prove theories, estimations and a hypothesis*
- **Data mining**
  - *Analysis of happenstance data, to identify hidden correlations between data*
- **Predictive Analytics**
  - ***Statistic and Data mining procedure to predict a future behavior with existing data sets***

Source: 2011 IBM Corporation

What is predictive data analytics?

- **The application of statistical analysis of historic data to predict future trends, patterns, and behavior to improve the outcomes in automated and human processes**

Source: 2011 IBM Corporation

Where to use predicitve data analysis in rubber manufacturing?

- **IBM SPSS predictive analytics solutions enable manufacturers to:**
- **Proactively identify equipment reliability and product quality issues**
- **Decrease equipment failures with reliability-centered maintenance**
- **Reduce costs associated with MRO (repair and overhaul) inventory and labor**

Source: 2011 IBM Corporation

Where to use predictive data analysis in rubber manufacturing?

- **Across every phase of production, predictive analytics helps manufacturers:**
  - **Efficiently perform root-cause analyses**
  - **Reduce machine/appliance/asset downtime due to the failure of critical parts**
  - **Minimize supply chain problems due to product issues**
  - **Improve productivity of maintenance resources**
  - **Avoid costs of machine/appliance/asset failure**
  - **Realistically forecast warranty accruals**

Source: 2011 IBM Corporation

How to do predictive data analysis?

- **Classification**
  - **Uses a known outcome field (target) and its relationship to predictor inputs to build a model that can predict the target value in new data**
  - ***C&RT, QUEST, Linear Regression, Logistic Regression, Neural Network, SVM***
- **Association**
  - **Builds a model that shows the patterns of entities (events, purchases, attributes) in a data set**
  - ***Apriori, CARMA, Sequence***
- **Segmentation**
  - **Divides the data set into clusters of records that are similar**
  - ***K-Means, Kohonen, TwoStep Cluster***
- **Forecasting**
  - **Produces future estimates for time based data**
  - ***ARIMA, Exponential Smoothing***

Why not predictive analytic?

- Software is available on the market
- Modern controls deliver all kind of data

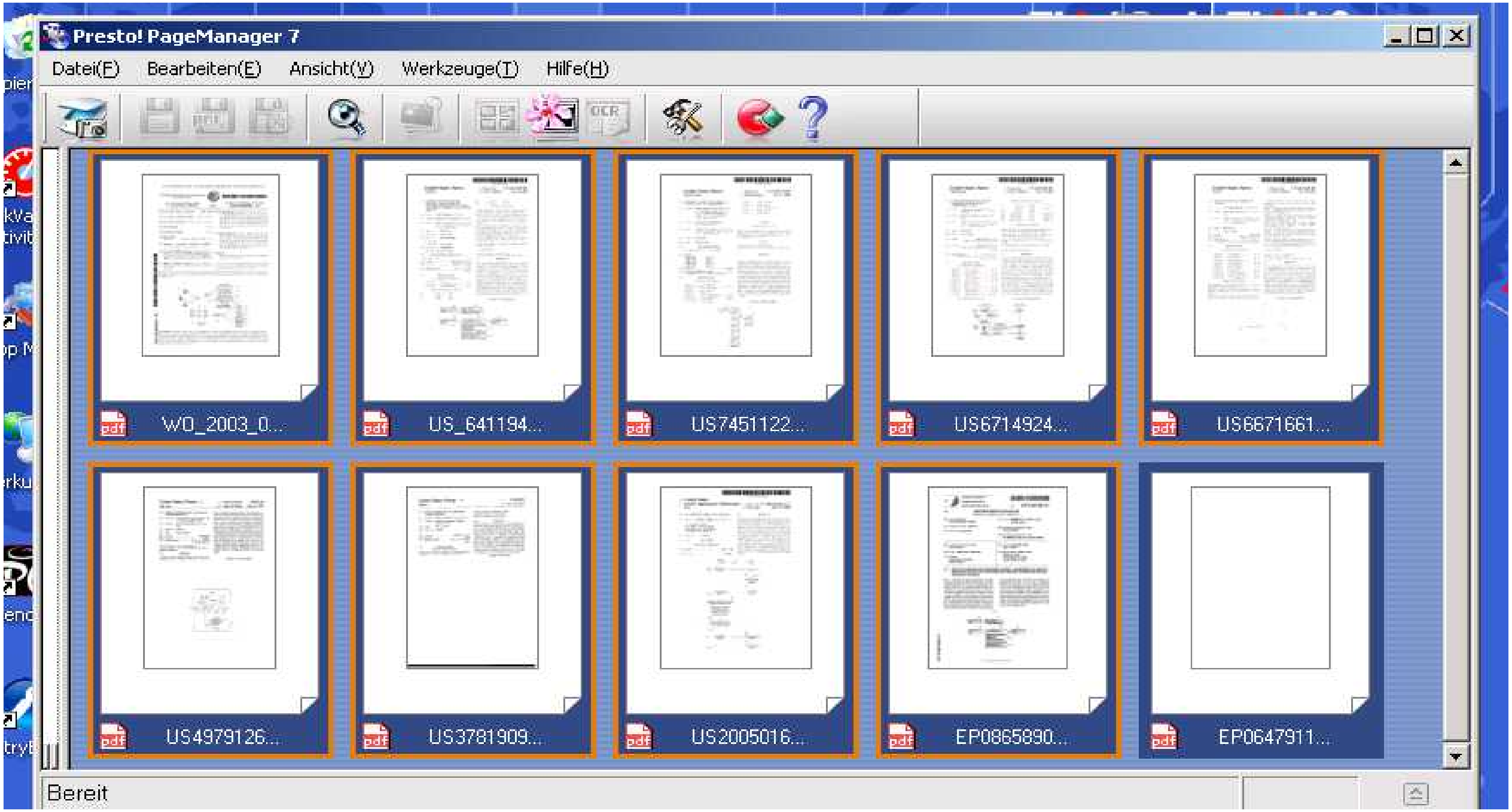
- What is needed:
  The application of statistical analysis of historic data to predict future trends, patterns, and behaviors to improve the outcomes in automated and human processes

Why I should not use this way of thinking and analysis to "forecast" a compound using historic set of data?

- **Correlation of ingredients and properties.**
  - **DoE tells us: most are linear!**
    Example: Filler / Oil loading and ratio on basic physicals
- **Estimate effects of changes of ingredients on properties.**

- **Selection of mathematical model**
  - **Linear – none linear**
  - **Iteration**
  - **Approximate function**

Actually an older idea:
9 patents identified dealing with this type of analytics:



Compound ingredient / property relation

Influences: Effects:

F_1 →
F_2 →
F_3 →

Compound Recipe

→ $R_1, R_2, .. R_n$

- **Objective of the Experiment should be the indentifcation of the most important factors ($F_{1,}..F_n$), to be able to measure Effects (Responses $R_{1,}...R_n$) and to describe there dependency in a mathematical equation:**

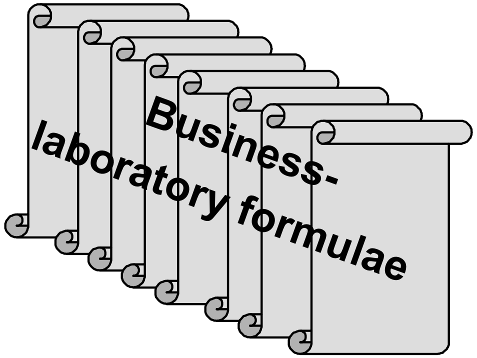
$$R_{i(1...n)} = f(A_0 + A_1F_1 + ...A_nF_n + ...)$$

Recipe database

- **Useful, if following information available:**
  - **Historical knowledge around ingredients and their effect on processing in the accompanying mixtures**
  - **Data about conspicuous features of the mixture in production**
  - **Database should contain information about the article manufactured from this mixture and its behaviors in use.**

- **Design guide for updating the database**

- **Design guide for formula development**



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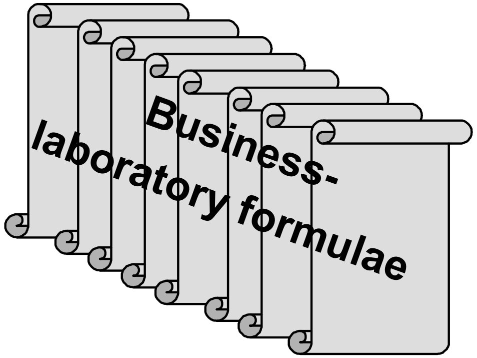
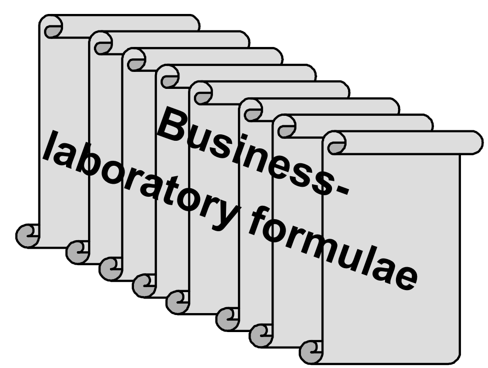


Recipe database and the use

- **Comparative analysis of formulas analogous an inquiry in a library**

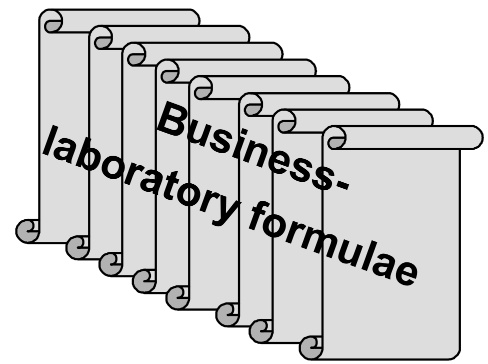
- **Comparison of parts made of the formula**
  - **Accelerator system as an example**

- **Choice of a formula,**
  - **Change after arbitrary criteria (Trial and Error)**
  - **Possibly processing according to a DOE in addition**



Source: Scarabaeus GmbH

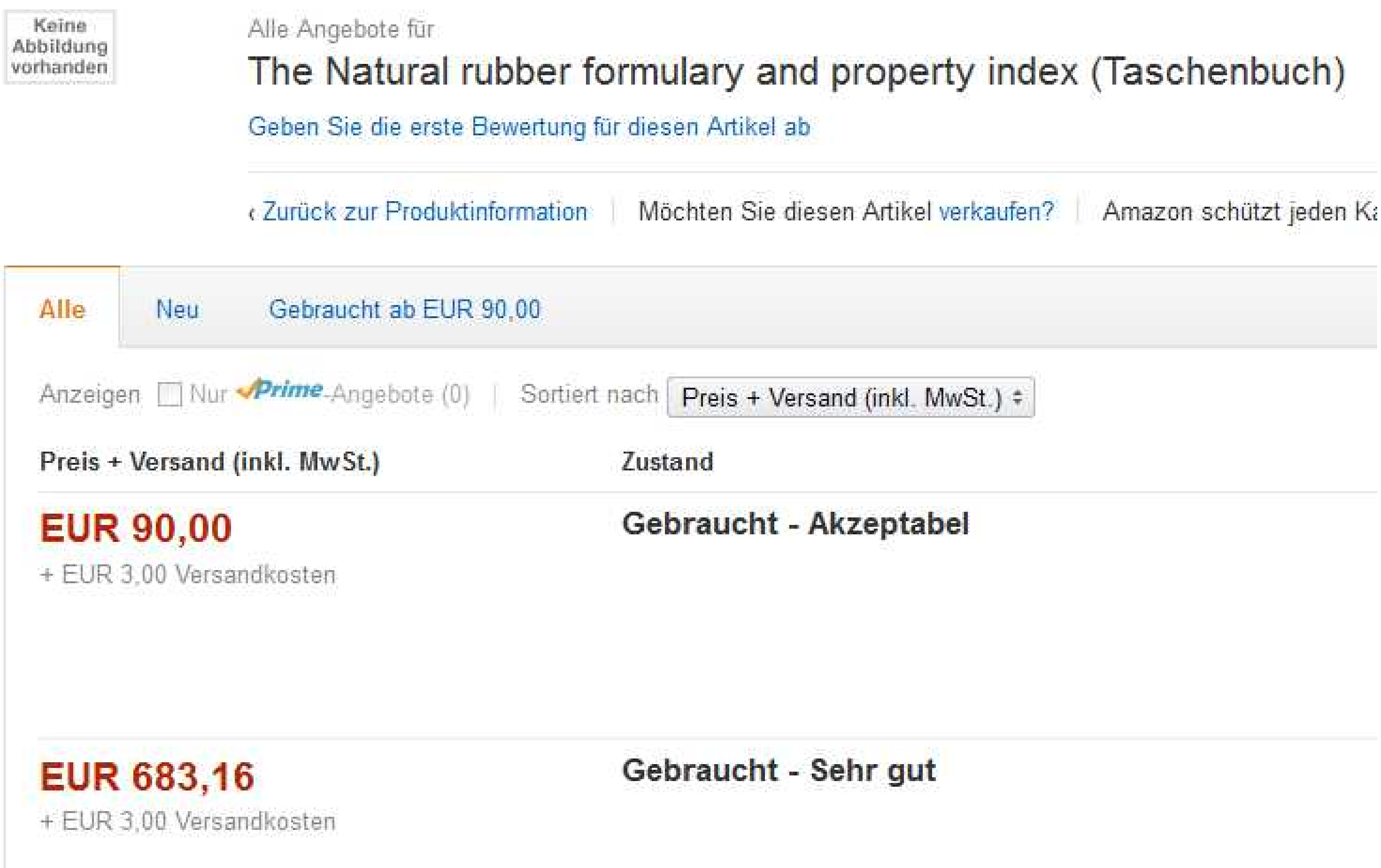
Recipe database organization



- **Cure Kinetic at 3 different Temperatures**
- **Basic physicals**
  - **H, TB, EB, M³,E,**
  - **C-Set 70°C / C-Set 150°C for HT-Polymers**
- **Aging Properties**
  - **Hot Air 7d/70°C 7d/150°C for HT-Polymers**
- **Viscosity at 3 different Temperatures**
  - **SIS-50 / RPA**
- **Other set of data**
  - **FEM – Data**
  - **Dynamic properties**

Figure: Scarabaeus GmbH

Source: Amazon



Source: Amazon

Keine Abbildung vorhanden

Alle Angebote für

The Natural rubber formulary and property index (Taschenbuch)

Geben Sie die erste Bewertung für diesen Artikel ab

‹ Zurück zur Produktinformation | Möchten Sie diesen Artikel verkaufen? | Amazon schützt jeden Ka

Alle | Neu | Gebraucht ab EUR 90,00

Anzeigen ☐ Nur Prime-Angebote (0) | Sortiert nach Preis + Versand (inkl. MwSt.)

Preis + Versand (inkl. MwSt.)	Zustand
EUR 90,00 + EUR 3,00 Versandkosten	**Gebraucht - Akzeptabel**
EUR 683,16 + EUR 3,00 Versandkosten	**Gebraucht - Sehr gut**

Most complete set of NR data!!

Predictive Data Analysis

5.1 Moderate damping rubbers — **40–60 IRHD**

Damping is given by a high viscosity oil with high filler loading and a cure system to produce a low crosslink density. Not suitable for use at elevated temperatures.

Formulation

	1	2	3	4	5	6	7	8
Nominal hardness	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	60	60
SMR 10	100	100	100	100	100	100	100	100
N330, HAF black	10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Coated calcium carbonate[a]	20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
High viscosity aromatic oil[b]	5	25	45	5	25	45	5	25
Zinc oxide	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Stearic acid	2	[illegible]	2	2	[illegible]	2	[illegible]	[illegible]
Antidegradant, HPPD[c]	2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Sulphur	1.5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
CBS	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5

a. *eg Calofort S* (John & E Sturge).
b. *eg Dutrex 729UK* (Shell).
c. *eg Santoflex 13* (Monsanto).

Data Sets contain:

- **Formula**
- **Rheological Properties**
- **Vulcanizate Properties – Laboratory sheet**
- **Vulcaniczate Properties – Molded part**
- **Other Properties (dynamic,..), depending on the article**

Rheological properties

	1	2	3	4	5	6	7	8
Mooney viscosity, 100°C	32	36	31	34	30	42	60	39
Mooney scorch, 120°C, min	28	28	32	28	32	22	20	25
Monsanto *Rheometer*, 150°C								
M_{HR}, torque units	21.5	19	15	23.5	21	21.5	31	29
M_L, torque units	6.5	6	3.5	5.5	5	3	9	6.5
scorch, t_{s1}, min	5.5	4.8	5.2	5.6	5.5	5.0	4.5	5
cure, $t_c'(95)$, min	14	14	13	15	15	11.5	14	12
cure, $t_c'(100)$, min	17	18	18	19	18	16	19	17

Reference: Technical Information Sheet D110 1982

5.1 (cont)

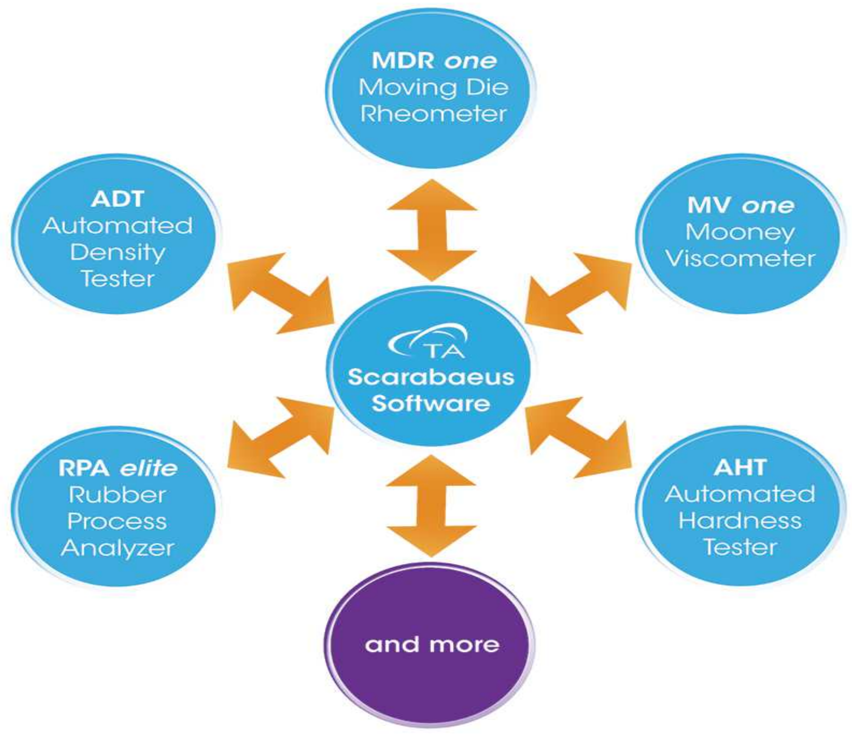
Vulcanizate properties, unaged

Formulation	1	2	3	4	5	6	7	8
Cure: 14min at 150°C								
Hardness, IRHD	42	41	40	48	48	52	61	60
Density, Mg/m^3	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20
MR100, MPa	0.65	0.65	0.61	0.90	0.85	0.91	1.40	1.15
Resilience, Lupke, %	78	66	54	70	52	40	58	43
Tensile properties								
M100, MPa	0.6	0.7	0.7	1.0	0.9	1.0	1.7	1.4
[illegible]	[illegible]	[illegible]	3.0	4.4	4.6	5.3	8.0	7.6
[illegible]	[illegible]	[illegible]	15.0	25	20	15.3	23	18
EB, %	785	725	690	715	705	615	560	590
Tear, ISO trouser								
23°C, median, kN/m	[illegible]	7.1	8.6	[illegible]	[illegible]	[illegible]	[illegible]	33
high/low ratio	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.6
100°C, median, kN/m	2.4	28	5.9	28	32	7.2	17	34
high/low ratio	2	1.4	1.2	2.9	1.4	1.2	4	2
Ring fatigue life, 0–100% strain								
median, kc	120	130	66	210	230	128	130	210
high/low ratio	2.7	2.4	3.2	2.2	3.2	5.6	2.4	2.3
Compression set, %								
1 day at −26°C	22	28	30	17	19	35	29	27
1 day at 0°C	10	14	14	8	12	16	13	12
3 days at 23°C	8	10	14	9	13	16	10	17
1 day at 70°C	39	50	61	44	50	54	44	50
Stress relaxation rate, 20% compression								
% per decade	2.1	2.3	3.9	2.6	3.9	4.2	3.4	4.3

Source: Scarabaeus GmbH

Database

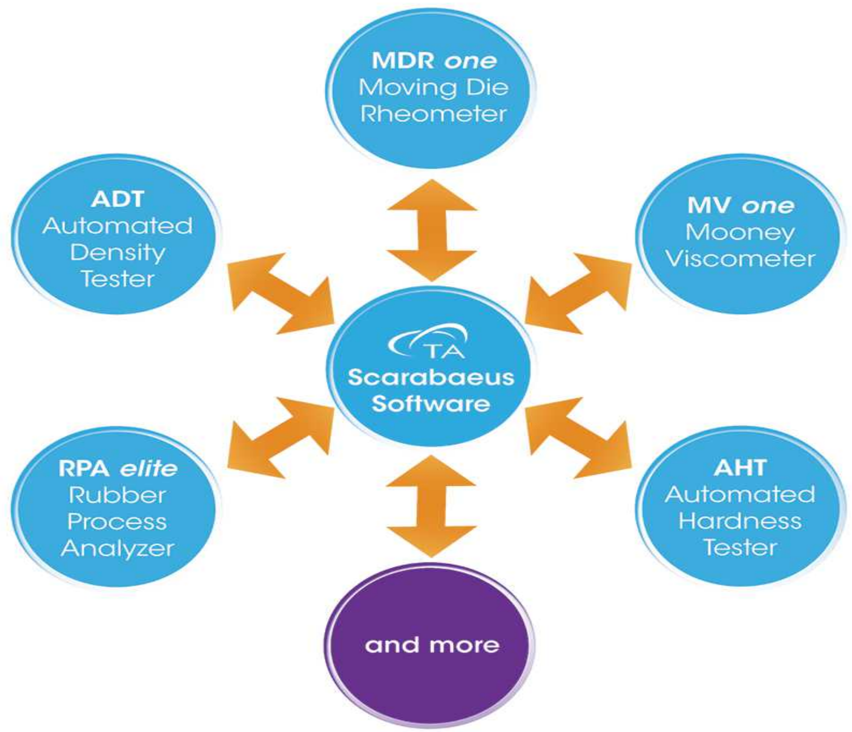
- **Raw Material Data Base**
- **Field for**
  - **Recipe**
  - **Property**
- **Search Functions**
- **Export of complete set of compound data**
- **Document organization**



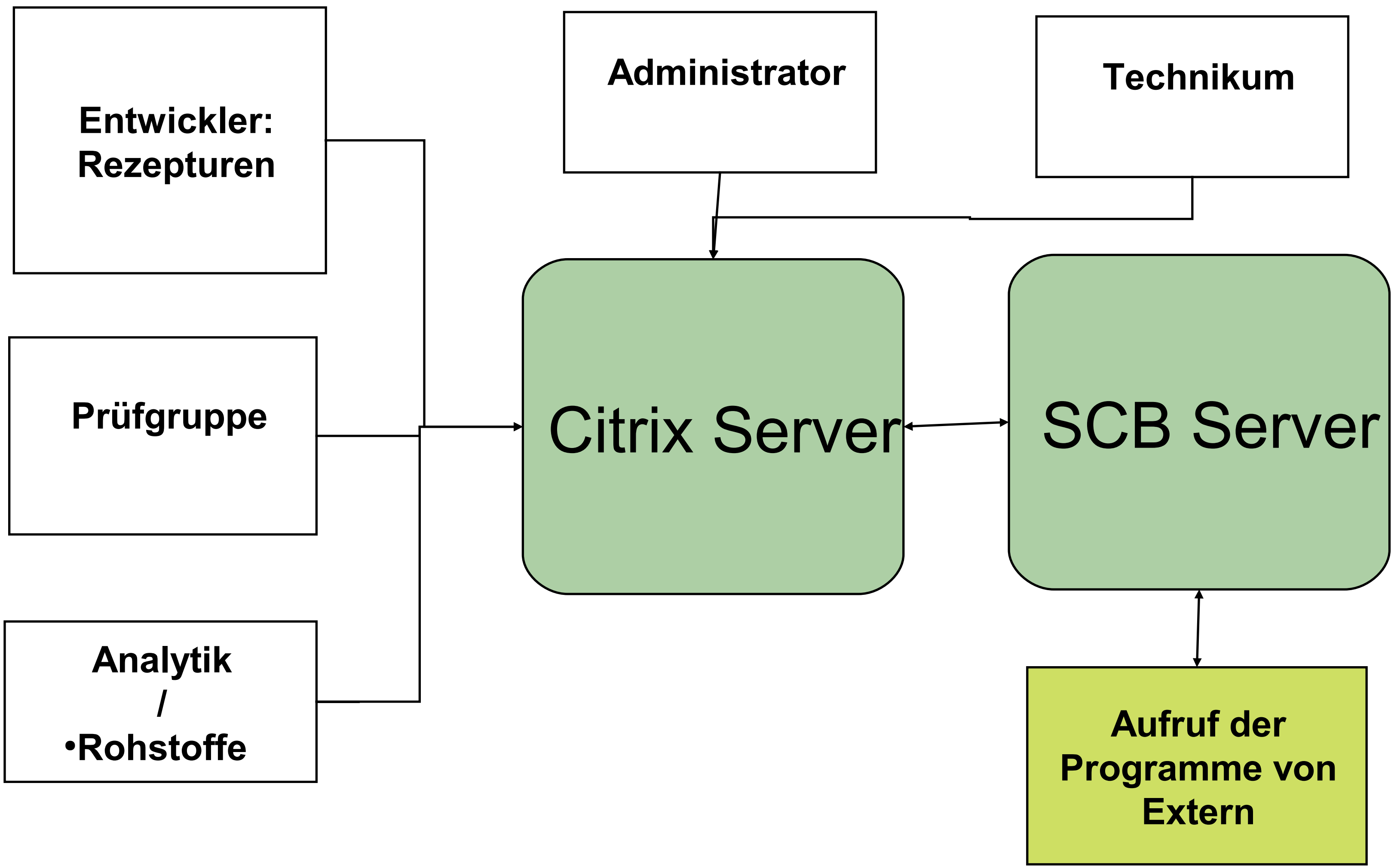
Source: Scarabaeus GmbH

Database

- **Without error because of automated transfer of measurement results**
- **Link with recipe**
- **Link with processing data possible**
- **Export to table calcula-tion programs**

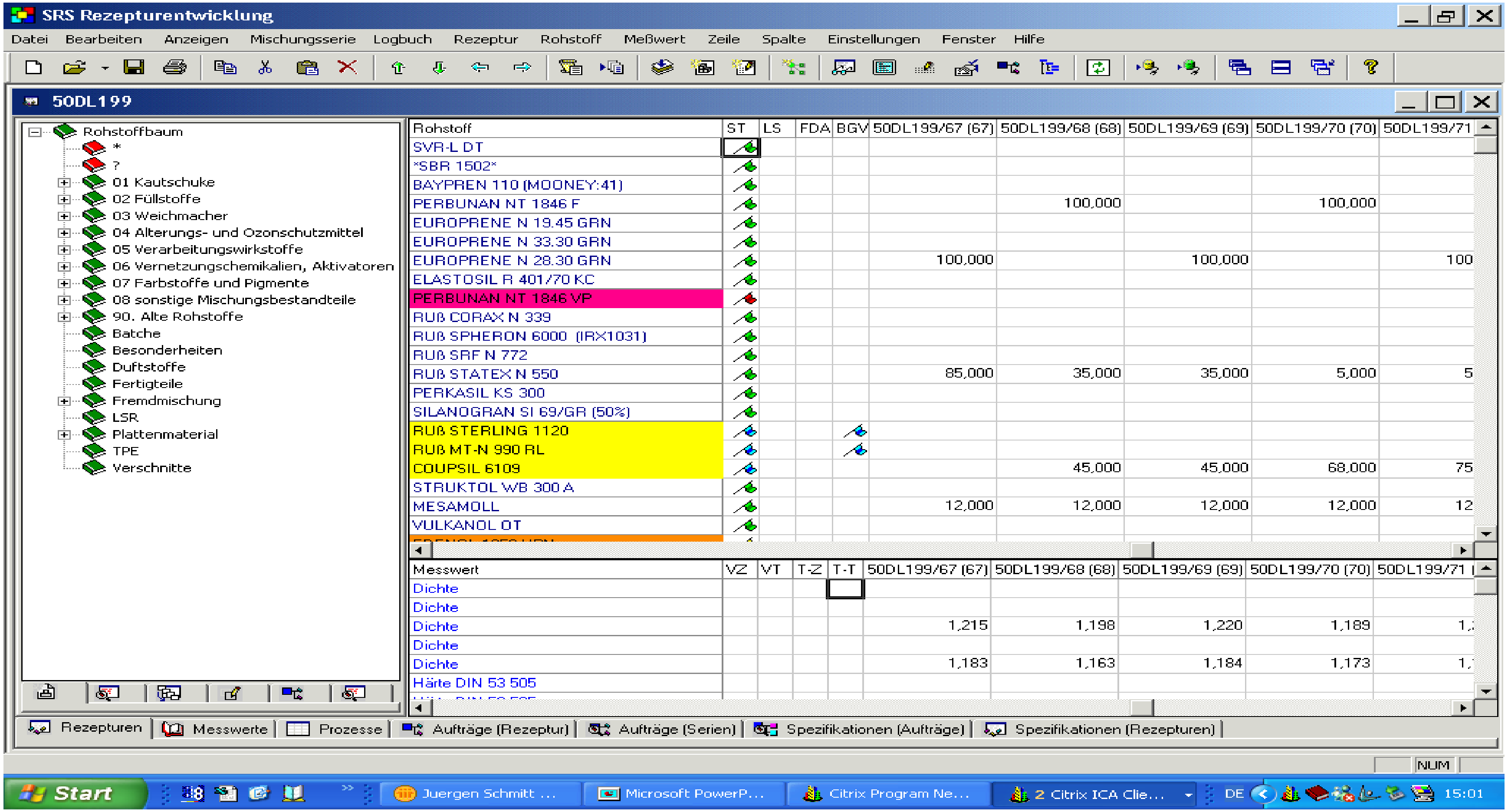


Organisation of IT for LIMS



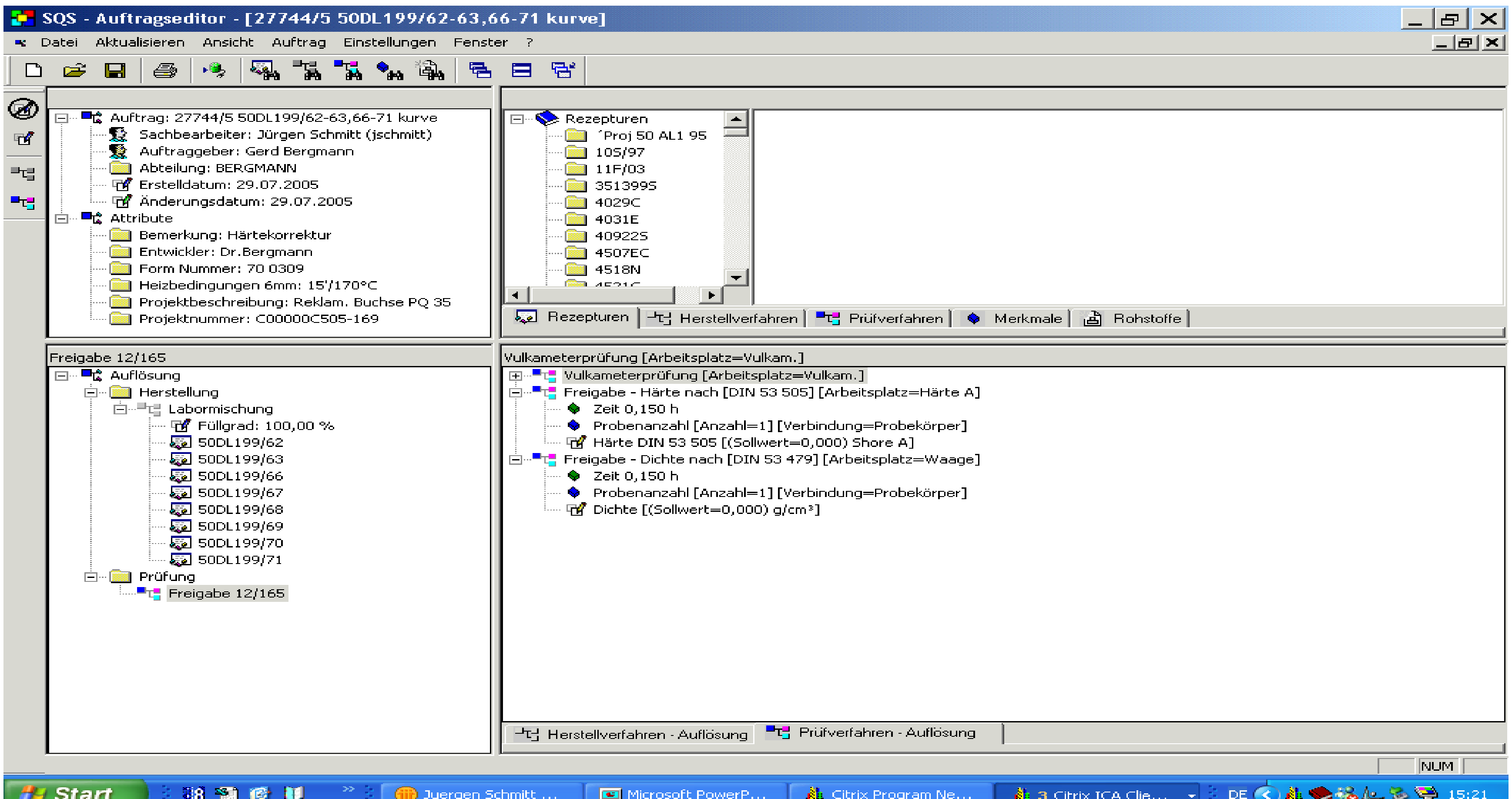
Source: Scarabaeus GmbH

Compound / Property Dataset



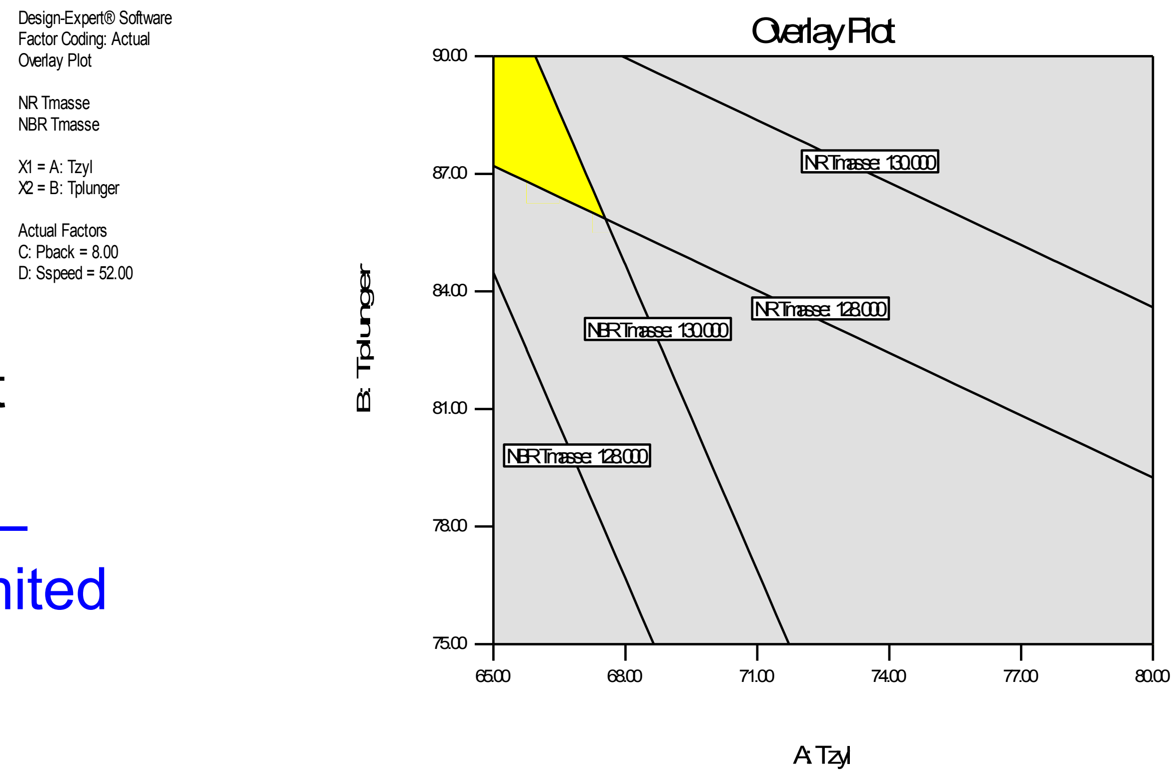
Source: Scarabaeus GmbH

Laboratory Testing Order



Introduction
Predictive data analysis
Organization of data
Database software
Tools for analysis
Conclusion

- Statistic Experimental Design Software
  - Optimization tool
    - Numerical
    - Graphical
    - Point prediction
    - Confirmation report

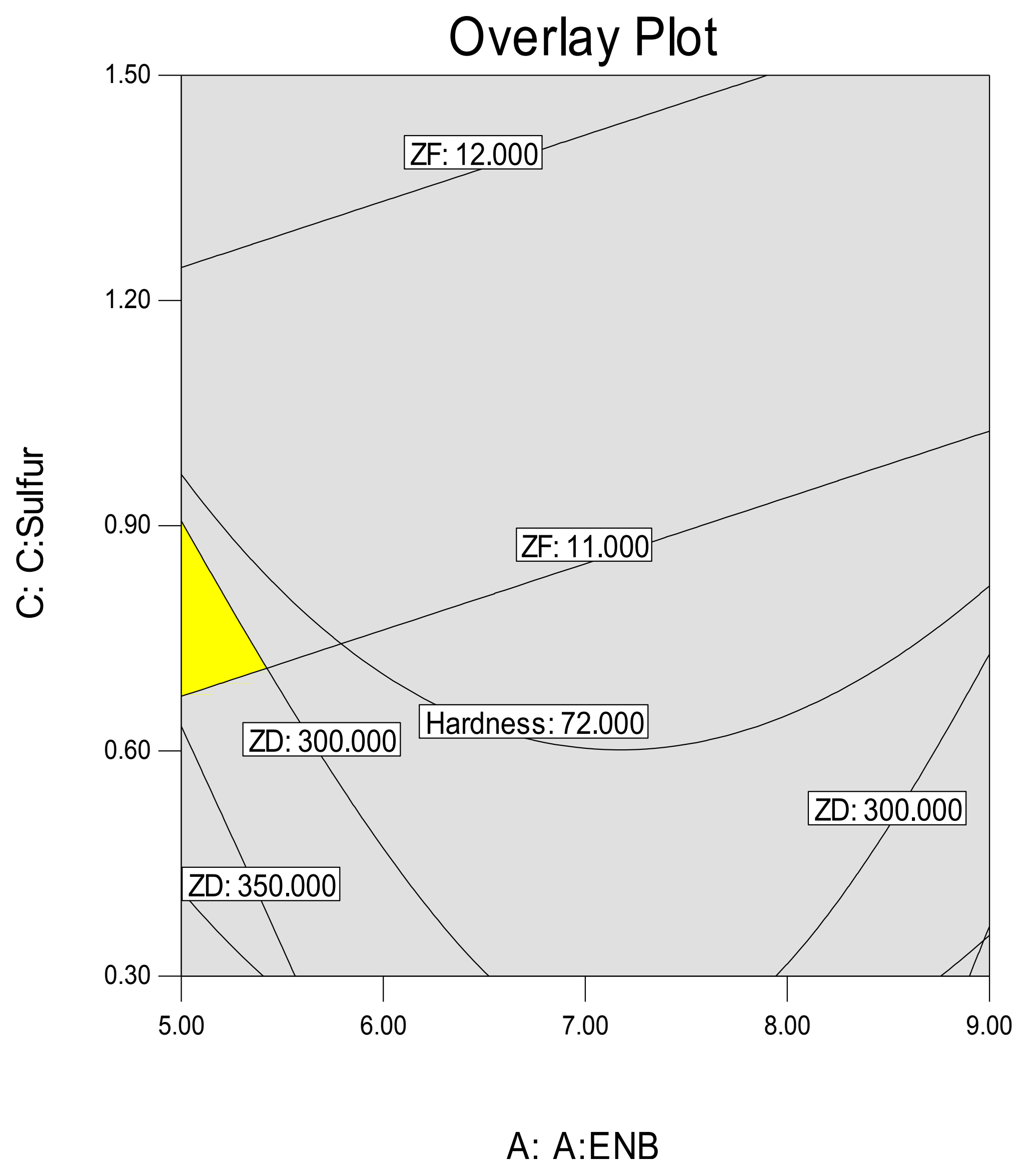


- Calculation of ingredient – property relations with limited organized set of data

Optimization

- **Design Expert® has several tools for optimization:**
  - **Numerical**
  - **Graphical**
  - **Point prediction**

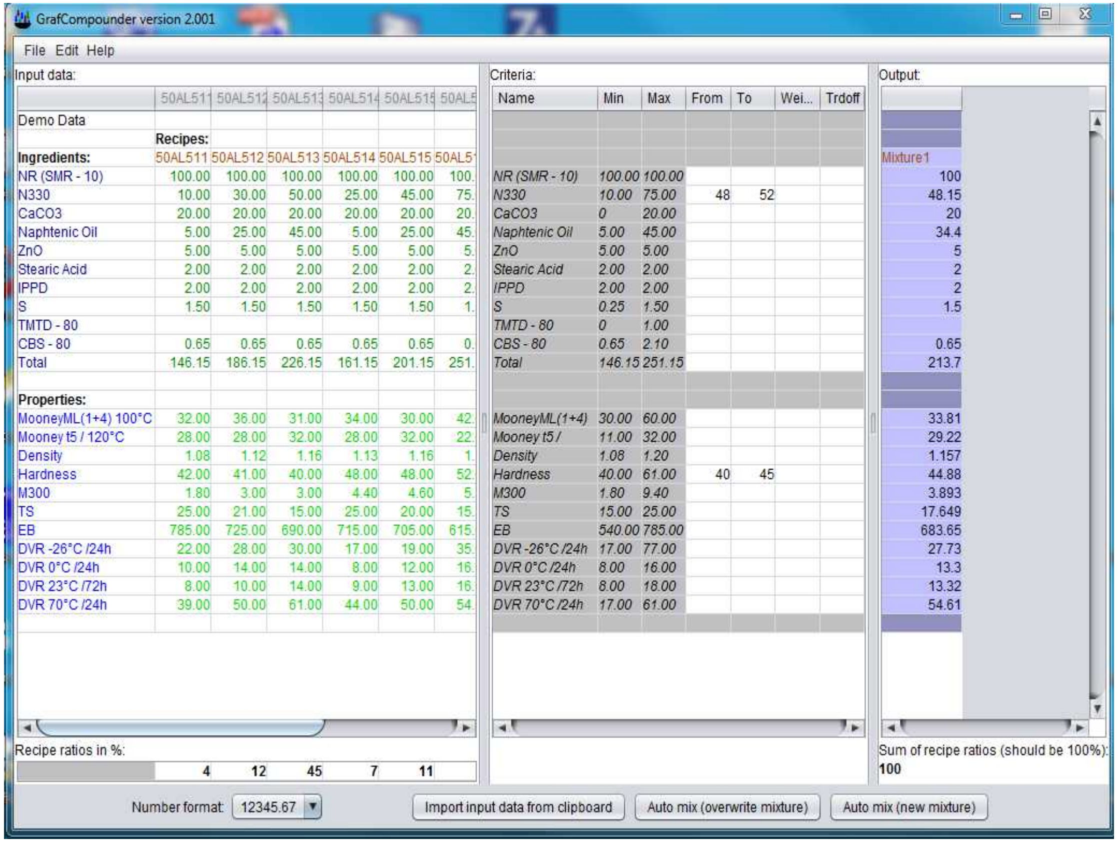
- **The graphical optimization allows to visualize the targets as an overlay plot in one graph.**
  - **You can run the numerical first and then transfer the values in the graphical optimization**



Source: GrafCompounder

GrafCompounder 2.001

- Table calculation software using happenstance data sets
  - Based on Java
  - Import / Export function for communication
  - Allows automatic mixing of compounds and manual mixing
  - Calculates property data
  - Shows data composition of the result
  - Import / Export of result



GrafCompounder version 2.001

File Edit Help

Input data:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL5
Demo Data						
	Recipes:					
Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL5
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.
N330	10.00	30.00	50.00	25.00	45.00	75.
CaCO3	20.00	20.00	20.00	20.00	20.00	20.
Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.
ZnO	5.00	5.00	5.00	5.00	5.00	5.
Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.
IPPD	2.00	2.00	2.00	2.00	2.00	2.
S	1.50	1.50	1.50	1.50	1.50	1.
TMTD - 80						
CBS - 80	0.65	0.65	0.65	0.65	0.65	0.
Total	146.15	186.15	226.15	161.15	201.15	251.
Properties:						
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.
Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.
Density	1.08	1.12	1.16	1.13	1.16	1.
Hardness	42.00	41.00	40.00	48.00	48.00	52.
M300	1.80	3.00	3.00	4.40	4.60	5.
TS	25.00	21.00	15.00	25.00	20.00	15.
EB	785.00	725.00	690.00	715.00	705.00	615.
DVR -26°C /24h	22.00	28.00	30.00	17.00	19.00	35.
DVR 0°C /24h	10.00	14.00	14.00	8.00	12.00	16.
DVR 23°C /72h	8.00	10.00	14.00	9.00	13.00	16.
DVR 70°C /24h	39.00	50.00	61.00	44.00	50.00	54.

Criteria:

Name	Min	Max	From	To	Wei...	Trdoff
NR (SMR - 10)	100.00	100.00				
N330	10.00	75.00	48	52		
CaCO3	0	20.00				
Naphtenic Oil	5.00	45.00				
ZnO	5.00	5.00				
Stearic Acid	2.00	2.00				
IPPD	2.00	2.00				
S	0.25	1.50				
TMTD - 80	0	1.00				
CBS - 80	0.65	2.10				
Total	146.15	251.15				
MooneyML(1+4)	30.00	60.00				
Mooney t5 /	11.00	32.00				
Density	1.08	1.20				
Hardness	40.00	61.00	40	45		
M300	1.80	9.40				
TS	15.00	25.00				
EB	540.00	785.00				
DVR -26°C /24h	17.00	77.00				
DVR 0°C /24h	8.00	16.00				
DVR 23°C /72h	8.00	18.00				
DVR 70°C /24h	17.00	61.00				

Output:

Mixture1
100
48.15
20
34.4
5
2
2
1.5
0.65
213.7
33.81
29.22
1.157
44.88
3.893
17.649
683.65
27.73
13.3
13.32
54.61

Recipe ratios in %:

	4	12	45	7	11

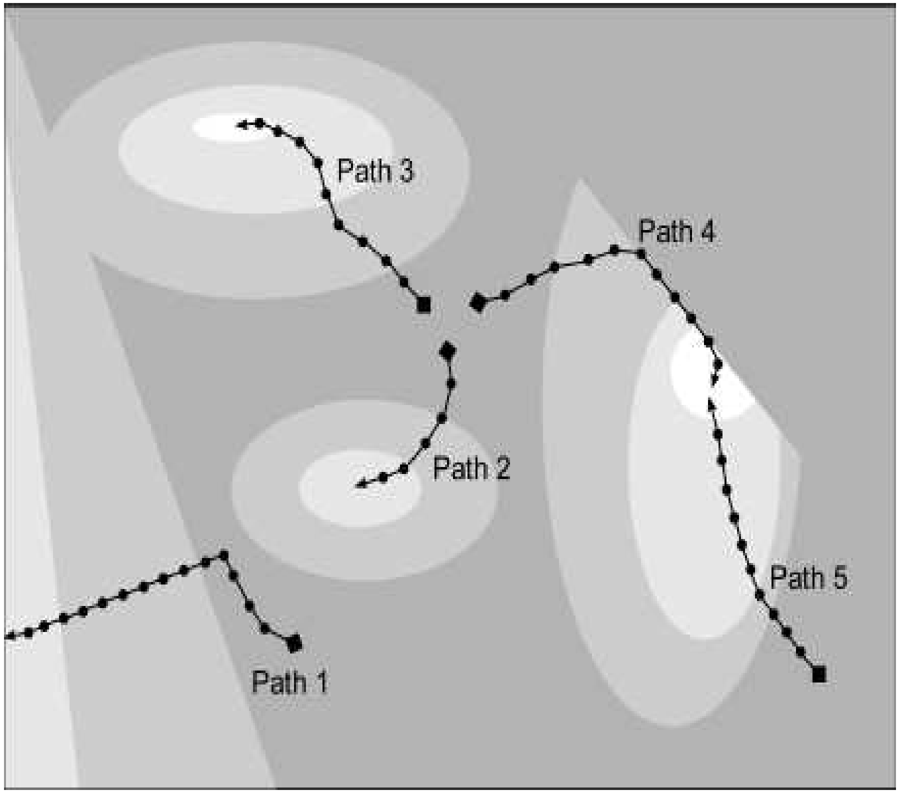
Sum of recipe ratios (should be 100%):
100

Number format: 12345.67

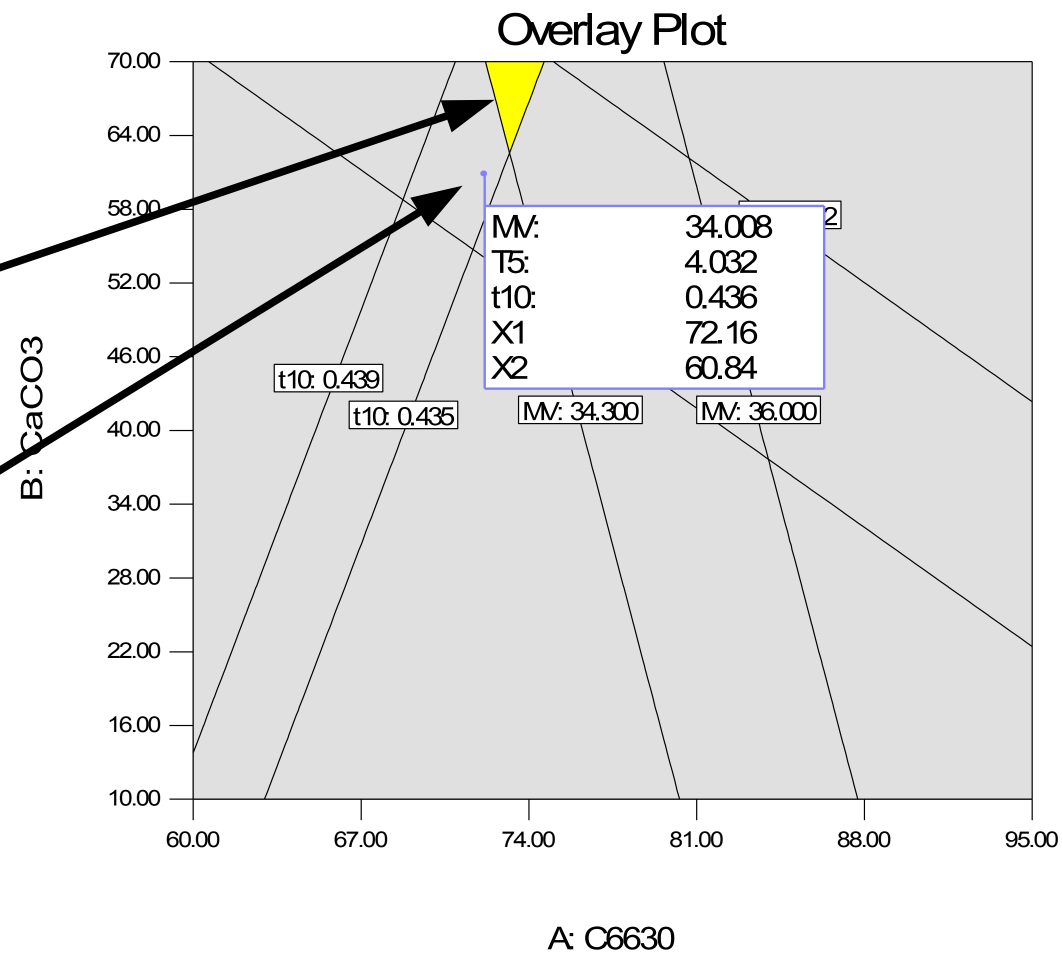
Import input data from clipboard | Auto mix (overwrite mixture) | Auto mix (new mixture)

- Analysis based on
  - **Measurables**
  - **Targets**
  - **Weights**
  - **Rating functions shows the distance between values and target**
  - **Iteration in small steps from different starting points**
  - **Check of maximum agreement with the target**

- Report of Results
  - **Recipe**
  - **All calculable physical properties**
    - **Missing data left out**
  - **Show all Recipes with their percentage used in the analysis**



- Analysis with data fitting on linear regression model equation
  - Optimization area calculated with Design Expert
- Analysis without fitting of data
  - Solution given by GrafCom-pounder



- **Full set of data in Recipe, resp. Compound development is of advantage for:**
  - **Comparison multiple recipes which each other**
  - **Correlation between ingredients and performance of compounds**
  - **Mathematical handling to virtual create compound with such data sets**

- **Considerations**
  - **A database with little to no errors is required, which should be possible with LIMS and an infrastructure accordingly**

- **Finally we should accept, that we are in the computer age**

Thanks for your attention.
What are your comments?