

# DKG SÜD / SÜD WEST

# Vorausschauende Daten Analyse und Organisation von Daten in der Mischungsentwicklung

April 3-4, Würzburg, Germany

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



## Introduction

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

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## 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

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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

Predictive	Data	Ana	lysis
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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



Source: 2011 IBM Corporation

### 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

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





Objective of the Experiment should be the indentification 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:

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

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### 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.
- $_{\ensuremath{\mathbb{C}}}$  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



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Source: Scarabaeus GmbH

### **Recipe database organization**

- Cure Kinetic at 3 different Temperatures
- Basic physicals
  - → H, TB, EB, M<sup>3</sup>,E,
- C 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

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Source: Amazon





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Damping is given by a high	viscos	ty oil w	ith high	filler loc	aoing an												
produce a low crosslink de	nsity. N	lot suiti	ble for	use at el	evated t	empera	tures.		Formulation	1	2	3	- 4	5	6	7	8
Formulation									- There are a second				_				
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	•	F	rm	ามไร	a				MR100, MPa	(1,65	0.65	0.61	0.90	0.85	0.93	1.40	1.1
SMR 10	tixy	100	100	100	100	100	100	100	Resilience, Lupke, %	78	- 50	54	70	52	-40	-58	-0
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	. 6	25	45	5	25	45	.5	25	M100, MPa	9.6	0.7	9.7	1.0	0.9	1.0	2.7	1.4
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High viscosity aromatic off Zinc oxide Sisearic acid Antidegradant, HPPEP Sulphur CBS a. eg Calofort 5 (John & E b. eg Duares 729UK (Shell c. eg Somofles 13 (Mensan Rheological properties	2 2 1.5 0.5 Sturge ). to).	Vi Vi O	ulc ulc the	anı ani r P	zat cza roj	ate oer	ro Pro ties	perties – operties s (dynam	Laboratory – Molded pa ic,), depen- love median, eNin highlow ratio Ring fatigue life, 0-100% median, ke		eet 725	15.0 690 0 1.2 60	25 715 the 28 2.9 210	20 705 23 1.4 230	15.3 615 ticl 7.2 1.2	23 560 <b>2</b> 9 1.7 4 130	18 590 33 1.6 34 2 210
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High viscosity aromatic off Zinc oxide Sicaric axid Antidegradant, HPPEP Sulphur CBS a. eg Calofort 5 (John & E b. eg Duares 729UK (Shell c. eg Santoffes 13 (Mensan Rheological properties Mooney viscosity, 10IPC Mooney secorch, 120°C, min Monuanto Rheometer, 150°C	2 2 1.5 0.5 Sturge ). to).	Vi Vi 0 36 28		ani ani r P				perties – operties s (dynam	Laboratory – Molded pa ic,), "depen 100'C.median, CN/m high/low ratio Ring fatigue life, 0-100% median, ke high/low ratio Compression sct, % 1 day at -26'C 1 day at 0'C	strain 27 120 27 27 27 27 27	28 130 24 130 24 130 24	15.0 690 5.9 1.2 66 3.2 30 14	25 715 the 29 210 212 17 8	20 705 32 1.4 230 3.2 1.4	15.3 615 <b>ticl</b> 7.2 1.2 128 5.6 35 16	23 560 <b>1</b> ,7 4 1,7 4 1,30 2,4 29 13 10	1.6 18 590 33 1.6 34 2 210 2.1 210 2.1 27 12
High viscosity aromatic off Zinc oxide Sizearic axid Antidegradant, HPPD Sulphur CBS a. eg Calafort 5 (John & E b. eg Duarex 729UK (Shell c. eg Santoffex 13 (Mensan Rheological properties Mooney viscosity, 100°C Mooney secoreh, 120°C, min Monanto Rheometer, 150°C Mon, torque units	2 2 15 0.5 Sturge 1. to). 32 28 21.5	VI VI 0 0 0 0 0		ani ani r P		215		perties – operties s (dynam	Laboratory – Molded pa Tear. 50 House ic,), "depen 100°C.median, cN/m high/low ratio Ring fatigue life, 0–100% median, ke high/low ratio Compression set, % 1 day at -26°C 1 day at 23°C 2 days at 23°C	24 2 3train 120 2.7 22 10 8 120	25 13 26 14 130 24 28 14 28 14 28	15.0 690 <b>D</b> 15.9 1.2 66 3.2 30 14 14 60	25 715 <b>the</b> 29 210 222 17 8 9 4	20 705 32 1.4 230 3.2 1.4	15.3 615 <b>10</b> 7.2 1.2 128 5.6 35 16 16 54	23 560 *9 17 4 130 2.4 29 13 10 44	1.0 18 590 33 1.6 34 2 210 2.3 27 12 17 50
High viscosity aromatic off Zinc oxide Stearie acid Antidegradant, HPPD Sulphur CBS a. eg Calofort 5 (John & E b. eg Duarex 729UK (Shell c. eg Santoflex 13 (Mensan Rheological properties Mooney viscosity, 100°C Mooney secorch, 120°C, min Monanto Rheometer, 150°C M <sub>410</sub> , torque units	2 2 15 0.5 Sturge 1, to). 32 28 21.5 6.5	56 28 19 6		aņi aņi r P	2at C2a ror 30 32	42 21.5 3		perties – operties - s (dynam	Laboratory – Molded pa ic., 23), dependent bigb/low ratio Ring fatigue life, 0–100% median, kc high/low ratio Compression sct, % 1 day at -25°C 1 day at 0°C 3 days at 23°C	strain 2785 24 2 120 27 22 10 8 39	225 130 2.4 14 130 2.4 14 130 2.4 14 130 2.4 14 130 30	15.0 690 5.9 1.2 66 3.2 30 14 14 14 61	<sup>25</sup> 715 <b>the</b> <sup>28</sup> 29 210 210 22 17 8 9 4	20 705 32 1.4 230 3.2 19 12 13 50	15.3 615 100 128 5.6 100 100 100 100 100 100 100 10	23 560 <sup>39</sup> <b>C</b> 1.7 4 1.70 2.4 29 13 10 44	1.0 18 590 33 1.6 34 2 210 2.3 27 212 17 50
High viscosity aromatic off Zinc oxide Stearie acid Antidegradant, HPPD Sulphur CBS a. eg Calofort 5 (John & E b. eg Duares 729UK (Shell c. eg Santofles 13 (Mensan Rheological properties Mooney viscosity, 100°C Mooney viscosity, 100°C Mooney secreth, 120°C, min Monuanto Rheometer, 150°C Mign, torque units secreth, f <sub>4</sub> , min	2 2 15 0.5 Sturge 1 to). 32 28 21.5 6.5 5.5	36 28 19 6 48	11C 11C 11C 15 15 15 15 15 15 15 15 15 15	aņi ani r P	2at CZa rOr 30 32	42 21.5 35.0		perties – operties - s (dynam	Laboratory – Molded pa ic., 23), adependent 100°C.median, Evin high/low ratio Ring fatigue life, 0–100%, median, ke high/low ratio Compression set, % 1 day at -26°C 1 day at 20°C 3 days at 20°C 1 day at 70°C	24 2 3train 120 2.7 22 10 8 39	225 130 2.4 14 130 2.4 14 10 50 mion	15.0 690 5.9 1.2 66 3.2 30 14 14 61	25 715 <b>the</b> 28 2.9 210 222 17 8 9 4	20 705 32 1.4 230 3.2 1.4 19 12 13 50	15.3 615 100 128 128 128 128 128 106 16 16 54	23 560 <b>99</b> <b>17</b> 4 130 2.4 29 13 10 44	1.6 18 590 33 1.6 34 2 210 23 27 12 17 50
High viscosity aromatic off Zinc oxide Stearie acid Antidegradant, HPPD Sulphur CBS a. eg Calofort 5 (John & E b. eg Duarez 729UK (Shell c. eg Santoflex 13 (Mensan Rheological properties Mooney viscosity, 100°C Mooney viscosity, 100°C Mooney viscosity, 100°C, min Monauto Rheometer, 150°C M <sub>100</sub> , torque units M <sub>410</sub> , torque units	5 2 2 15 0.5 Sturge ) to). 32 28 21.5 6.5 55 14	36 28 19 6 4 14	31 22 31 32 33 33 33 33 33 33 33 33 33 33 33 33	ani ani r P	2at CZa rO rO 30 32	42 21.5 3 5.0 11.5	() Pro ties	perties – operties - s (dynam	Laboratory – Molded pa ic., 23), mdepen ic., 23), mdepen 100°C.median, ENim highlow ratio Ring fatigue life, 0–100%, median, ke highlow ratio Compression set, % 1 day at -25°C 1 day at 0°C 3 days at 23°C 1 day at 70°C Stress relexation rate, 29%	2.4 2.4 2.4 2.4 2.4 2.4 2.4 2.4	24 10 24 14 10 50 14 10 50 14 10 50 14 10 50 14 10 50 14 10 50 14 10 50 14 14 10 50 14 14 14 15 14 15 14 15 16 16 16 16 16 16 16 16 16 16	15.0 6900 5.9 1.2 66 3.2 30 14 14 61 3.9	25 715 <b>the</b> 29 210 22 17 8 9 44 2.6	20 705 32 1.4 230 3.2 19 12 13 50 3.9	15.3 <b>5</b> 15 <b>1</b> 10 <b>1</b> 28 5.6 10 10 10 10 10 10 10 10 10 10	23 560 <sup>39</sup> <b>C</b> 1.7 4 1.30 2.4 29 13 10 44 3.4	1.0 18 590 33 1.6 34 2 210 2.3 27 12 17 50 4.3

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Source: Scarabaeus GmbH

### Database

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



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Source: Scarabaeus GmbH

### Database

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



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### Organisation of IT for LIMS



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Source: Scarabaeus GmbH

### **Compound / Property Dataset**

🚰 SRS Rezepturentwicklung														_ & ×
Datei Bearbeiten Anzeigen Mischungsserie Log	jbuch Rezeptur Rohstoff Meßwert	Zeile S	ipalte i	Einstel	lungen Fo	enster	Hilfe							
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50DL199														
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	*SBR 1502*	1												
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Weichmacher	EUROPRENE N 19.45 GRN	_ ∕�												
	EUROPRENE N 33.30 GRN	∕♦												
06 Vernetzungschemikalien, Aktivatoren	EUROPRENE N 28.30 GRN	_ ∕�			10	0,000				100,0	00			100
😥 🔖 07 Farbstoffe und Pigmente	ELASTOSIL R 401/70 KC	_∕∕₅												
🗄 較 08 sonstige Mischungsbestandteile	PERBUNAN NT 1846 VP	∕∙												
😟 😥 90. Alte Rohstoffe	RUB CORAX N 339	_ ∕�												
Batche	RUB SPHERON 6000 (IRX1031)	_ ∕♦												
Besonderheiten	RUB SRF N 772													
	RUB STATEX N 550				8	5,000		35,000		35,0	00	5,	000	5
Eremdmischung	PERKASIL KS 300													
LSR -	SILANOGRAN SI 69/GR (50%)													
🗄 💀 😣 Plattenmaterial	RUB STERLING 1120	1		1										
TPE	RUB MT-N 990 RL	1		1										
Verschnitte	COUPSIL 6109	<u></u>						45,000		45,0	00	68,	.000	75
	STRUKTOL WB 300 A	∕♦												
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	VULKANOL OT	<u></u>												
				· · · ·										
	Messwert	VZ V	/T  T-Z	T-T 5	50DL199/67	7 (67) !	50DL199/6	8 (68)	50DL1	199/69 (6	9) 50DI	.199/70 (	70) 50	DL199/71 🔼
	Dichte													
	Dichte													
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Source: Scarabaeus GmbH

### Laboratory Testing Order



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Factor Coding: Actual

Overlay Plot NR Tmasse

NBR Tmasse

X1 = A: Tzvl

X2 = B: Tplunger Actual Factors

C: Pback = 8.00 D: Sspeed = 52.00



### Statistic Experimental Design Software

- Optimization tool
  - Numerical
  - Graphical
  - Point prediction
  - Confirmation report
- Calculation of ingredient property relations with limited organized set of data



A Tzyl



### 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



A: A:ENB

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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

and Lot Holp							Contraction (							0.1.1	
nput data:	במא בלל במא ביל במא בלל במא בלל במא בלל במא				1221012	Criteria:	14423		Output						
	50AL51	50AL512	50AL513	50AL514	50AL515	50AL5	Name	Min	Max	From	10	Wei	Irdoff		
Demo Data															
	Recipes:														
Ingredients:	50AL511	50AL512	50AL513	50AL514	50AL515	50AL51								Mixture1	
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.	NR (SMR - 10)	100.00	100.00					100	
N330	10.00	30.00	50.00	25.00	45.00	75.	N330	10.00	75.00	48	5	2		48.15	
CaCO3	20.00	20.00	20.00	20.00	20.00	20.	CaCO3	0	20.00					20	
Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.	Naphtenic Oil	5.00	45.00			_		34.4	
ZnO	5.00	5.00	5.00	5.00	5.00	5.	ZnO	5.00	5.00					5	
Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.	Stearic Acid	2.00	2.00					2	
PPD	2.00	2.00	2.00	2.00	2.00	2.	IPPD	2.00	2.00					2	
S	1.50	1.50	1.50	1.50	1.50	1.	S	0.25	1.50					1.5	
TMTD - 80							TMTD - 80	0	1.00						
CBS - 80	0.65	0.65	0.65	0.65	0.65	0.	CBS - 80	0.65	2.10			-		0.65	
Total	146.15	186.15	226.15	161.15	201.15	251.	Total	146.15	251.15					213.7	
Properties:															
MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.	MooneyML(1+4)	30.00	60.00					33.81	
Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.	Mooney t5 /	11.00	32.00					29.22	
Density	1.08	1.12	1.16	1.13	1.16	1.	Density	1.08	1.20					1.157	
Hardness	42.00	41.00	40.00	48.00	48.00	52.	Hardness	40.00	61.00	40	4	5		44.88	
M300	1.80	3.00	3.00	4.40	4.60	5.	M300	1.80	9.40					3.893	
TS	25.00	21.00	15.00	25.00	20.00	15.	TS	15.00	25.00					17.649	
EB	785.00	725.00	690.00	715.00	705.00	615.	EB	540.00	785.00					683.65	
DVR -26°C /24h	22.00	28.00	30.00	17.00	19.00	35.	DVR -26°C /24h	17.00	77.00					27.73	
DVR 0°C /24h	10.00	14.00	14.00	8.00	12.00	16.	DVR 0°C /24h	8.00	16.00					13.3	
DVR 23°C /72h	8.00	10.00	14.00	9.00	13.00	16.	DVR 23°C /72h	8.00	18.00					13.32	
DVR 70°C /24h	39.00	50.00	61.00	44.00	50.00	54.	DVR 70°C /24h	17.00	61.00					54.61	
•				t		7.							7.6		
Recipe ratios in %:	4	12	45	7	11									Sum of recipe ratio	os (should be

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#### Analysis based on

- ♂ Measurables
- Targets
- Weights
- Rating functions shows the distance between values and target
- E 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



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A: C6630



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

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

Thanks for your attention. What are your comments?