



H-JG Consulting

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**Compound Simulation Tool
„GrafCompounder“
Version 2.004**

Advantages to the Customer

Computer Aided Compound Development

- ⌘ Better utilization of historic compound data base
- ⌘ Faster results - minimizes efforts and time in development
- ⌘ Increases creativity through compound simulation

Compound calculation and simulation goes beyond „trial and error“ and typical statistical design of experiment (DoE) algorithms

Specifics of GrafCompounder

- ⌋ **The GrafCompounder uses the Multiple Linear Iteration method [MLI] to calculate a new recipe according to properties targeted**
- ⌋ **The GrafCompounder enables the user to analyze and improve their compound database via identification of faulty data sets**
- ⌋ **Each compound is taken into account for the calculation and the influence of each on the final result is visualized as a ratio**
- ⌋ **The GrafCompounder is a fast and easy to use tool without utilizing a complex “hidden” mathematical and analytical method**

Specifics of GrafCompounder

- ┌ **The resulting formulas calculated correspond to the general rules of compounding**
- ┌ **These formulas will show property scores larger than the 90% confidence interval**
- ┌ **Only one confirmation experiment is needed as opposed to multiple trials**

Example of Program Working Screen

Screenshot of GrafCompounder with demo data, targets and a calculated compound

GrafCompounder version 2.003

File Edit Help

Input data:

	50AL511	50AL512	50AL513	50AL514	50AL515	50AL516	50AL517	50AL518	50AL542
Demo Data									
Ingredients:									
NR (SMR - 10)	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
N330	10.00	30.00	50.00	25.00	45.00	75.00	45.00	65.00	50.00
CaCO3	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	
Naphtenic Oil	5.00	25.00	45.00	5.00	25.00	45.00	5.00	25.00	10.00
ZnO	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
Stearic Acid	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
IPPD	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
S	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	0.25
TMTD - 80									1.00
CBS - 80	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	2.10
Total	146.15	186.15	226.15	161.15	201.15	251.15	181.15	221.15	172.35

Properties:

MooneyML(1+4) 100°C	32.00	36.00	31.00	34.00	30.00	42.00	60.00	39.00	41.00
Mooney t5 / 120°C	28.00	28.00	32.00	28.00	32.00	22.00	20.00	25.00	11.00
Density	1.08	1.12	1.16	1.13	1.16	1.19	1.19	1.20	1.11
Hardness	42.00	41.00	40.00	48.00	48.00	52.00	61.00	61.00	59.00
M300	1.80	3.00	3.00	4.40	4.60	5.30	8.00	7.60	9.40
TS	25.00	21.00	15.00	25.00	20.00	15.30	23.00	18.00	23.00
EB	785.00	725.00	690.00	715.00	705.00	615.00	560.00	590.00	540.00
DVR -26°C /24h	22.00	28.00	30.00	17.00	19.00	35.00	29.00	27.00	77.00
DVR 0°C /24h	10.00	14.00	14.00	8.00	12.00	16.00	13.00	12.00	16.00
DVR 23°C /72h	8.00	10.00	14.00	9.00	13.00	16.00	10.00	17.00	18.00
DVR 70°C /24h	39.00	50.00	61.00	44.00	50.00	54.00	44.00	50.00	17.00

Criteria:

Name	Min	Max	From	To	Weig...	Trdoff
NR (SMR - 10)	100	100				
N330	10	75	48	52		
CaCO3	0	20				
Naphtenic Oil	5	45				
ZnO	5	5				
Stearic Acid	2	2				
IPPD	2	2				
S	0.25	1.5				
TMTD - 80	0	1				
CBS - 80	0.65	2.1				
Total	146.15	251.15				

Output:

Mixture 1	
	100
	48.35
	17.8
	23.75
	5
	2
	2
	1.3625
	0.11
	0.8095
	201.182
	39.08
	24.62
	1.1562
	50.96
	5.467
	19.957
	646.95
	32.42
	13.19
	13.31
	46.36

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

Recipe ratios in %:

5	11	10	11	11	19	11	11	11
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Number format: 12345.67

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

Projects done with GrafCompounder

Samples of Projects successfully developed with GrafCompounder before market release:

- Non-bronzing iridescence EPDM compound
- SBR/EPDM blend for automotive profile
- Sponge corner moulding EPDM compound
- EPDM Compound for body mounts
- Seal for drinking water application
- NBR/PVC blend in automotive air ducts
- Very low temperature resistance NBR/PVC grommets

Market Situation

There is no program on the market available with features like the GrafCompounder

- There are 9 US, 3 EP and 2 WO patents in the literature but nothing has been marketed
- Software CAD-Chem was taken from the market in approximately 2004

Similar programs

- **Alfa-Technologies: Compound**
 - A flexible recipe management system that provides a knowledge base that can be easily searched

Market Situation

References (Selection)

- PT Hung A, Korea
- Dunlop - Belt, Thailand
- Weros Technolgy, Germany
- Weir Minerals, Australia + USA
- Kozato Kizai, Malaysia
- Medical rubber products, Malaysia
- Ryco Hydraulics, Malaysia
- Loadstar, Srilanka
- Zeon, Thailand + USA
- Mahidol University, Thailand
- Rubber Research Institute, Malaysia
- LS Cable, Korea
- Carlisle Transportation Products, Thailand + USA
- Emerald Resident Tyre, India
- Lanxess, India
- Nisco Aegis Polymers, India
- Vitillo, Italy
- Royal Tires, India
- Parker, USA
- Trelleborg, USA
- Hexpol, USA
- Trico Products, USA
- National Oilwell Varco, USA

Next steps

- Release of the „GrafCompounder“ Version 2.004 will come at the end of 2014
- A comparison will be conducted between standard DoE software and GrafCompounder on correlations calculated between ingredients and physicals on a set of formulations