H-JG Consulting

Dr. Hans-Joachim Graf

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Tire Technology Conference 2015

The Smart Tire Factory

CARD - Computer Aided Recipe Development

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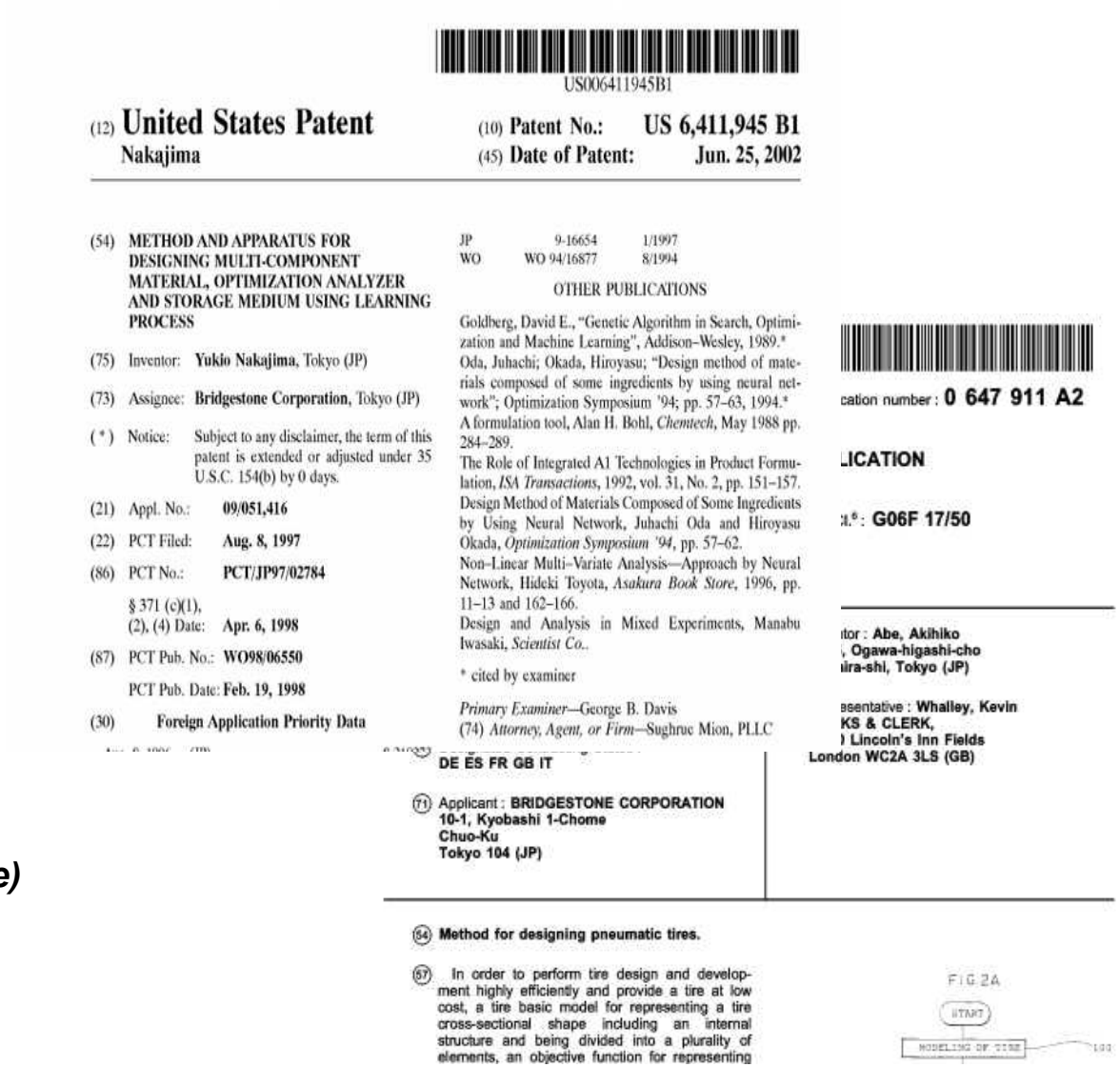
Content of this presentation

1. Introduction
2. Program idea
3. Justification of calculation method
4. Comparison with DoE Software calculation
   - Filler / Oil Design
   - Accelerator Design
   - DoE Simulation
5. Outlook

Computer Aided Compound Development

- **Bridgestone Patent 1994**
  Inventor: Akihiko Abe
- **Bridgestone Patent 2002**
  Inventor: Yukio Nakajima
- ***Colour Matching***
  Patents from
  BASF, CyanAmid, DuPONT
- ***Empirical DoE Patent:***
  Honeywell
- ***Recipe Libary Search and***
  Comparison
  CombiChem, GE, Hunt (Private)



US006411945B1

(12) **United States Patent**
Nakajima

(10) **Patent No.: US 6,411,945 B1**
(45) **Date of Patent: Jun. 25, 2002**

(54) **METHOD AND APPARATUS FOR DESIGNING MULTI-COMPONENT MATERIAL, OPTIMIZATION ANALYZER AND STORAGE MEDIUM USING LEARNING PROCESS**

(75) Inventor: **Yukio Nakajima**, Tokyo (JP)

(73) Assignee: **Bridgestone Corporation**, Tokyo (JP)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

(21) Appl. No.: **09/051,416**

(22) PCT Filed: **Aug. 8, 1997**

(86) PCT No.: **PCT/JP97/02784**

§ 371 (c)(1),
(2), (4) Date: **Apr. 6, 1998**

(87) PCT Pub. No.: **WO98/06550**

PCT Pub. Date: **Feb. 19, 1998**

(30) **Foreign Application Priority Data**

JP 9-16654 1/1997
WO WO 94/16877 8/1994

OTHER PUBLICATIONS

Goldberg, David E., "Genetic Algorithm in Search, Optimization and Machine Learning", Addison-Wesley, 1989.*
Oda, Juhachi; Okada, Hiroyasu; "Design method of materials composed of some ingredients by using neural network"; Optimization Symposium '94; pp. 57-63, 1994.*
A formulation tool, Alan H. Bohl, *Chemtech*, May 1988 pp. 284-289.
The Role of Integrated AI Technologies in Product Formulation, *ISA Transactions*, 1992, vol. 31, No. 2, pp. 151-157.
Design Method of Materials Composed of Some Ingredients by Using Neural Network, Juhachi Oda and Hiroyasu Okada, *Optimization Symposium '94*, pp. 57-62.
Non-Linear Multi-Variate Analysis—Approach by Neural Network, Hideki Toyota, *Asakura Book Store*, 1996, pp. 11-13 and 162-166.
Design and Analysis in Mixed Experiments, Manabu Iwasaki, *Scientist Co.*.

* cited by examiner

Primary Examiner—George B. Davis
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cation number : **0 647 911 A2**

LICATION

G06F 17/50

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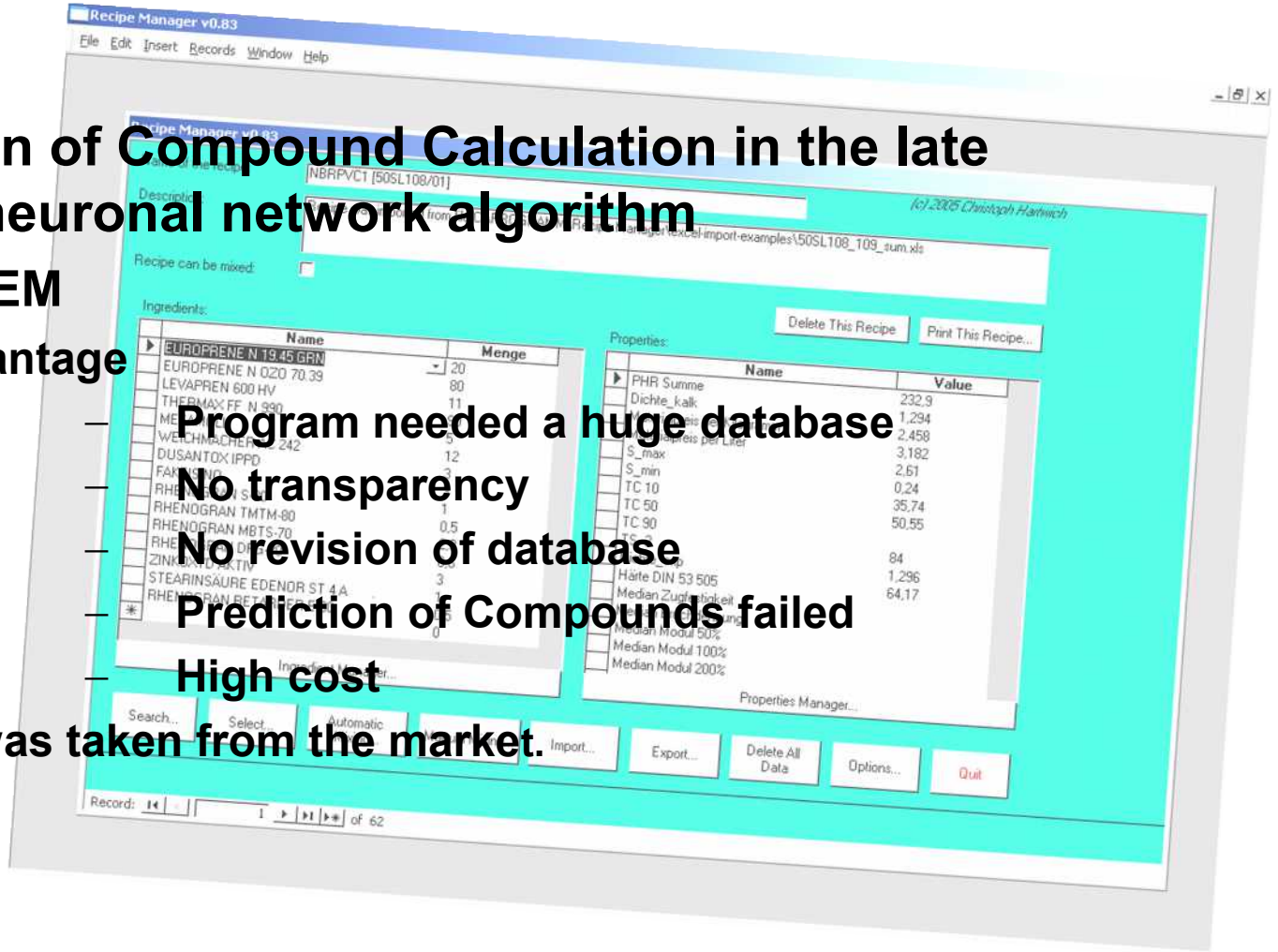
(54) **Method for designing pneumatic tires.**

(57) In order to perform tire design and development highly efficiently and provide a tire at low cost, a tire basic model for representing a tire cross-sectional shape including an internal structure and being divided into a plurality of elements, an objective function for representing

FIG 2A
START
MODELING OF TIRE

Commercialization of Compound Calculation in the late 90ties based on neuronal network algorithm

- Called CAD-CHEM
  - Disadvantage
    - Program needed a huge database
    - No transparency
    - No revision of database
    - Prediction of Compounds failed
    - High cost

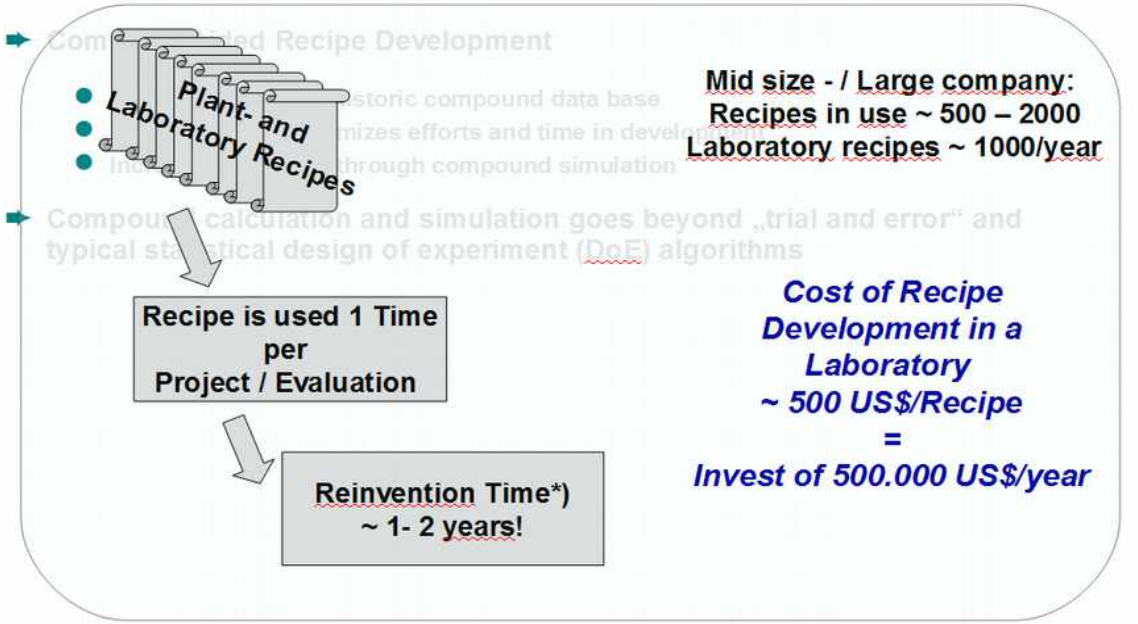


- Program was taken from the market.

Computer Aided Recipe Development

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

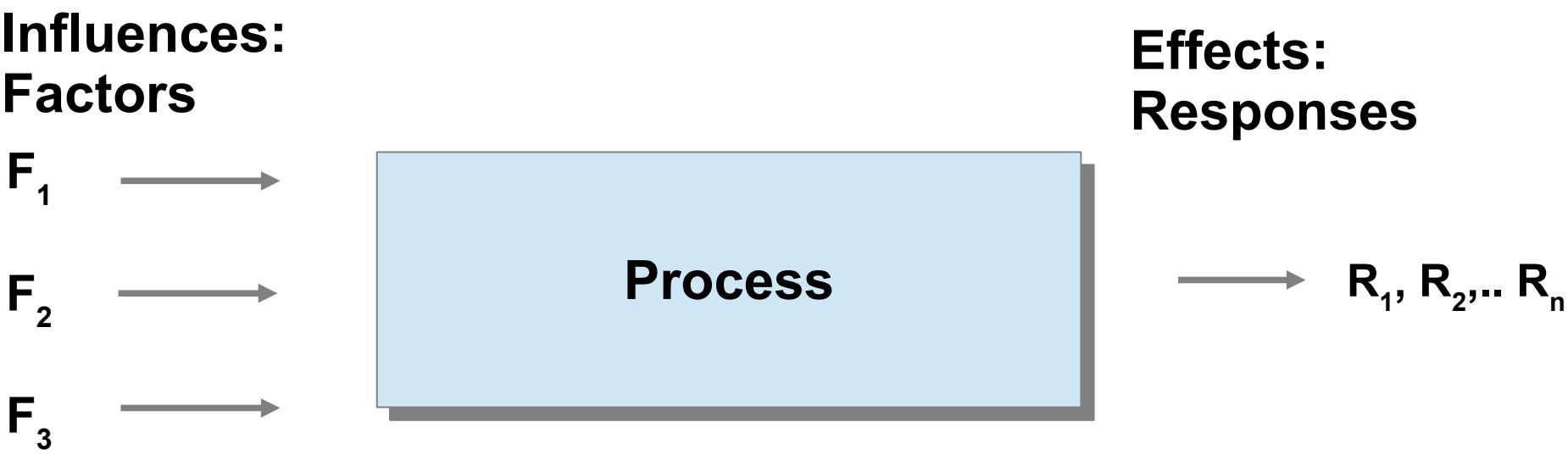
Compound calculation and simulation goes beyond „trial and error“ and typical statistical design of experiment (DoE) algorithms



Question:

Why we can hardly take Compound Databases as working capital,
Saving time and effort in our daily work?

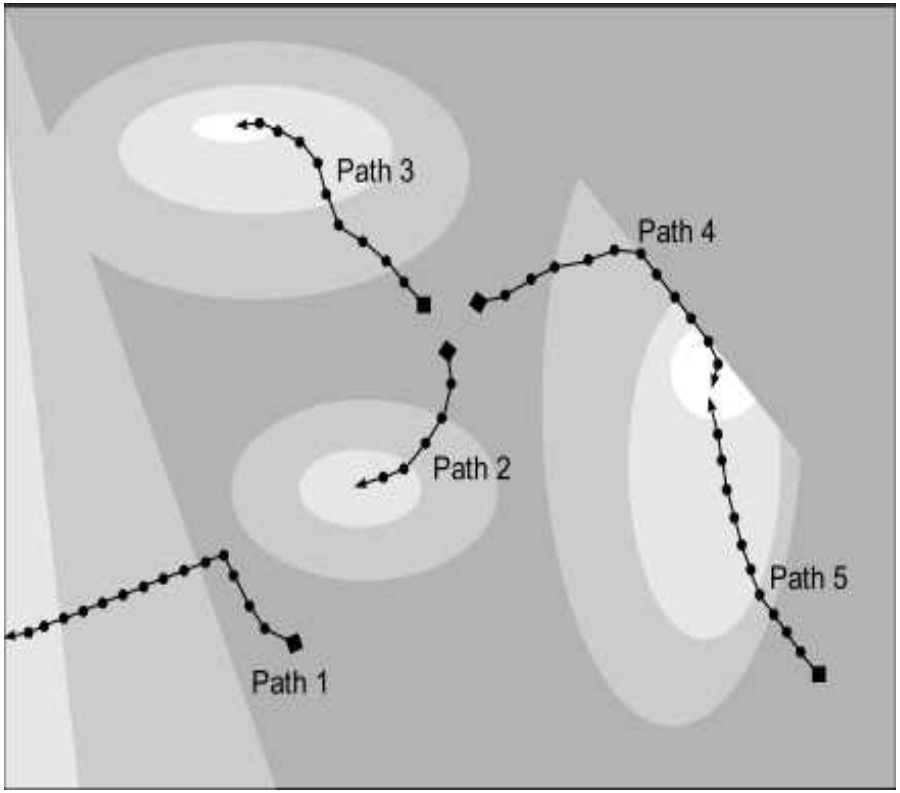
- **Avoiding reinvention**
- **Increase our compounding knowledge.**
- **Gaining room for really new ideas in compound development**



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:

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

- **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**



- **Database created with Statistic Experimental Design (DoE)**
  - **Organized / limited size**
  - **Variation of few factors according DoE**
  - **Optimization, numerical and graphical / prediction Tool available in the software**
- **CARD Computer Aided Recipe Development with GrafCompounder Database created historically**
  - **Unorganized / Unlimited**
  - **Multiple factor variation**
  - **Prediction according specification**

Justification of calculation method

- **If the majority of factor / response relations are linear the MLI – method gives sufficient accurate results (95% confidence interval)**

Line call out:

- **SEA J200: AA/BA/CA – NR, SBR, EPDM...and other Material**
- **SAE J200 M4 AA621 A13 B13 F17**

AA 610 **Suffix 2**	**Rubber** **Hardness** **Tensile** **Elongation**	**NR** **60°ShA** **21 Mpa** **350%**
A13	**Heat Aging** **Hardness Change** **Change Tensile** **Change Elongation**	**70h / 70°C** **± 15 °ShA** **± 30 %** **- 50%**
B13	**C-Set (22h/70)**	**< 25%**
F17	**Low Temperature Res.** **Non Brittle (3Min)**	**- 40 °C** **pass**

Properties of MB is determined by Polymer, CB and Oil content and the ratio or CB and Oil.

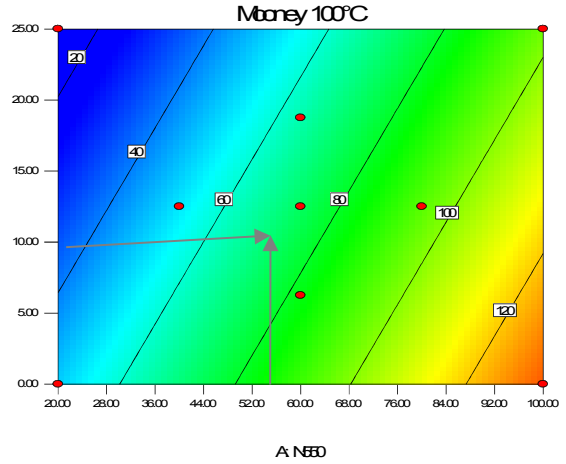
- Unit 2 as a reference (based on Cabot TG RG-135
- …

- CB 550: 55 phr
- Oil: 10 phr

- Mooney Viscosity: 71 M-Units
- Hardness: 60 °ShA
- Tensile: 21 MPa
- Elongation: 460 %
- C-Set: 28%

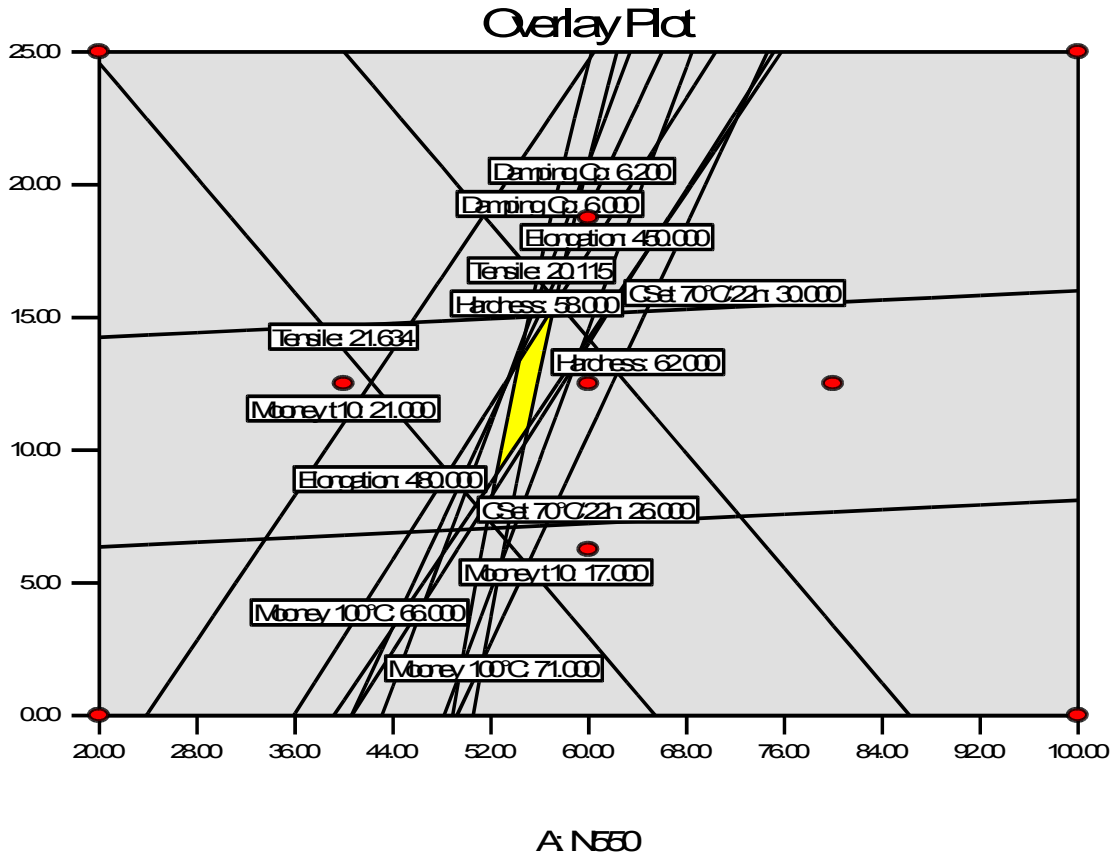
NR Compound

- *SMR 5CV – 100 phr*
- *CB – Var*
- *Oil – Var*
- *ZnO – 5 phr*
- *StAc – 1 phr*
- *AO – 1 phr*
- *NR 100 phr*
- *MBTS – 0.6*
- *S – 2.5 phr*



Properties of MB is determined by Polymer, CB and Oil content and the ratio or CB and Oil.

- **Unit 2 as a reference (based on Cabot TG RG-135)**
- **…**
- **CB 550: 55 phr**
- **Oil: 10 phr**
- **Mooney Viscosity: 66 – 71 M-Units**
- **Hardness: 58 – 62 °ShA**
- **Tensile: 20 – 22 MPa**
- **Elongation: 450 – 480 %**
- **C-Set: 26 – 30%**



Calculation method confirmation

- **Prove with**
  1. **NR Filler / Oil DoE – most of basic physicals are linear**
  2. **Filler / Oil DoE**
  3. **Accelerator DoE**

DoE with 4 Factors

Polymer used: EPDM (Vistalon 8600)

1.

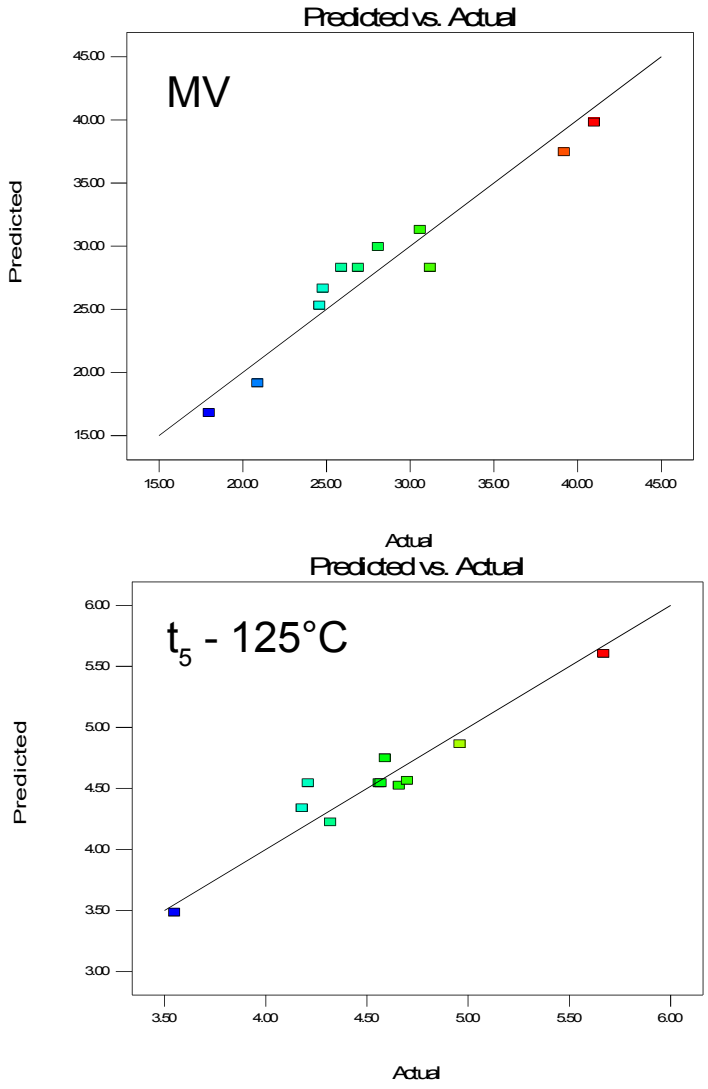
Factor	Name	Units	Min	Max
A	C6630	phr	60.00	95.00
B	CaCO3	phr	10.00	70.00
C	Clay	phr	10.00	50.00
D	Oil	phr	70.00	95.00

- **A fractional factorial DoE with 11 compounds only!**

Rheological Data are examined

- **MV and t_5 - 125°C can be measured quite accurate.**

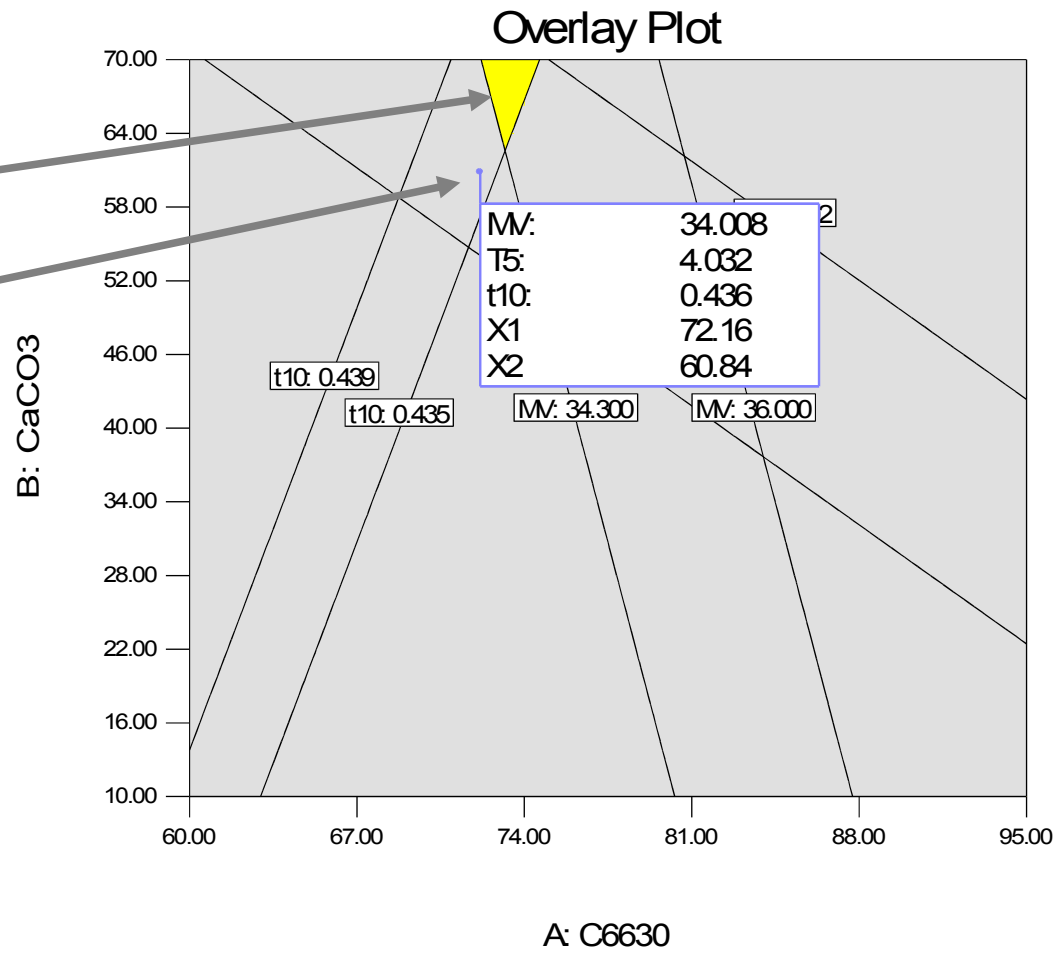
Both are significant with a linear model equation



Optimization area calculated with Design Expert

Solution given by GrafCompounder

with the additional condition (CC 6630 – 73 phr)



2.

DoE published by DuPont Dow in 1998

- **Factors: ENB, DTDC, S, MBT, TiTBD, ZdiBC, DTP**
- **DoE with 41 Experiments**

Tensile at break is significant with linear model

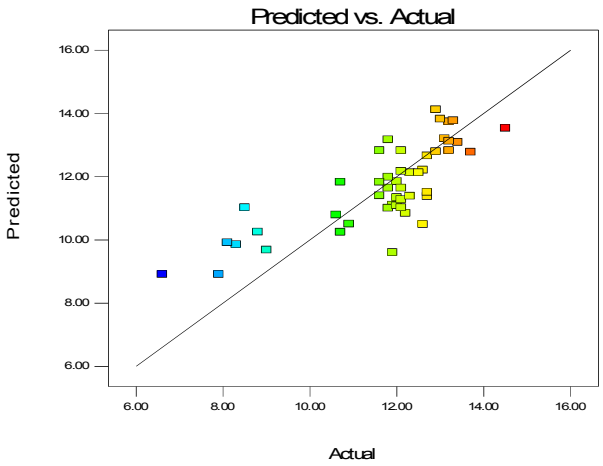
- **Sulfur has larger influence followed by DTDC and TiBTD, but negative**

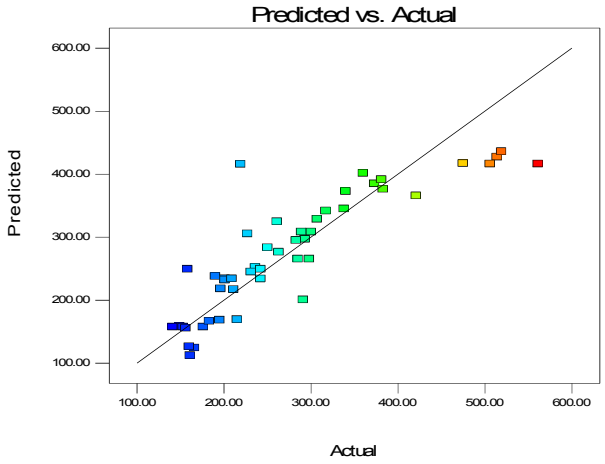
Elongation is significant with quadratic model, but linear model is a more than sufficient fit

- **Sulfur has the largest influence followed by DTDC**

Hardness is sufficient significant with linear model as well

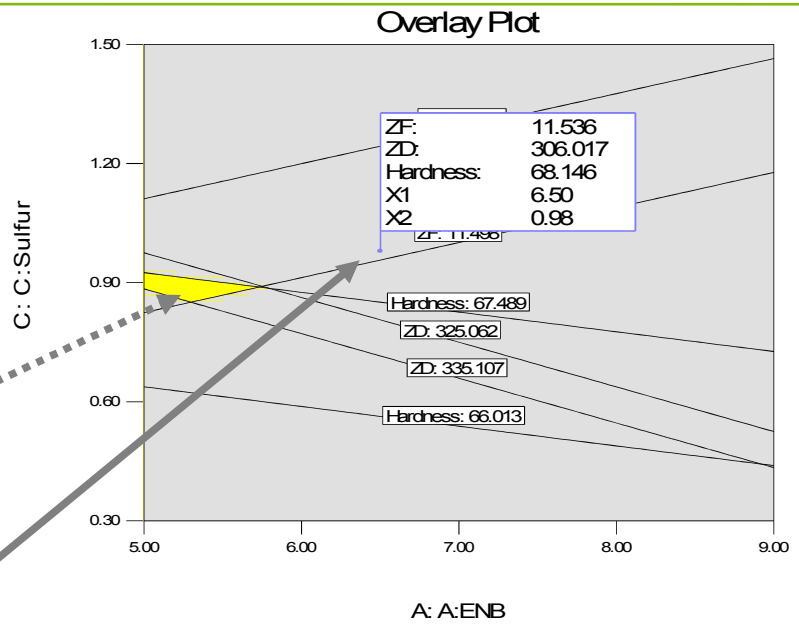
- **Main influence Sulfur, DTDC**





Boundary Conditions

- **Select boundaries**
- **ZF-MPa : 11.5-12.0**
- **ZD-% : 325-335**
- **H-°ShA : 65-67**



The Design Expert optimization graph shows the location of the result as a yellow area, but

GrafCompounder result is tagged with a flag.

Ingredients	GrafCompounder	Design Expert®
ENB	**6.5**	**5.45**
C:Sulfur	**0.93**	**0.88**
B:DTDC	**0.98**	**0.98**
D:MBT	**1**	**1**
E:TiBTD	**1.51**	**1.51**
F:ZDiBC	**1.33**	**1.33**
G:DTP	**1.45**	**1.44**
ZF	**11.5**	**11.5**
ZD	**325**	**330**
Hardness	**67**	**67.5**

3.

- **Simulation of a DoE**
- **Experiments made in the Laboratory**
  - **NR based Compound** — **LL** — **UL**
    - **Filler 1: CB 336** — **30 phr** — **70 phr**
    - **Filler 2: CB 550** — **0 phr** — **20 phr**
    - **Oil: Naphtenic Oil** — **5 phr** — **45 phr**
  - **Type of DoE: fractonal factorial**
  - **Software: Design Expert®**
- **Calculation made with GrafCompounder**
  - **NR Formula index from MRPRA**
  - **Formula data adjusted, but responses taken as is.**

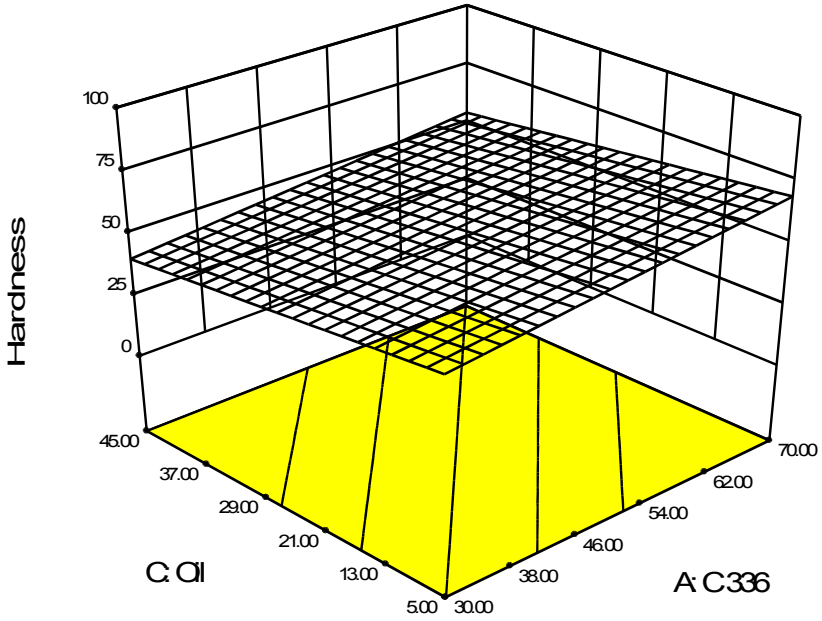
★ **For comparison: Hardness, Tensile - / Elongation at break**

Hardness:

X1 – A: CB 336

X2 = C: Napht oil

B: CB 550 = 10.00 phr

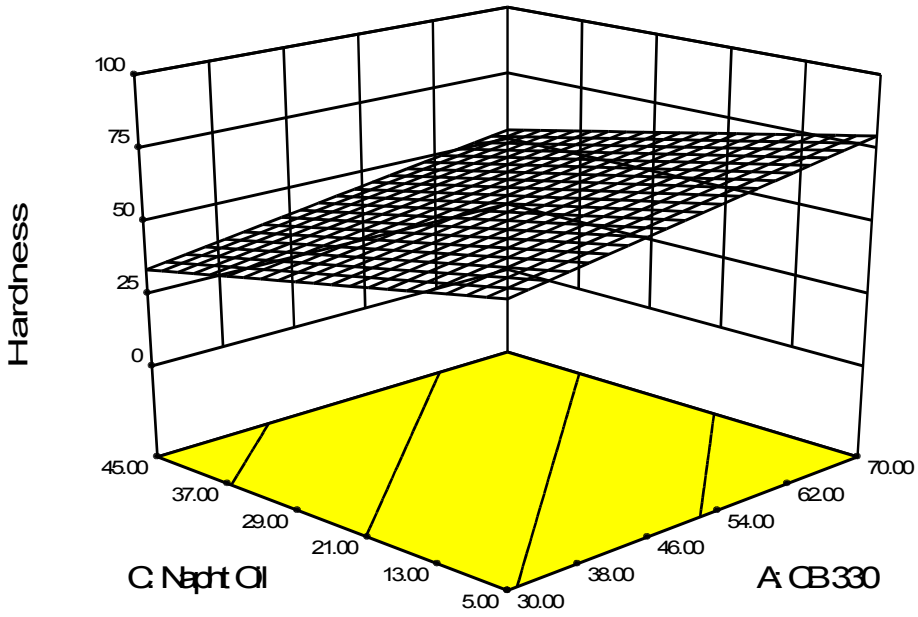


Hardness Simulation

X1 – A: CB 330

X2 = C: Napht oil

B: CB 550 = 10.00 phr

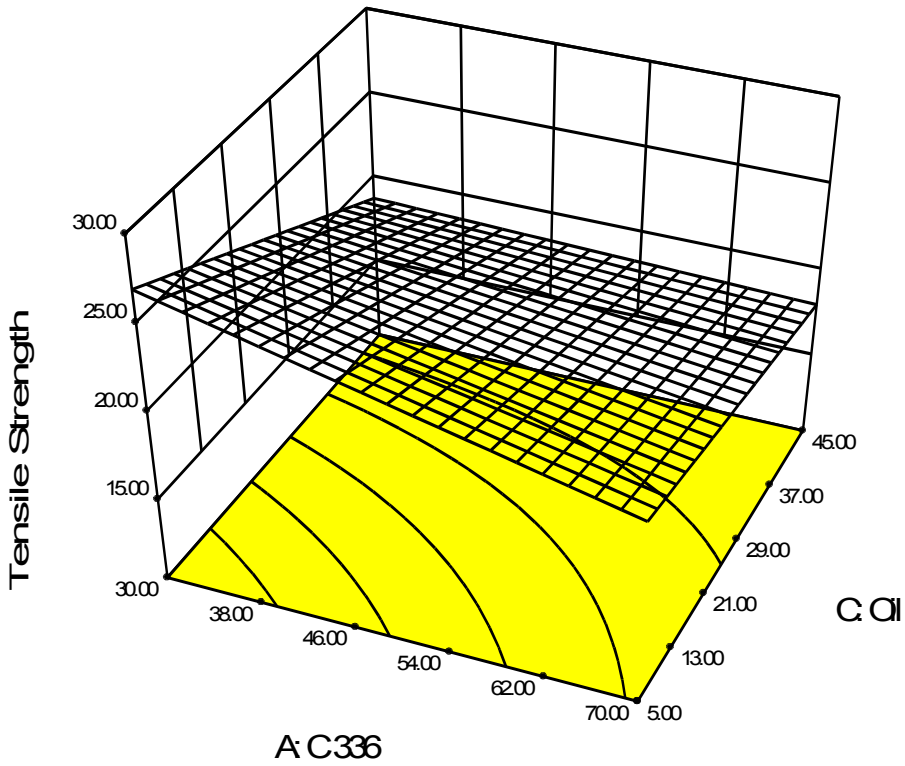


Tensile at break:

X1 – A: CB 336

X2 = C: Napht oil

B: CB 550 = 10.00 phr

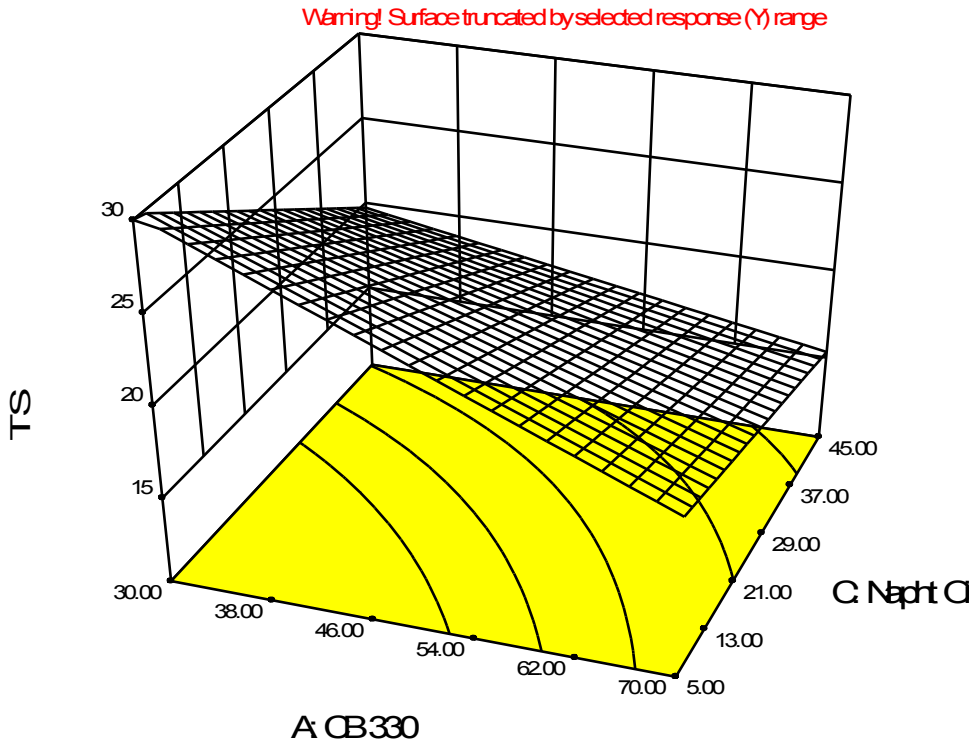


Tensile at break Simulation

X1 – A: CB 330

X2 = C: Napht oil

B: CB 550 = 10.00 phr

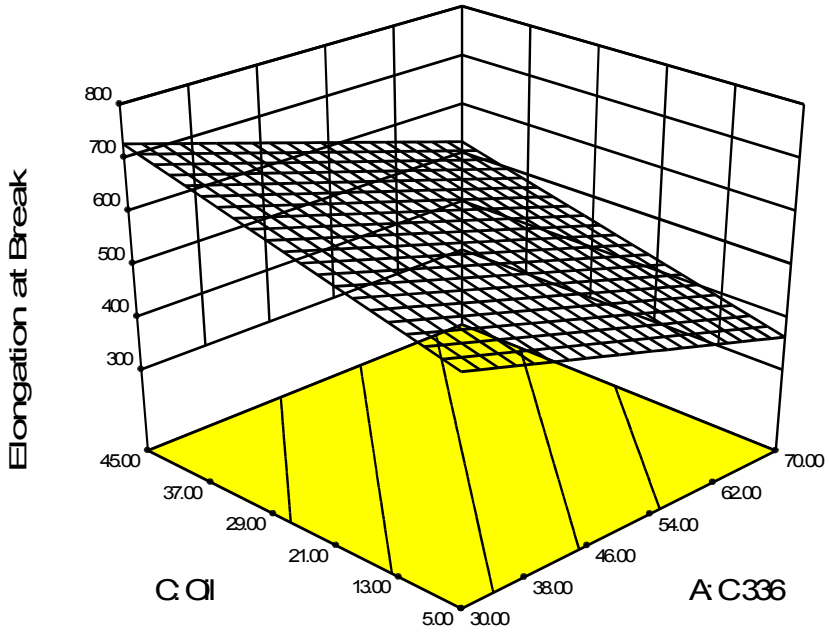


Elongation at break:

X1 – A: CB 336

X2 = C: Napht oil

B: CB 550 = 10.00 phr

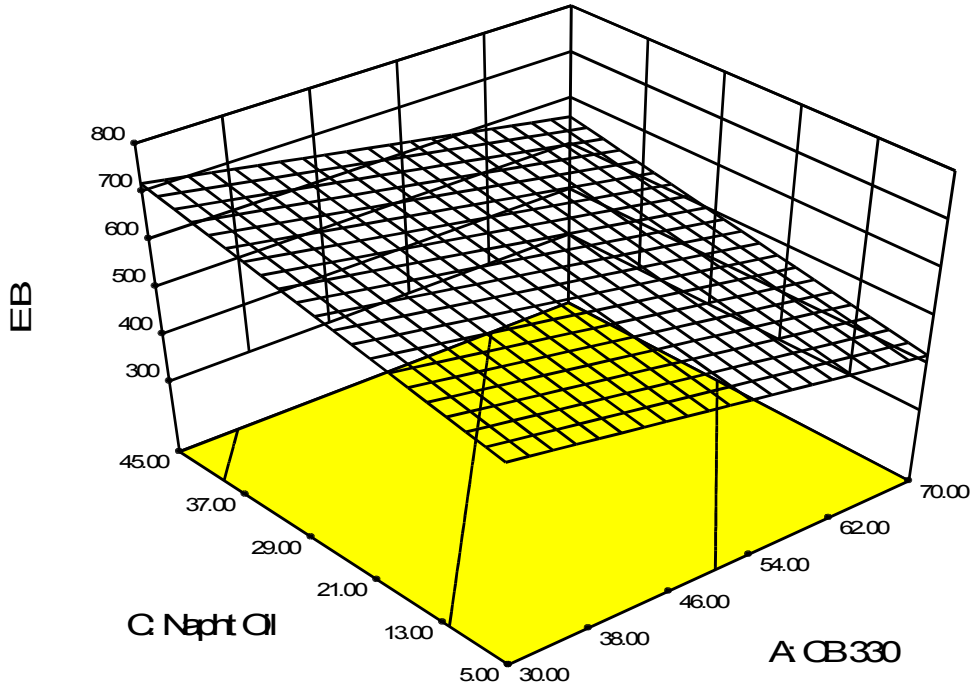


Elongation at break Simulation

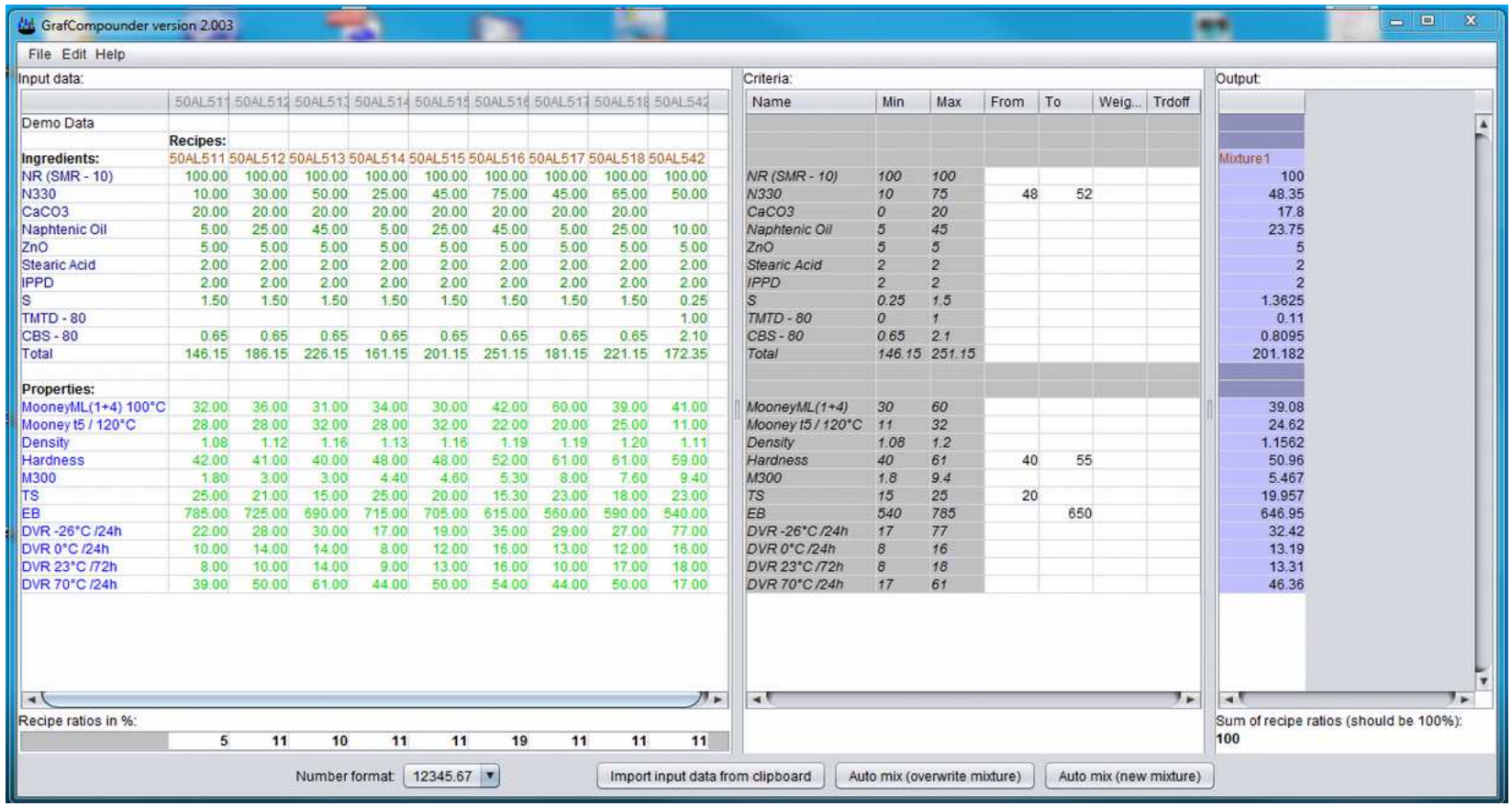
X1 – A: CB 330

X2 = C: Napht oil

B: CB 550 = 10.00 phr



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



Recipe manager

- **Creation of a formula according predefined criteria**
  - **Ingredients**
  - **Properties**
- **Traceability back to the starting formulas**
  - **Analysis of outliers and their correction or elimination in the database is possible.**
  - **Integration of results from statistical experimental designs.**
  - **Inquiry of databases of different origin, provided that an export of the data is possible with Office programs.**

Result of the calculations MUST be confirmed by an experiment.

- **Probability of a match between calculation and confirmation experiment result is about 90-5% according first experience**

- **Examples show:**
- **The resulting formulas calculated correspond to the general rules of compounding**
  - **Differences with calculations based on regression is marginal**
- **The formulas will show property scores larger than the 90 % – 95 % confidence interval in confirmation experiment**
- **Only one confirmation experiment would be needed as opposed to multiple trials in case of development targets.**

More information under: **www.grafcompounder.com**

- **Release of the „GrafCompounder“ Version 2.004 November 2014**
- **A simulation of a statistic experimental design is conducted between standard DoE software and GrafCompounder will be presented in more detail at IRC / DKT 2015 in Nueremberg / Germany**

Thank you for joining this presentation.

- **Any question, comment?**

More information under: **www.grafcompounder.com**