Navigating the Complexities of Rubber Development:

Bridging AI and DoE

Dr. Hans-Joachim Graf

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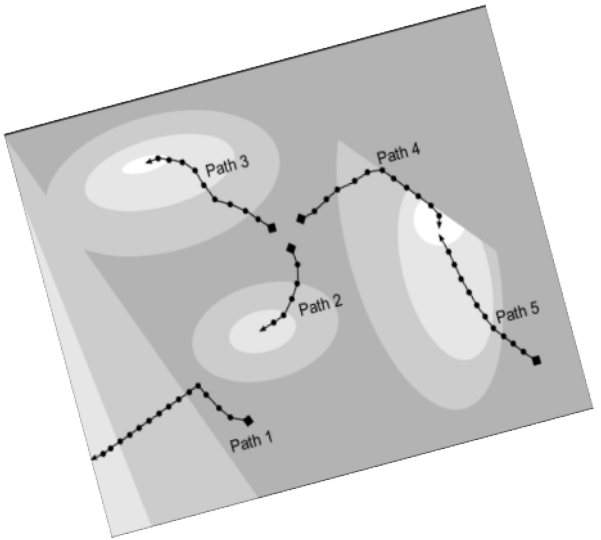
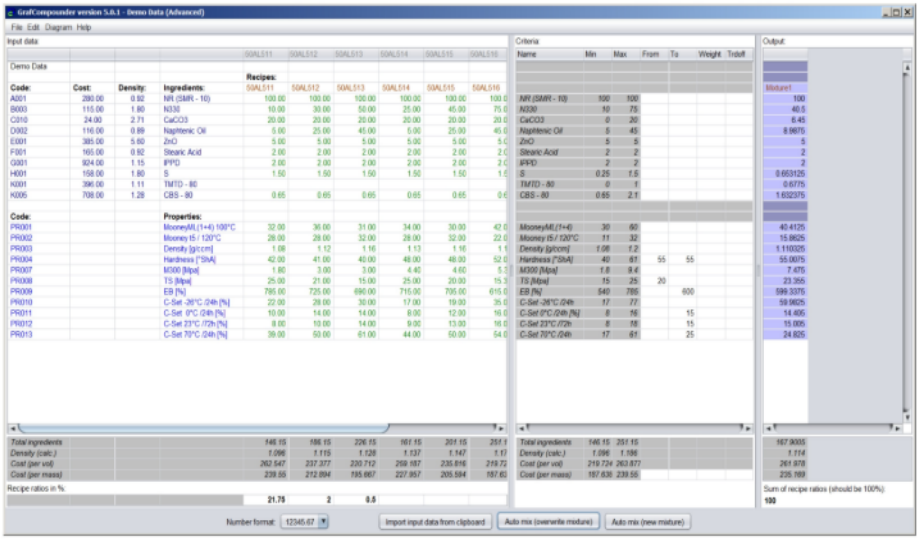


Development Tools

- **DoE – New Materials / Processes**
  - **Model** / Ingredient Selection & Limits / *Perform Experiments* / Select Result / Confirmation Experiment
- **AI – Historic Compound / Process Data**
  - **Data** / Criteria / *Prediction* / Select Result / Confirmation Experiment

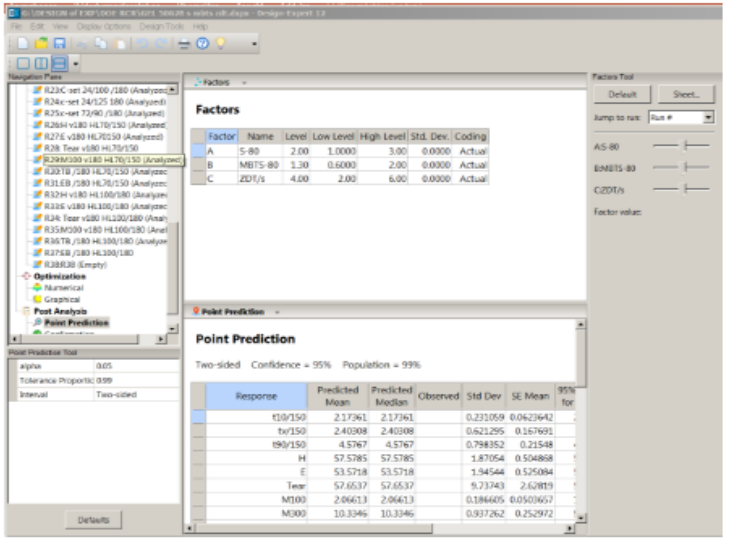
Navigating the Complexities of Rubber Development

- **Prediction based on AI**



GrafCompounder 5.0 (Screen shot

- **Prediction based on DoE**

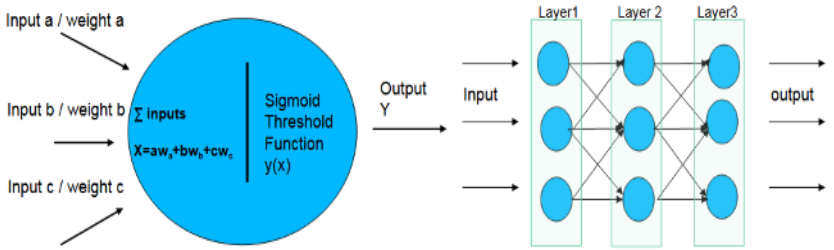


Point Prediction Tool in Design Expert®12 Software (Screen shot)

Navigating the Complexities of Rubber Development

- ## Data Calculation AI

Artificial Intelligence: Neuronal Network and Algorithm



Extended model of an artificial neuron with moderated input weights

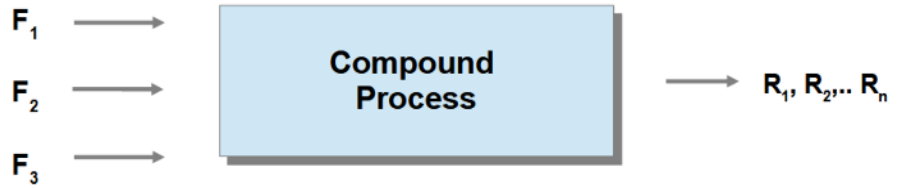
A model with multiple layers of neurons, each connected to the preceding and succeeding layer.
- Weights could be assigned to the connections between nodes

Source: T. Rashid, Neuronal Nets, 2017

- ## Data Calculation DoE

Experimentation: Variation of Factors

Measurements: Responses



Objective of the Experiment is the identification of the factors (F_1..F_n) type of influence on the responses (R_1...R_n) and description with mathematical equations for further processing.
ANOVA is used for statistical evaluation.

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

Navigating the Complexities of Rubber Development

- **Algorithm AI**

Matrix multiplication with the terminology of neuronal nets
*(**w** – weight, **I** = Input, **O** – X-Matrix multiplied sigmoid function)*

$$\begin{bmatrix} w1,2 & w2,1 \\ w1,2 & w2,2 \end{bmatrix} = \begin{bmatrix} I1 * w1,1 & I2 * w2,1 \\ I2 * w1,2 & I2 * w2,2 \end{bmatrix}$$

The input values for the subsequent layer is in each case:
X = w * I

Each x must be treated with the sigmoid, respective activation function:
Y =
Values for subsequent layers change to:
O = sigmoid (**X**)

- **Algorithm DoE**

The Prediction is calculated with the
- **Intercepts and**
- **Regression Factors:**

(*Table shows case for linear regression*)

Response	Intercept	F1	F2	Fn
R1	A_1	$A_{F1.1}$	$A_{F2.1}$	$A_{Fn.1}$
R2	A_2	$A_{F1.2}$	$X_{F2.2}$	$A_{Fn.2}$
.....	.....	.....	.....	.....
Rn	A_n	$A_{F.n}$	$A_{Fn.n}$	$A_{Fn.n}$

Mathematic basics of Development Tools

- **DoE**
  - Linear and 2nd, 3rd order regression: *Experimental effort*.
- **AI**
  - Feed Forward
    - Depending on data accuracy: Experimental effort
  - Machine Learning ?
    - **Limited resources, time constraints a hint for machine learning models**
      Dependency on property

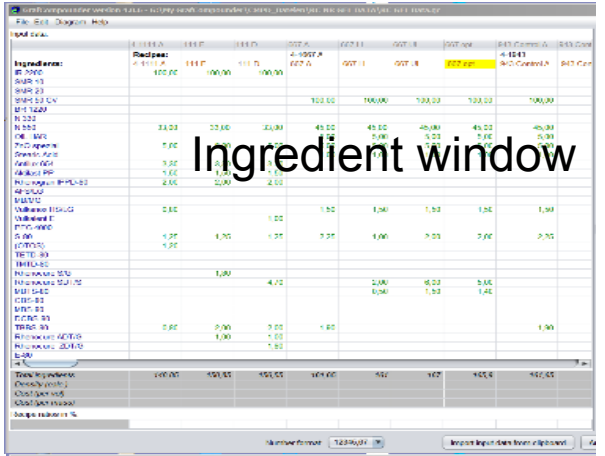
Graf Compounder

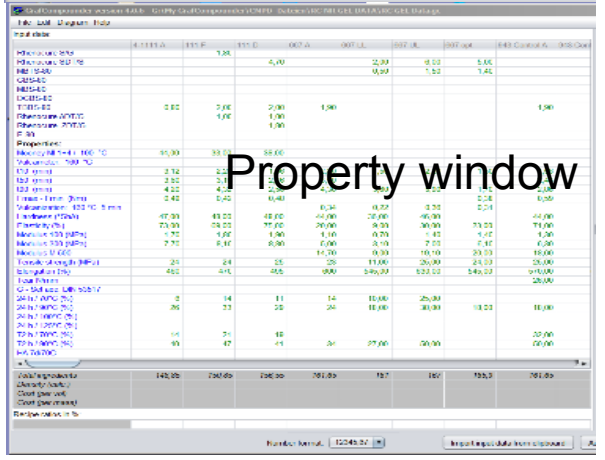
Ingredients

Properties

Data Structure Rubber Compounds

- Ingredients
  - Normalized to 100 parts polymer = phr
- Properties
  - Rheological properties
  - Physicals
    - Other
      - Appearance
      - Dynamics



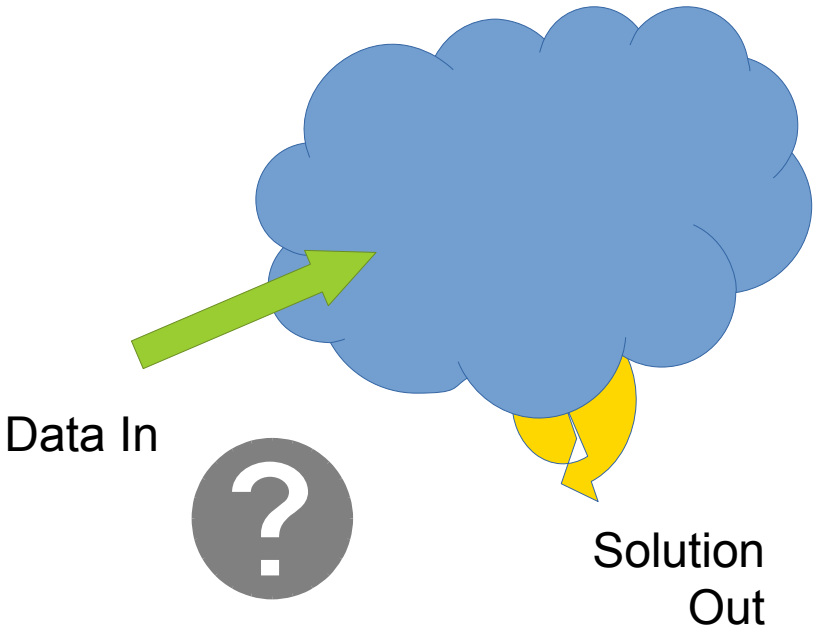


- **AI Data Structure**
  - Trial&Error Data Collections
  - OFAT Data Blocks
  - DoE Data blocks
    - Property Data
      According Customer / Market
      Specification
    - Data Diversity

- **DoE Data Structure**
  - Data Sets
    - Blocks of 9 – 20 Sets
    - Property Data
      Project related
    - Data Diversity: blockwise

- **Data Quality**
  - **Faulty Data in**
  - **No useful Solution out**
- **Sources of Error**
  - Lack of Standardization
    - Variation Mixing
    - Variation Testing

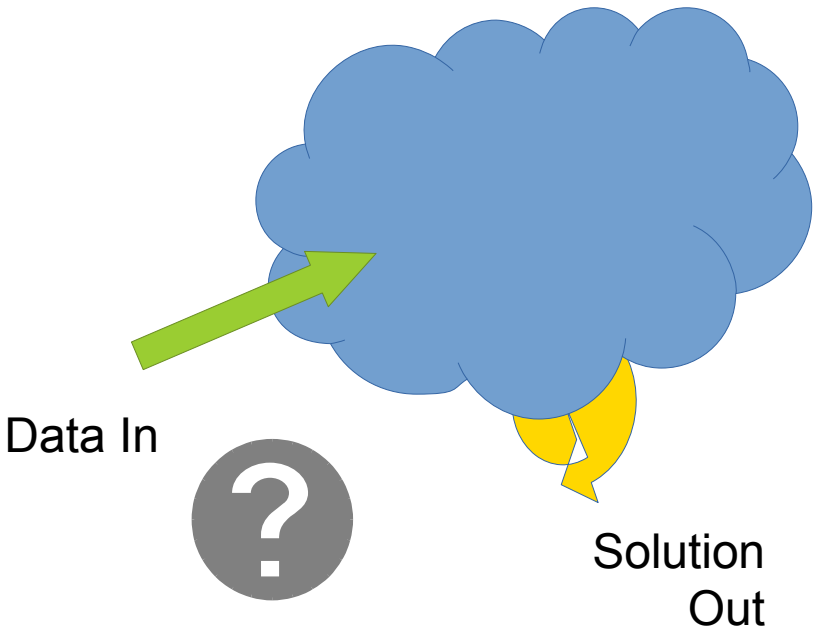
- **Data Cloud?**



Navigating the Complexities of Rubber Development

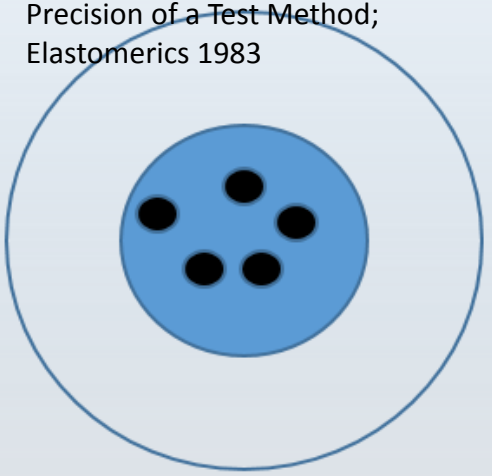
- **Standarization**
  - Eliminate Redundant Ingredients
    (Neutralization of Names)
- **Separation**
  - Polymer Compatibility
  - Ingredient Solubility
  - Crosslinking Systems

- **Data Cloud?**



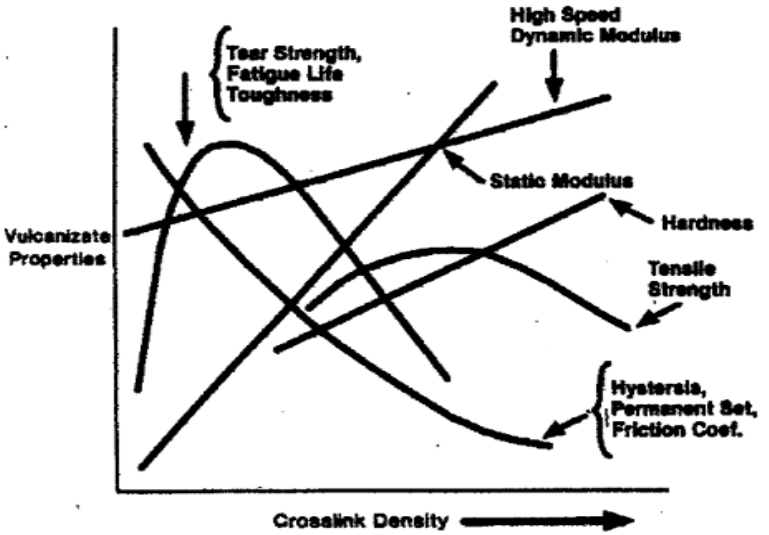
- **Decrease of Variation, Increase Precision**
  - **Laboratory Mixing Machine: Variation**
    - Raw Material / Process Protocol Influences
    - Testing
  - **Test Protocol: 5 instead of 3 samples per Test**
    - Evaluation of Measurement Error (Man – Machine – Material)
    - Design of Experiments: Number of Repeats
  - **Round Robin Testing with external Laboratories**

Source: C.E. McCormick, Evaluating and Utilizing the Precision of a Test Method; Elastomerics 1983



- **How to check / improve quality of a historic data pool?**
- **AI Prediction of compound inside 95% confidence interval**
  - Elimination of outliers possible, if ingredient – property relation can be demonstrated
    - Properties correlated to crosslink density (according Coran)
  - Correlation analysis of properties
  - Properties inter-correlated

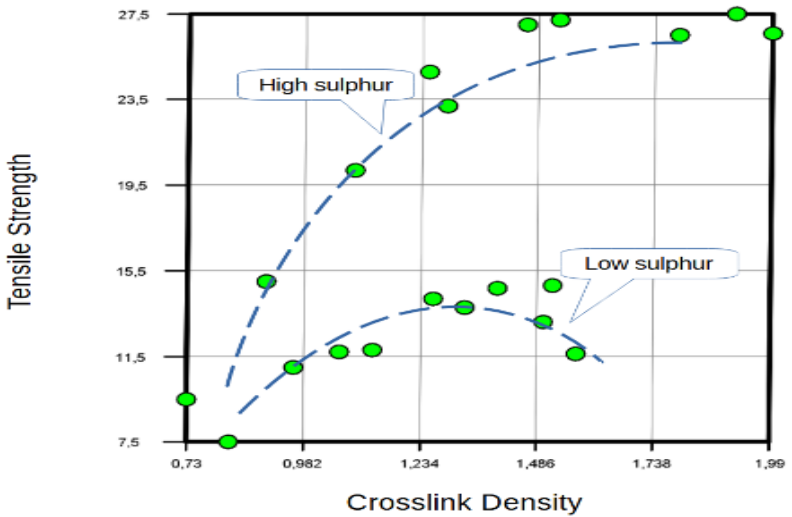
Correlation between crosslink density and physical properties



Source: D. Hertz, Elastomerics 1984,
A.Y. Coran, in Science Technology of Rubber, § Vulcanization, Academic Press 1994
M.L. Studebaker, RCT 39, 1966

- **Properties over Crosslink Density**
  - Variation of ingredients cause a shift of properties
    - Hardness / Modulus
    - Static- / Dynamic Force
    - Crosslink Density / CLD Concentration
    - ….

- **Variation of Ingredients: Example Sulphur**
  Source: L. Gonzales, et al., KGK 2005

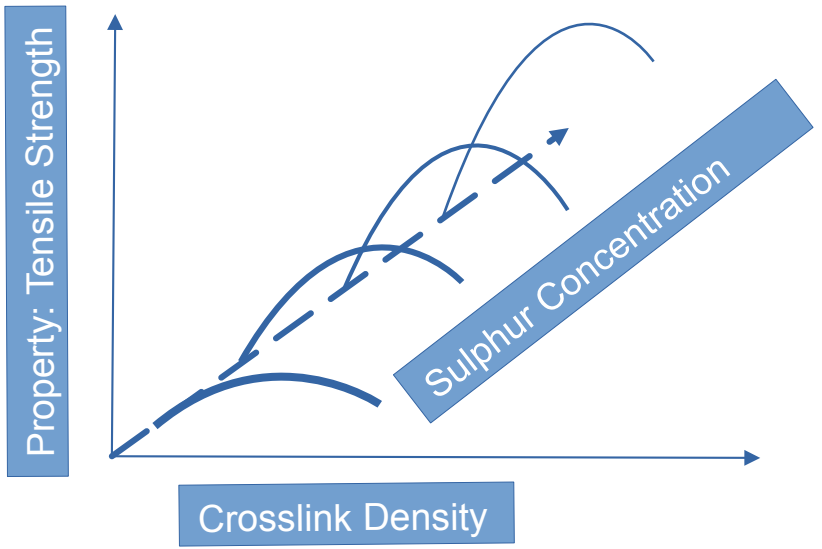


- **Checking Data**
  - Correlation of Related Properties
    - Hardness / Modulus
    - Static- / Dynamic Force
    - Crosslink Density / Cross Linker Concentration
  - Using a consistent sulfur content when cutting out a curve enables the assessment of accuracy by observing the dispersion or clustering of points along the curve.

- **Coran's Diagram**

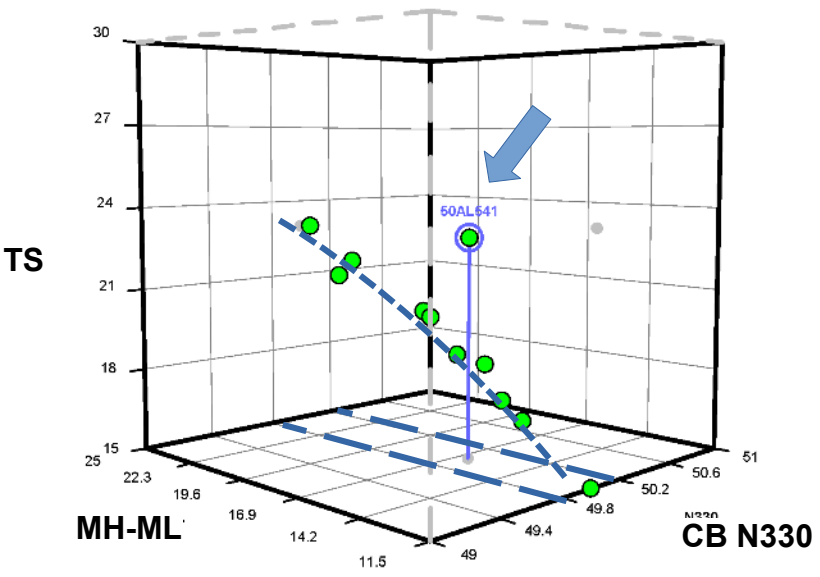
Variation of Ingredients: Example Sulphur

Source: L. Gonzales, et al., KGK 2005

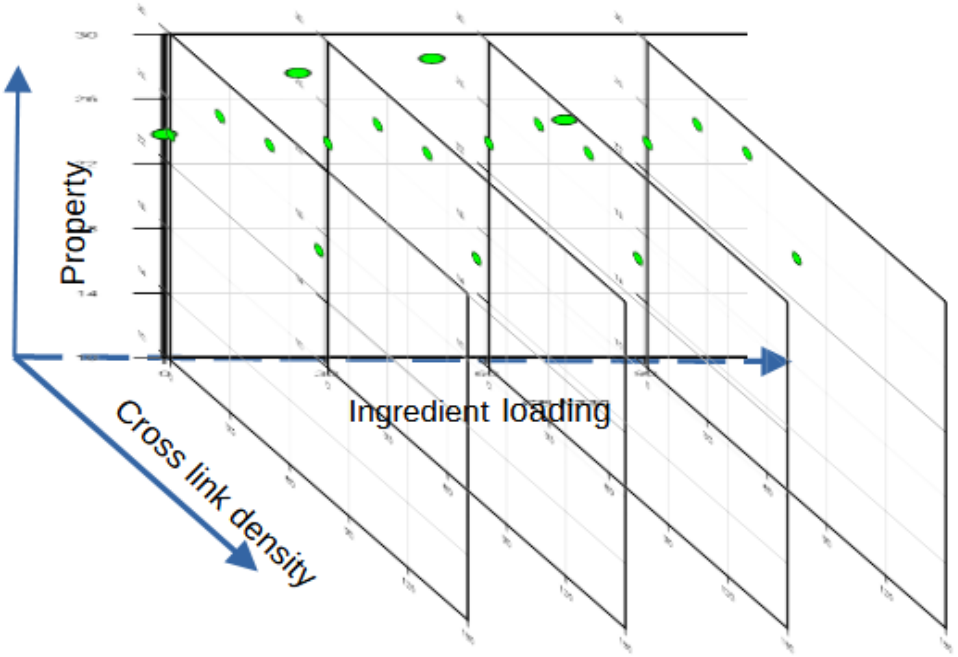


Navigating the Complexities of Rubber Development

- **Property Data Slice**
  - With outlier



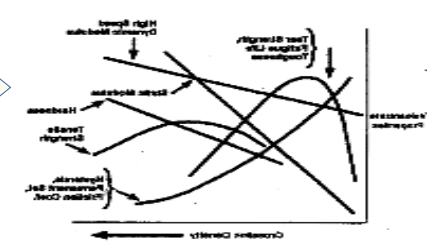
- **Property (TS) over XLD & Loading (CB N330)**
  - Cutting property-XLD slices

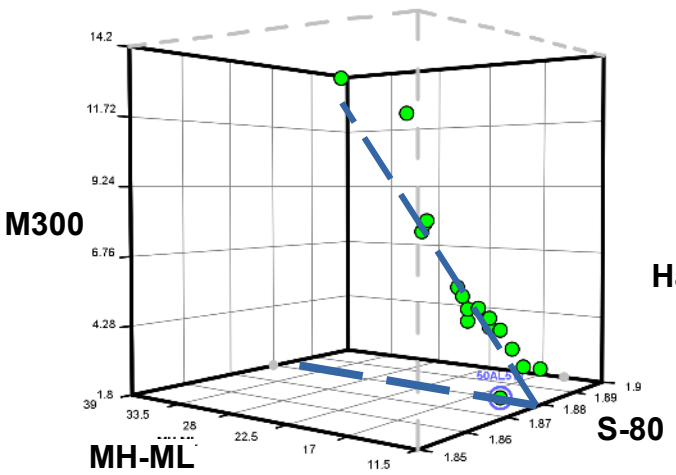


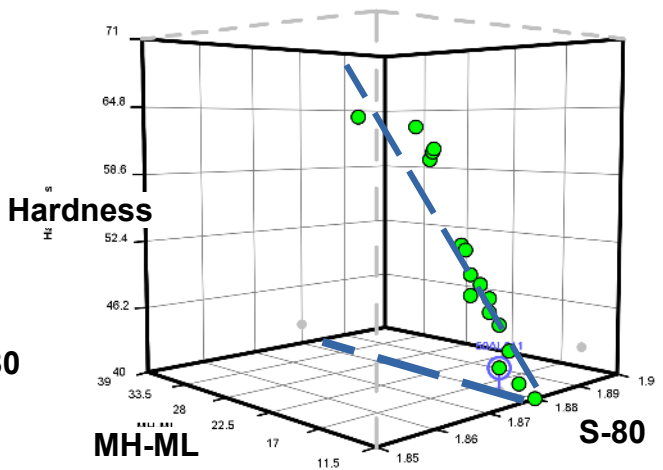
Navigating the Complexities of Rubber Development

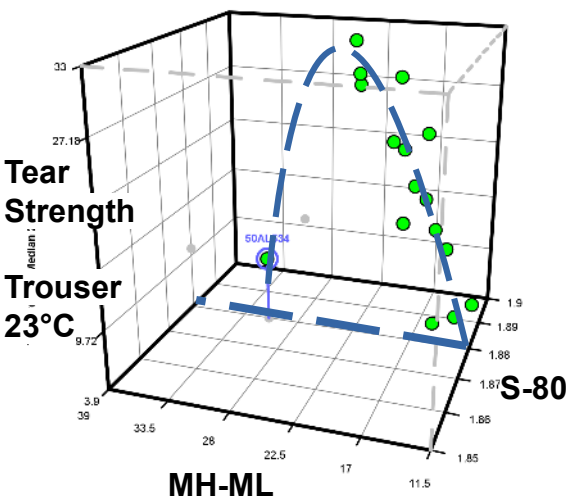
- **Property over XLD & Sulfur**
  - Cutting Property-XLD Slices

Coran's Diagram Reversed



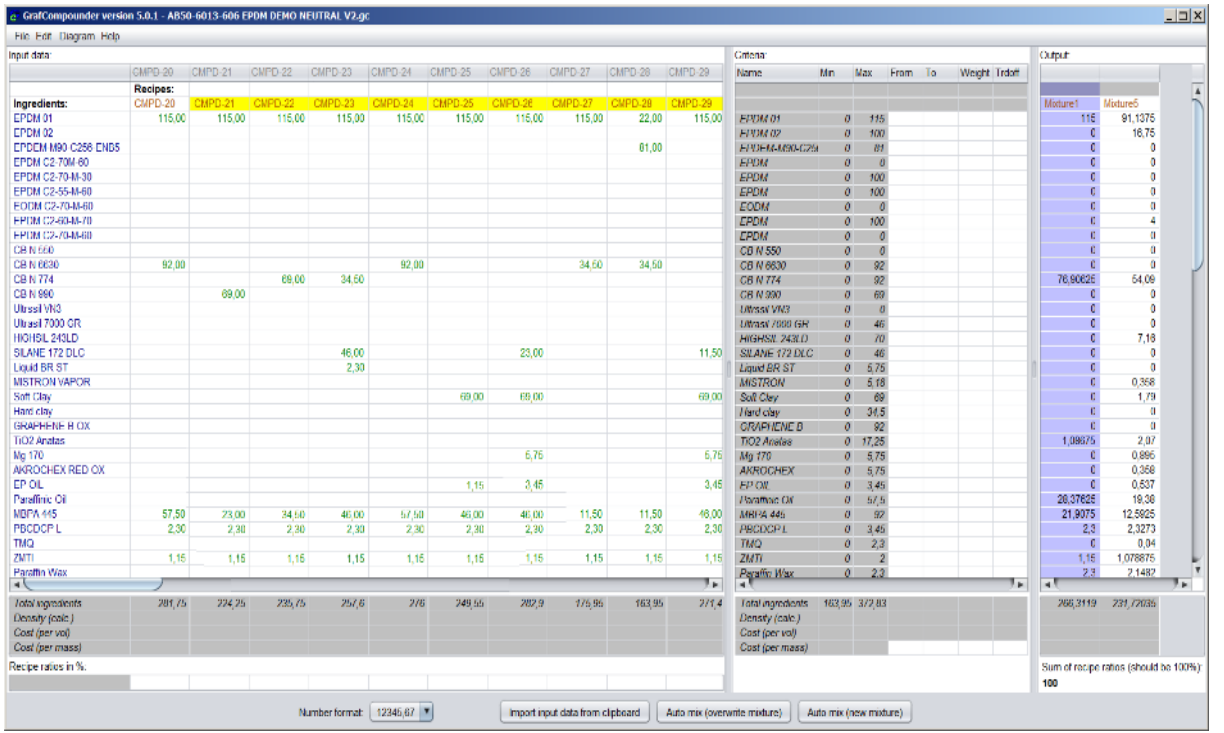






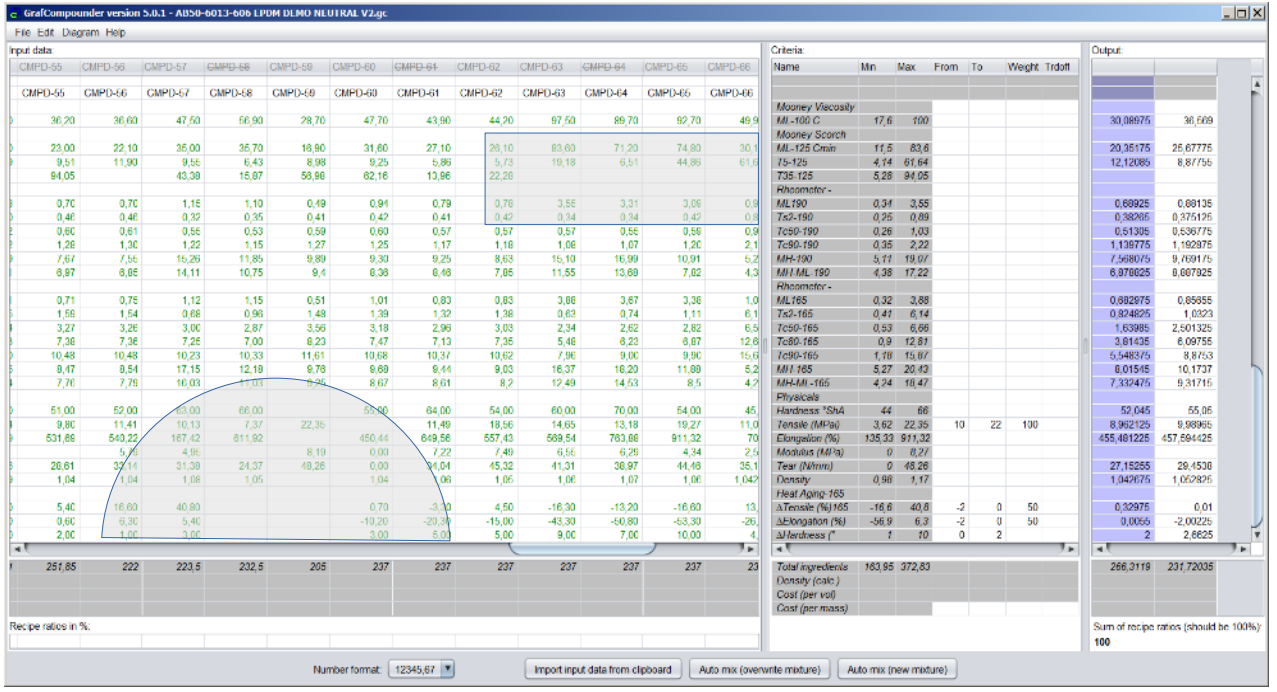
Navigating the Complexities of Rubber Development

- **Data Management**
  - **Ingredients**
    - Copy / Paste ingredients from **master ingredient file**
    - Neutralization
      - CAS No.
      - Chemical name



Navigating the Complexities of Rubber Development

- **Data Management**
  - **Properties**
    - Copy / Paste property names from **master property file**
  - **Standardization**
    - Standard properties
  - Custom properties.



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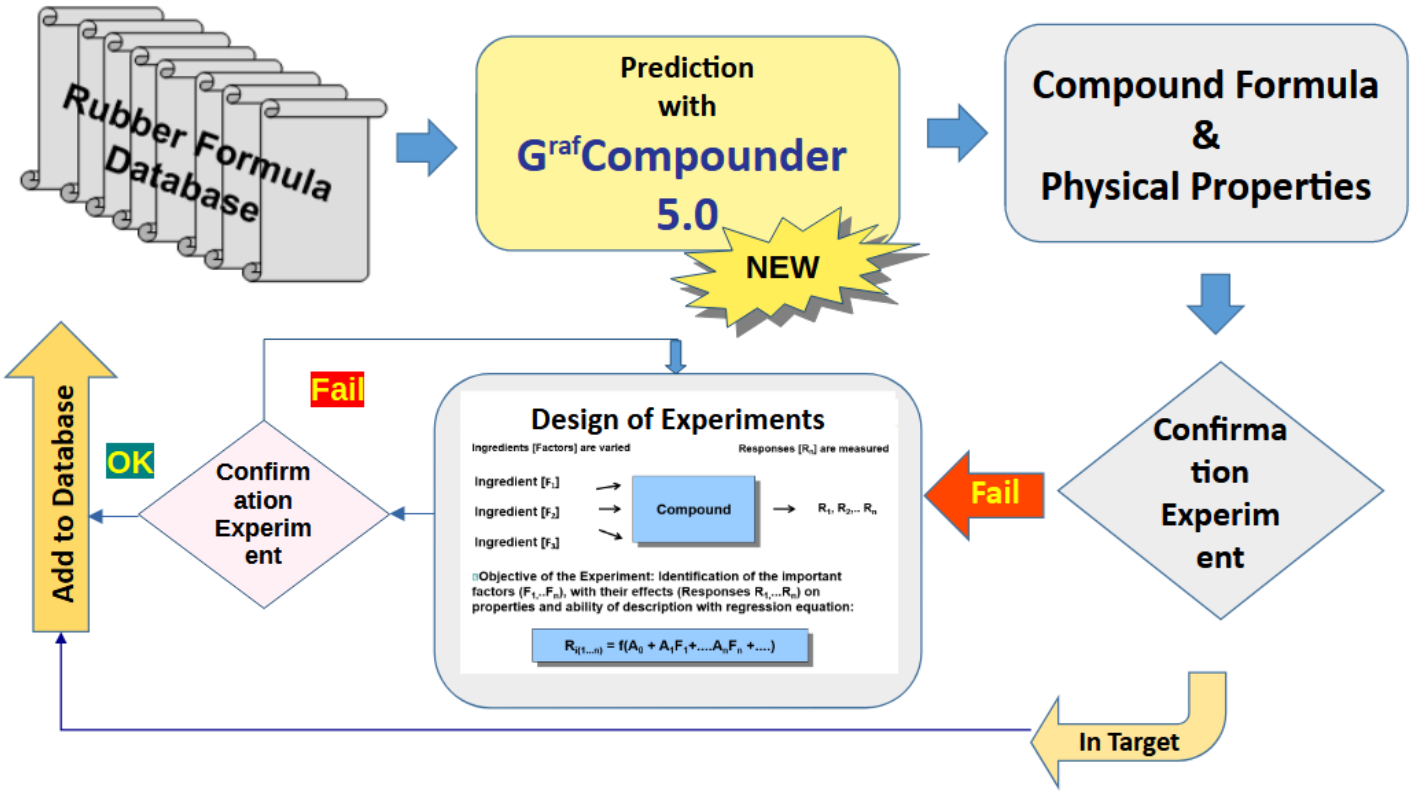
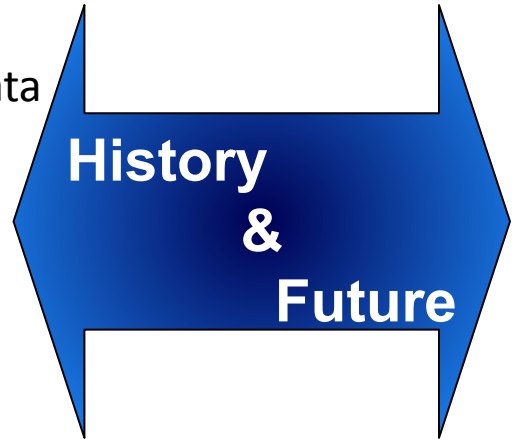


Navigating the Complexities of Rubber Development

Artificial Intelligence: G[raf]Compounder

- Compound History
- Analyze / Eliminate Foulty Data
- Simulate
- Select Solution for Confirmation Trial
- Confirm



EXPERIMENTAL DESIGN

- Explore Materials
- Evaluate
- Decide
- Select Possible Solution for Confirmation Trial
- Confirm

- **Conclusion**
  - DoE and AI complement each other perfectly.
  - All Data in the cloud is not recommended.
  - Quality of data remains an issue.
  - Database can be improved with suitable tools.
  - Management of data will enhance AI accuracy