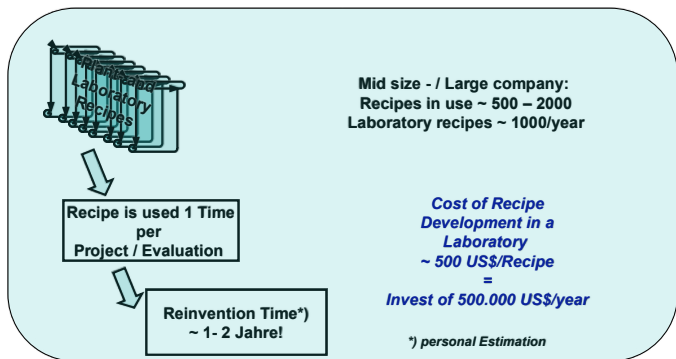


# Where we are with Artificial Intelligence & Machine Learning in Rubber Development

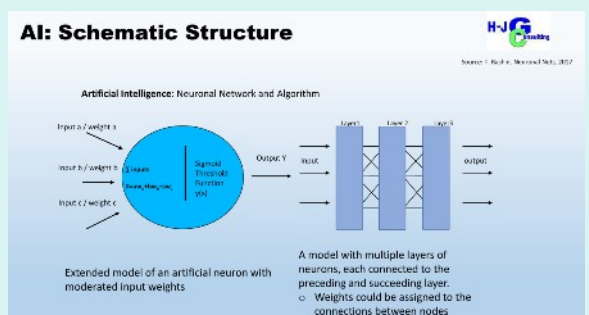
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Compounds in Rubber Industry are seen as intellectual property and a sensitive topic, due to its large influence on total manufacturing cost. Surprisingly development methods are quite conservative compared to other industries. While the use of CAD (Computer Aided Design) and Simulation becoming the new standard of part development and processing, compounds created based on experience, knowledge and rules evaluated in the last centuries. Nowadays the discussion is on, to use modern computer techniques like Artificial Intelligence [AI] and Machine Learning [ML] in compound development, but ML may find its way in processing much faster.

## Artificial Intelligence

To open up the limits of DoE, Artificial Intelligence (AI) and even ML is discussed since some time. AI is created to make use of existing data (for example "Words" for spell checking or "Pixels" for Face recognition). It processes data created in the past. It works with specific neuronal network algorithm, but needs large amount of data. In rubber development there is no lack of data, but this data are not publicly shared nor available in an organized standard format. Opposite to above examples the data have measurement errors. On top, the error values are not normal distributed due to influences from time, machine, man and material. This is an obstacle for ML and specifically the training of a ML program. The other issue, the training would take a large amount of time from weeks up to months.



However, happenstance database can be improved via cross correlation analysis via taking out outliers and other errors. Rubber technology teaches us, that some physical properties depending on cross link density and / or reinforcement. There are interdependent properties which are inter correlated as well. If such relations can be generalized and considered independent from the compound composition, then such analysis is a step forward to clean up the data. It would lead to a much better compound prediction even without ML programs, which is demonstrated already.

**Feed Forward AI: What is the advantage?**

- Compound Prediction is possible with any data set
  - Data set can be small or large
- All significant parameters should be included in the query simultaneously
  - 2-3 Properties in the query makes no sense.
  - Most specification values, but at tighter limits
    - Improve query with "Weights" and "Toloff"

AI and DoE replacing completely trial and error or any other development strategy like One Factor A Time (OFAT) procedure. AI and DoE have its advantages and disadvantages, which will be discussed in this presentation. In modern rubber development both are needed. But the use of ML in Rubber compound development seems far away and will take a new approach.

More Information:  
[www.grafcompounder.com](http://www.grafcompounder.com)

## Design of Experiments

Statistic Experimental Design [DoE] is a tool to explore new materials, it even can help, whether an ingredient in a compound is necessary or can be eliminated. This technique is based on factor – response correlations and regression analysis. However, conclusions are always limited to the limits of the experiments. Beyond extrapolation is hardly possible, if not forbidden. The smaller the DoE, the lack between confirmation experiment and prediction becomes large.

**Regression Analysis**

Experimentation: Variation of Factors  $F_1, F_2, F_3$

Compound Process

Measurements: Responses  $R_1, R_2, \dots, R_n$

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

$$R_{1(n)} = f(A_0 + A_1 F_1 + \dots + A_n F_n + \dots)$$

TS (Tensile at Break): Predicted over actual, top - linear, bottom - 2D

It depends highly on compound manufacturing variation and measurement precision. Compounding knowledge is, of course, helpful for the selection of factors with their upper and lower limits. In addition, the findings cannot easily be transferred to other compounds made of different ingredients like polymers, etc.

**DoE: Point Prediction based on Regression**

The Prediction is calculated with the

- Intercepts and
- Regression Factors:

(Table shows case for linear regression)

Response	Intercept	F1	F2	Fn
R1	A <sub>0</sub>	A <sub>1,1</sub>	A <sub>2,1</sub>	A <sub>n,1</sub>
R2	A <sub>0</sub>	A <sub>1,2</sub>	A <sub>2,2</sub>	A <sub>n,2</sub>
.....	.....	.....	.....	.....
Rn	A <sub>0</sub>	A <sub>1,n</sub>	A <sub>2,n</sub>	A <sub>n,n</sub>

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

