Advantage of Compound Development with the "GrafCompounder"

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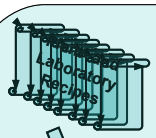


Recipe is used 1 Time per Project / Evaluation

Reinvention Time*) ~ 1- 2 Jahre!

*) personal Estimation

Mid size - / Large company:
Recipes in use ~ 500 – 2000
Laboratory recipes ~ 1000/year

Cost of Recipe Development in a Laboratory ~ 500 US$/Recipe = Invest of 500.000 US$/year

- **Analysis of a recipe database with Multiple Linear Iteration (MLI)**
  - Search criteria manageable with different weights!
  - Recipe Selection (Exclusion of unwanted recipes during analysis)
  - Avoid Analysis of none compatible Polymers
  - Automatic an Manual Mode
  - Simulation of Blends of Compounds
  - Property Data should be from a trustworthy source, if not your own
- **Advantages of Multiple Linear Interation**
  - GRAFCompounder enables to analyze any compound database and
  - Calculates a compound recipe with its properties predicted

Statistic Experimental Design [DoE] allows a Factor - Response Calculation with regression equations

Influental Factors are varied → **Compound** → **Effects Responses are measured**

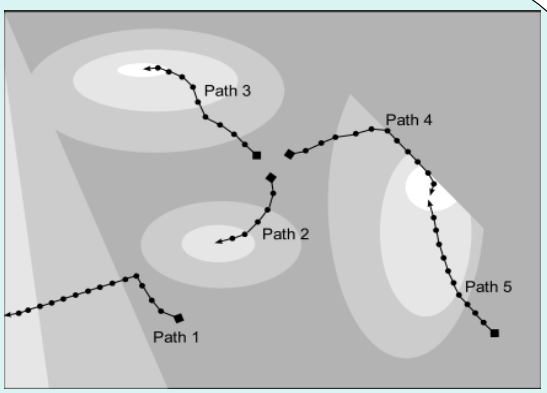
F_1, F_2, F_n → Compound → $R_1, R_2, \ldots R_n$

Objective ot the Experiment should be the identificatio of the most important factors (F_1..F_n) to be linked with measured effects (Responses R_1..R_n) and to describe their dependency in a mathematical equation.:

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

A dataset of organized Data / Result pairs is achieved, which allows further evaluation and investigation

Compound Database = unorganized Data
Impossible to Analyze with Regression



With „Multiple Linear Interation" [MLI] one can analyze unarganized, happenstance data, which is impossible with regression, neither linear or none-linear regression.

The Analysis is based on
- Ingredinets and Properties of Compound
- Targets
- Weights
- Rating Functions, which shows the distances between Values and targets
- Iteration in small steps from starting points
- Check of best agreement between conflicting targets

Report of result:
- One recipe with its properties
- Ratios of recipes used for the calculated compound

Bibliography

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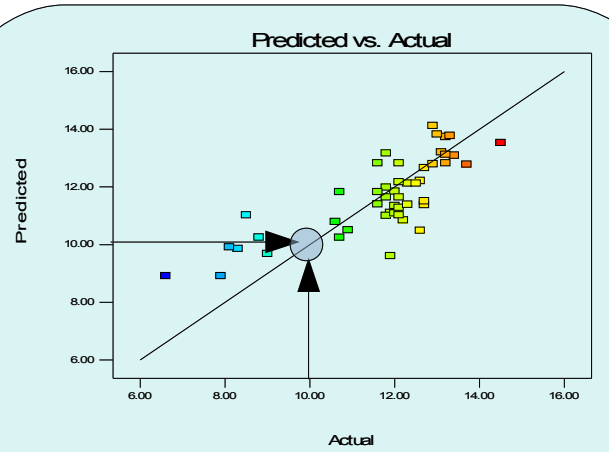
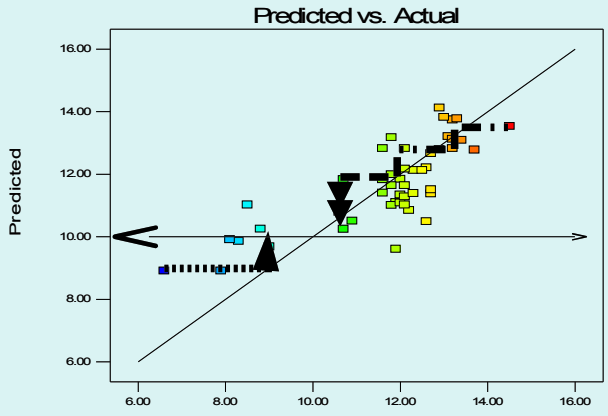
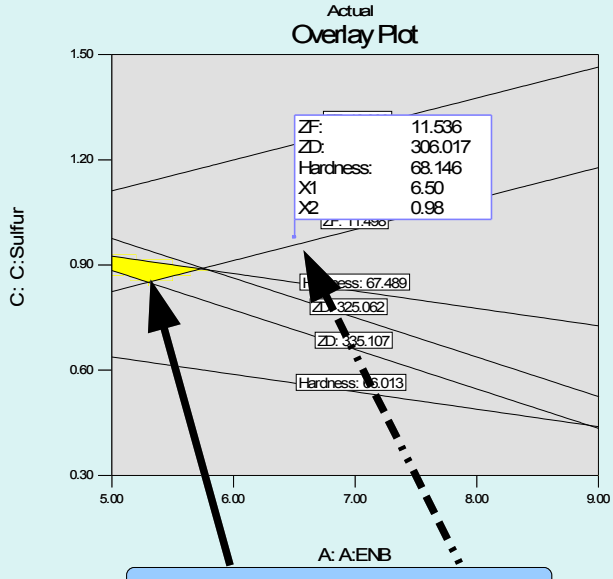
4: Novakovski, D.C., Profile of Cabot Carbon Blacks in EPDM Rubber, Technical Report RG – 135

5: Kirschbaum, Ronald J., Jones, Fred E., Profile of Cabot Carbon Blacks in Natural Rubber, Technical Report RG - 133

6: Ohm, Robert F., Vara, Rajan G., Buckley, Timothy M., Sulfur Cure System Development for EPDM Produced via Constrained Geometry Catalyst Technology, Paper presented at RDofACS1998, May 5-8







Design Expert(R) / GRAFCompounder