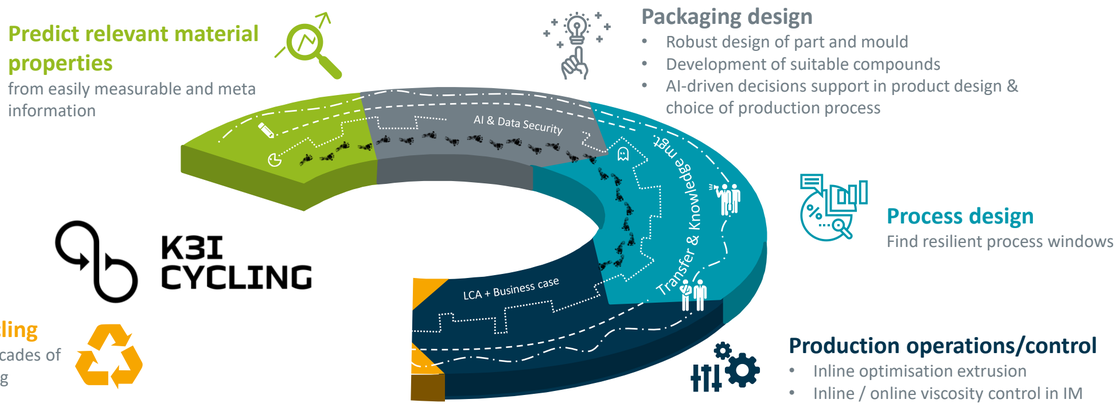
KI OPTIPACK

INSTITUTE FOR PLASTICS PROCESSING in Industry and Craft at RWTH Aachen University

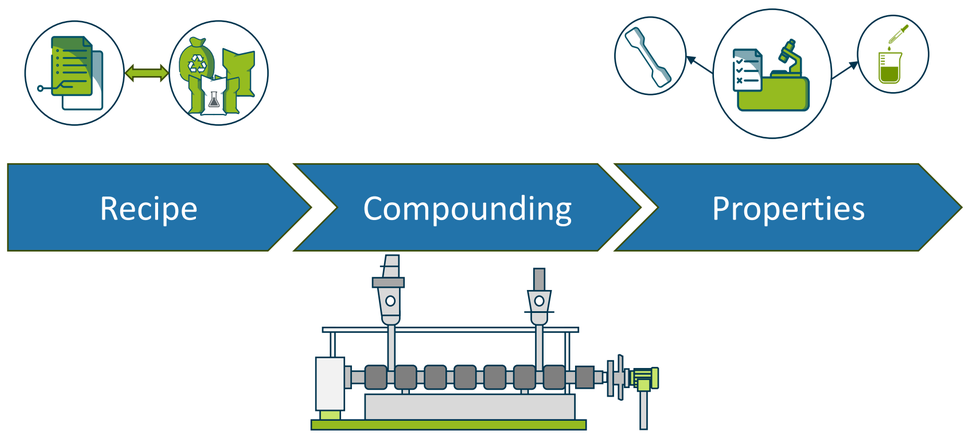
Designing sustainable plastics packaging compounds with machine learning

Goals and partner of KI OptiPack project



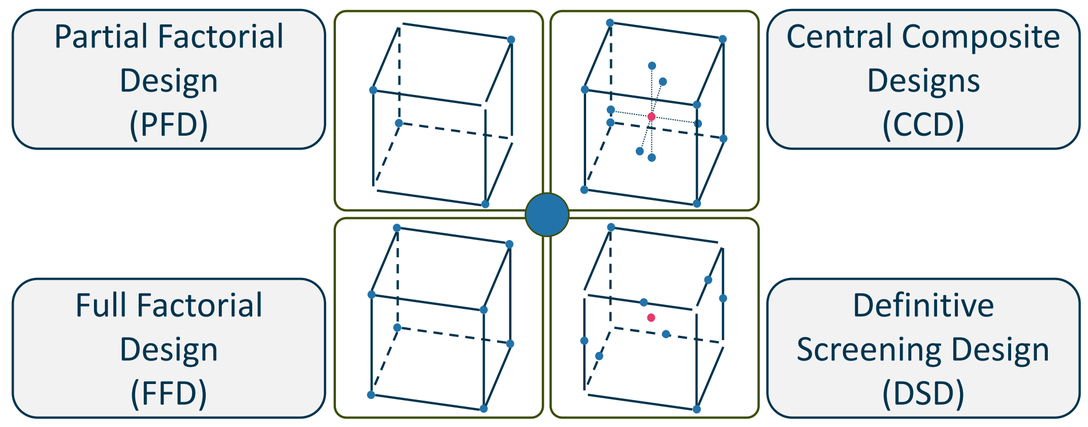
- Large number of stakeholders in design and production of plastic packaging
- Large amounts of data need to be considered, necessitating the usage of advanced methods like e.g. Artificial Intelligence
- Exemplary use case of compounds (i.e. the mix of polymers, additives and contaminants making up the packaging plastic)
- In order to develop new compounds using machine learning methods, the amount of training data required needs to be reduced and the achievable model quality of the machine learning methods needs to be increased.

Experimental trials to create a database



- Different types of polypropylene (PP) were mixed with a contractive peroxide additive at different concentrations.
- The blend was compounded at different machine settings.
- Tensile modulus and melt flow rate were determined for each compound produced.

Variation of DoE



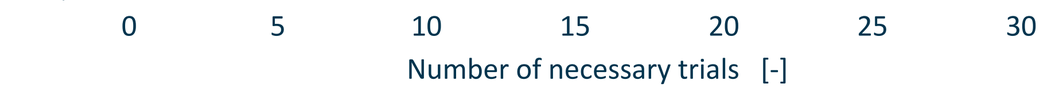
- Different types of design of experiments (DoE) were chosen.
- As process parameters, the barrel temperatures and twin screw revolutions per minute were variied.
- As recipe parameters, the polymer blend and the percentage of peroxide-containing additive were varied.

Prediction quality for the MFR

$$R^2 = \frac{\sum(\hat{y}_i - \bar{y})^2}{\sum(y_i - \bar{y})^2}$$

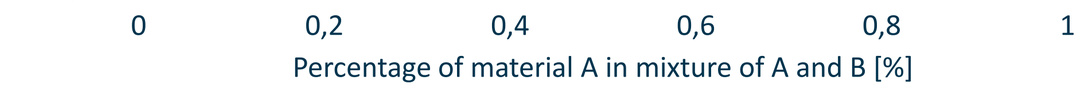
R² ~ 1 is a perfect model

R² ~ 0 is an inadequat model



- Model training with the Python framework PyTorch.
- Model scores of R^2=0.9 and above can be achieved for all DoEs used to predict melt flow rates.
- The best cost-benefit ratio can be achieved by using a definitive screening design.

Increasing the data base artificially



- Existing physical or empirical models can be used to increase the amount of training data for machine learning methods.
- By applying mixing rules such as Arrhenius or Cragoe, mixtures can be artificially interpolated between experiments.
- The model quality will increase with the same amount of data.

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FONA Research for Sustainability

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