39th Danubia-Adria Symposium on Advances in Experimental Mechanics
Sep 26-29, 2023
Siófok, Hungary
www.das2023.hu

Data Based Modelling Approaches on Impact Experiment Databases

Florian KIEHAS[1], Martin REITER[1], Juan Pablo TORRES[2], Michael JERABEK[2], Zoltan MAJOR[1]

1 Johannes Kepler University Linz – Institute of Polymer Product Engineering, Altenberger Straße 69, 4040 Linz, Austria

2 Borealis Polyolefine GmbH, St. Peter Strasse 25, 4021 Linz, Austria

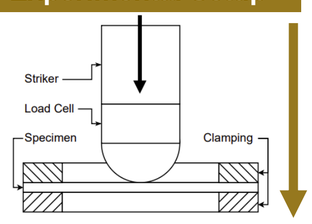
Introduction

Data based modelling approaches like machine learning have become more accessible in recent years. One major issue in material science is that mechanical characterization is very laborious, and generation of sufficient experimental data is not always feasible. Many studies circumvent this by generating artificial datasets by either numerical simulations or stochastic processes. In this study, we want to show how large amounts of experimental instrumentation signals can be used for model building. Specifically, we examine impact experiments to determine the ductile- to brittle transition temperature (DBTT) on a dataset of 7587 instrumented puncture tests according to ISO6603-2. Additionally, we show a classification task where we want to discern different fracture types according to this standard.

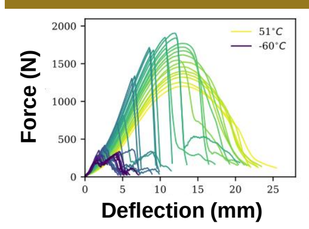
Methodology

Impact Experiments → Database → Feature Engineering → Unsupervised Machine Learning → Supervised Machine Learning

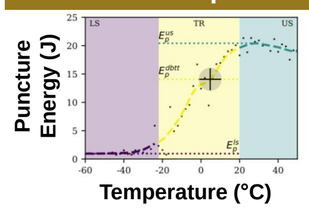
Experimental Setup



Instrumentation

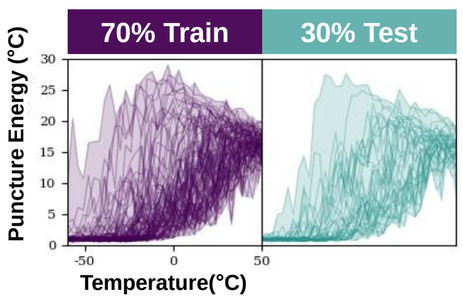


Transition Temperature



Database

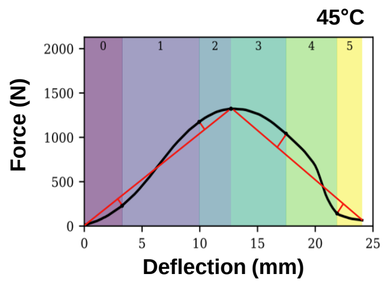
PE/PP-Compounds
181 Temperature Sweeps
7587 Puncture Tests
ISO6603-2 standard

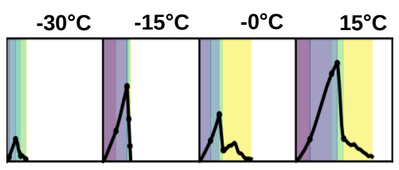


The ductile- brittle transition temperature is calculated by linear interpolation where puncture energy drops to 66% of the sweep maximum in the transition region between upper- and lower shelf.

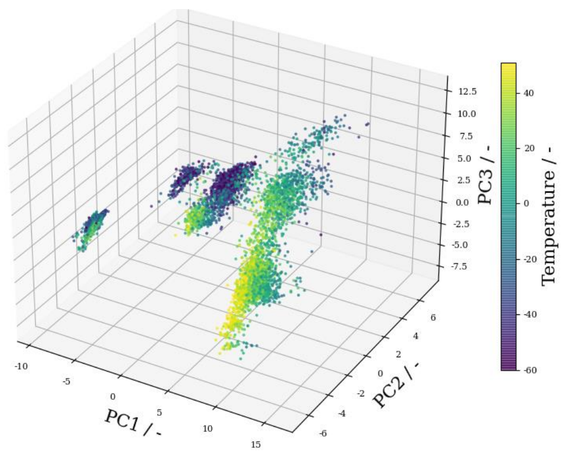
Feature Engineering

Signals are divided into regions. Statistical quantities from the distribution of deflection-, force- and energy values are extracted In each region (e.g. Mean, Std. etc).





Unsupervised Machine Learning



Extracted 97 features can be transformed by *Principal Component Analysis* to a new set of uncorrelated variables, called principal components, which are ordered according to the amount of explained variance in the original data. In this new coordinate system, clear correlation to the ductile-brittle transition and fracture types are visible.

Supervised Machine Learning

Features

↓

Principal Components

Random Forest Regressor → **Ductile-Brittle Transition Temperature (DBTT)**

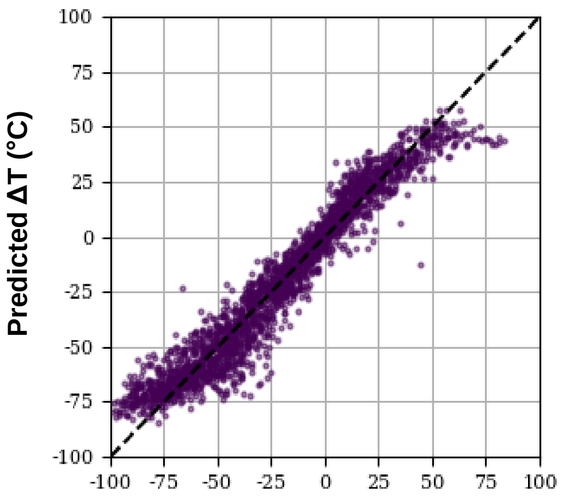
Random Forest Classifier → **ISO6603-2 Fracture Types**

Results

Evaluation of trained models on 2375 samples in the test set.

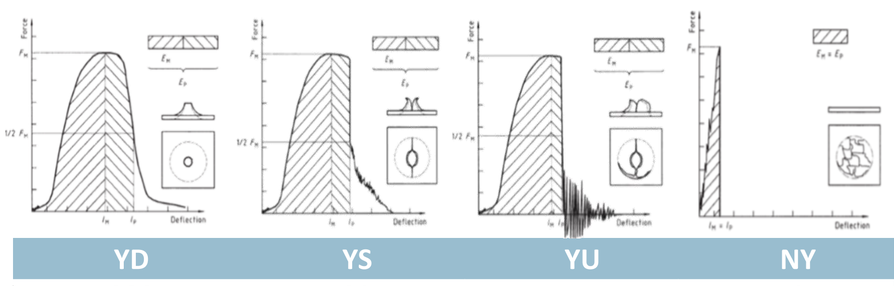
- **Regression:** a *coefficient of determination* of R2=0.935 is achieved. Predictions for very ductile or very brittle experiments shift because instrumentation signals become increasingly indistinguishable.
- **Classification:** considering unequal distribution of classes, the *accuracy* and *balanced accuracy* is 94.69% and 87.68% respectively.
- **Principal Component Analysis:** the first three principal components explain 72% of variance in the original training data.

Regression



Targets are defined as $\Delta T = T - DBTT$ where T is the measurement temperature and DBTT is the ductile-brittle transition temperature.

Classification ISO6603-2 Fracture Types



YD	YS	YU	NY	True / Predicted
289	32	4	0	YD
26	168	16	6	YS
5	3	117	9	YU
4	13	5	1677	NY

Fracture classification of force-deflection instrumentation signals according to ISO6603-2 categories: No Yielding (NY), Yielding Deep Drawing (YD), Yielding Stable Crack (YS) and Yielding Unstable Crack (YU).

Conclusion

We provided regression and classification examples to showcase how data driven modelling can tackle complex tasks on large scale experimental datasets that can not be modelled with traditional numeric or analytic approaches. Using PCA, the dataset was transformed into a coordinate system where fracture types and transition temperatures can be more easily inferred.

iPPE Institute of Polymer Product Engineering

JKU JOHANNES KEPLER UNIVERSITÄT LINZ