



Project duration: 01.06.23 - 31.05.26

## MSE - Material

**Polymers:** Rubber compounds

## MSE - Application areas

**Process optimization:** Improved characterization of mixing process.

**Material prediction:** Prediction of the product properties which are connected to the raw materials and processing parameters.

**Improved information along life cycle:** Development of an intelligent search engine.

## MSE - Product Lifecycle

**Raw materials:** Rubber, fillers (active, inactive), oils, additives

**Refining/Processing:** Mixing process / extrusion / injection moulding

**Product development:** Final product properties

## MSE - Material properties

**Mechanical:** Density, Physical parameters

**Thermodynamic:** Material temperature

**Chemical:** Mixing quality

**Rheological:** Viscosity of Compounds

**Structural:** Microstructure, Dispersion of fillers

## MSE - Approach

**Experiments:** Polymer processing, Rubber processing, Mixing, extrusion, injection moulding, characterization.

**Machine Learning/Statistical/Big data:** Search engine.

**Coupled:** Experiments and search engine.

## MSE - Material scales

**Micro-scale**

**Meso-scale**

**Continuum/Macro-scale**

## General - Types of data

**Raw data:** Machine protocols.

**Processed data:** Mathematical models of the processes, i.e., the mixing process.

**Analysed data:** Spec sheets, i.e., for materials

## General - Documentation and publishing of data

**Product life cycle management software**

**Publication in data focused journals**

## General - Proprietary/Non-proprietary

**Mostly proprietary data**

## Ontologies - Aspects of digitalization

**Procedures for ontology development:** We are contributing to the PMDco semantic modelling patterns that will be used for ABox and TBox modelling across all PMD projects. We also refine and extend the DIGIT RUBBER ontology and merge it with the new PMDco 3.0.

## Ontologies - Levels of structured data handled

**Ontologically described data (RDF data):** In a use case we attempt to demonstrate that data existing in a relational database can be described in RDF/OWL using the patterns we develop.

## Ontologies - Existing ontologies used

**MSE ontologies:** PMDco

**Complimentary ontologies:** IAO, OBI

**Ontologies for units:** QUDT

**Domain-specific ontologies:** DIGIT RUBBER ontology

## Ontologies - Tools for ontologies

**Editors and Collaborative tools:** TIB instance of WebProtégé

**Validation tools:** LinkML, ROBOT, ODK

**Templates:** YAML, SHACL

**Terminology services:** TIB Terminology Service

**Formats and Languages:** OWL, SHACL, YAML

**ML/LLMs:** Material-AI (MAT-AI)

## Workflows - Types of workflows

**Data acquisition from experiments:** Material parameters (Mw, MWD, Microstructure, Branching, Functionalization), Influences (Rotor speed, Machine temperature, Density, Physical parameters).

**Post-processing/analysis of raw data:** Models (Material temperature, Mixing quality) -> output variables (Compound, Process, Further processing).

**Machine-learning**

## Workflows - Workflow priorities

**Automation of workflows:** Automatic transfer of data from processing machines to the InSuKa database; ideally also from testing machines.

**Better documentation:** Documentation of data for different materials and respective processing chain in one tool.

**Better reproducibility:** Unified documentation of parameters, machine data and test results ensures better reproducibility.

## Workflows - Workflow challenges

**Data formats:** Heterogeneous data formats.

**User interfaces:** Managing heterogeneous user requirements for GUI implementation.

## Workflows - Publishing of workflow-related elements

**Software packages:** InSuKa LLM-Search

## Workflows - Use of PMD workflow store

**Publish own workflows/modules**

## Workflows - Tools for workflows

**Tools for ontologies/RDF data**

## IT & Security - Computational demands

**Usage of cloud resources:** AWS

## IT & Security - Data-federation

**With project partners:**

## IT & Security - Software user interface

**Desktop app:** Based on MAT-AI Software.

## IT & Security - Data encryption

**Encryption:** TLS

## IT & Security - Tools for IT-architecture and security

**Containerization tools:** Docker

**AAI (auth & access infra) tools:** Gitlab

## Use of PMD-Tools



**Workflowstore**



**PMDco**