

KEEN - KünstlichE IntElligenz INkubator Labore in der Prozessindustrie

(AI Incubator Labs in the Process Industry)

Gesamtprojekttreffen #6

TP6 Smart Engineering

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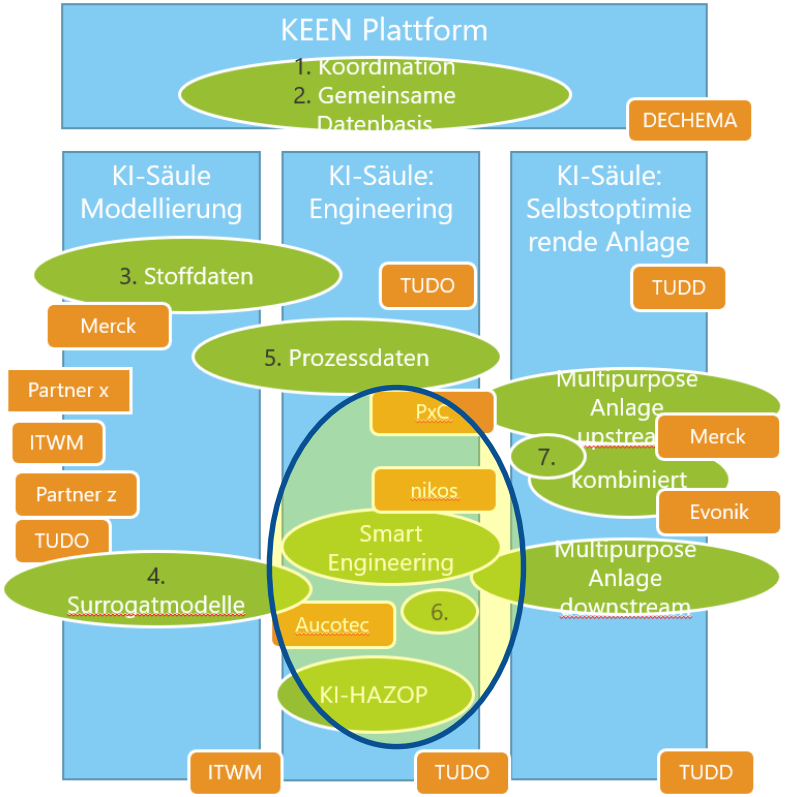
Federal Ministry for Economic Affairs and Energy

on the basis of a decision by the German Bundestag

KE-EN

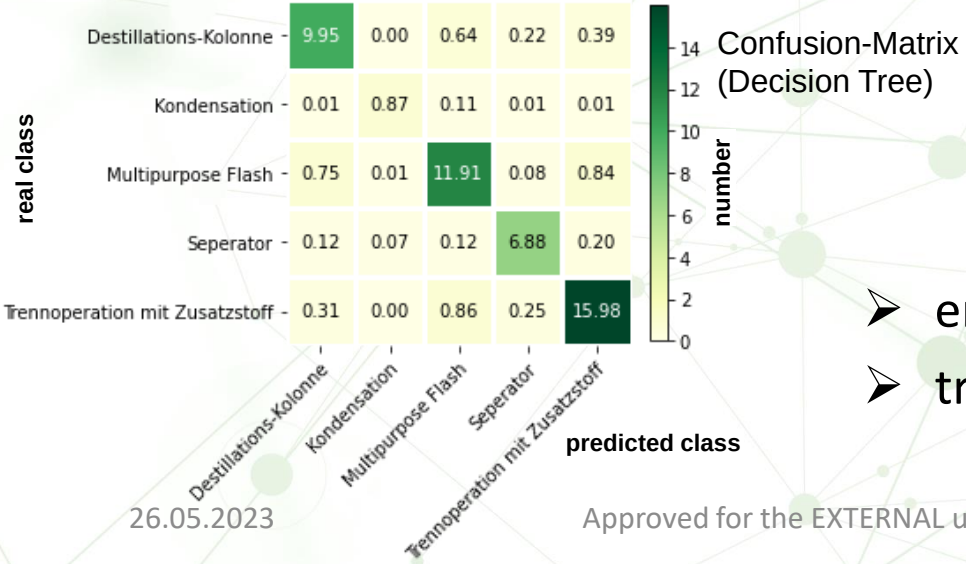
TP6 Smart Engineering - Start

- AP6.1 – Smart Process Design and Simulation
- AP6.2 – eHAZOP methodology
- AP6.3 – eCockpit & Innovation management, together with TP1.1

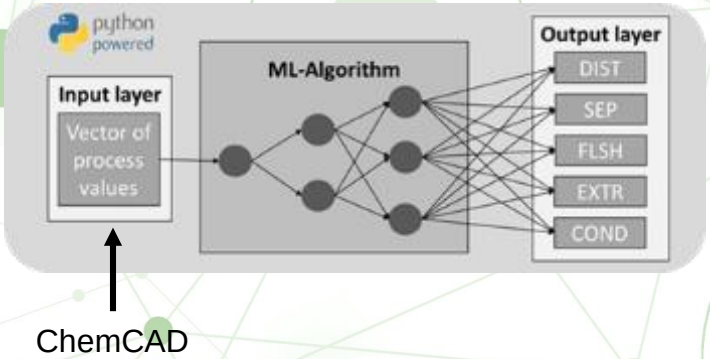


Process Simulation

- definition of process modules
- interface to ChemCAD and example processes
- good prediction on low data amount



Confusion-Matrix (Decision Tree)



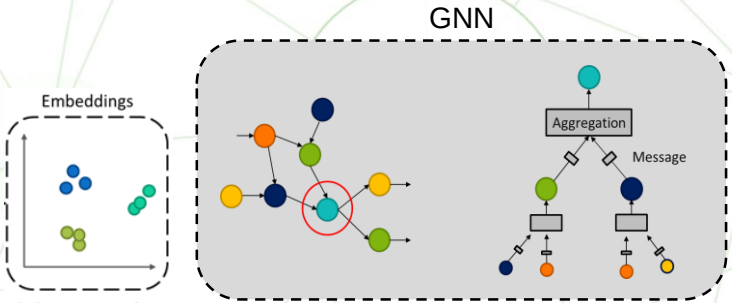
ChemCAD

- enlarged to 3 and 4 component mixtures
- transferred to process flow diagrams

Pipe & Instrumentation Diagrams

- **GNN**s (Graph neural networks) for DEXPI
- **Node classification** via GNN
  - Three-Layer-GraphSAGE[1]
- **Edge classification** via GNN
  - only few P&IDs at the beginning (13) with 377 nodes (DEXPI export)

➢ more P&IDs from partners and from own lab



True node class

Predicted node class	Category	Valves	Pumps	Vessels	Heat exchanger	Separation units	PCE – equipment	Piping equipment	Flanges	T-pieces
	Valves	**120**	1	1	5	0	5	2	0	6
	Pumps	1	**17**	0	0	0	0	0	0	2
	Vessels	2	0	**18**	0	0	0	0	0	1
	Heat exchanger	7	1	0	**18**	0	0	0	0	1
	Separation units	0	0	0	0	**5**	0	0	0	0
	PCE - equipment	10	0	0	1	0	**32**	0	1	1
	Piping equipment	8	0	0	0	0	0	**28**	0	3
	Flanges	2	0	0	0	0	0	0	**3**	2
	T-pieces	8	2	0	2	0	1	0	1	**59**

[1] N. Kipf, M. Welling (2017): „Semi-Supervised Classification with Graph Convolutional Networks“, conference paper at ICLR 2017

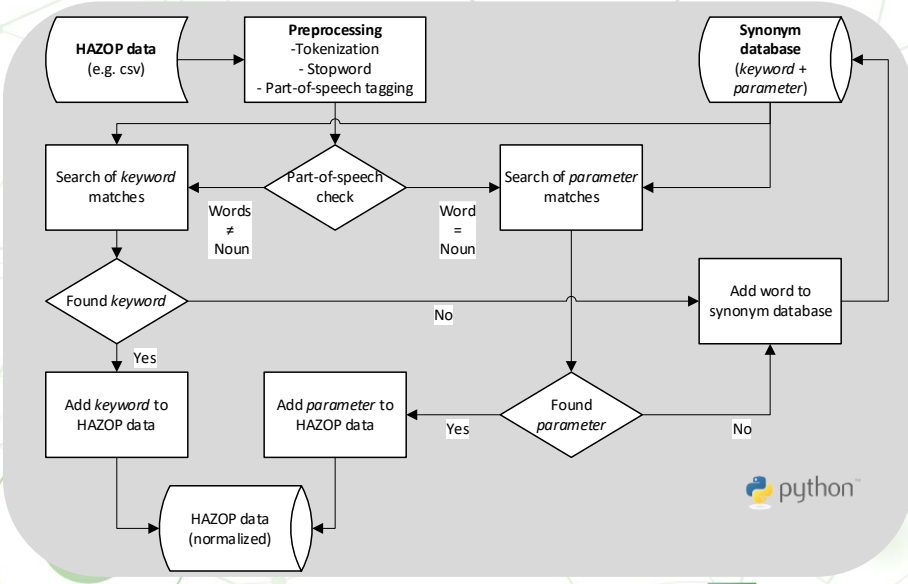
eHAZOP with industrial data

- first approach: HAZOP text analysis with NLP
  - phrase recognition and statistical analysis

- data scarcely machine-readable
  →no conclusions about topology possible
- information gain possible, but
  no application of the learned knowledge...

→Cost/benefit too high!

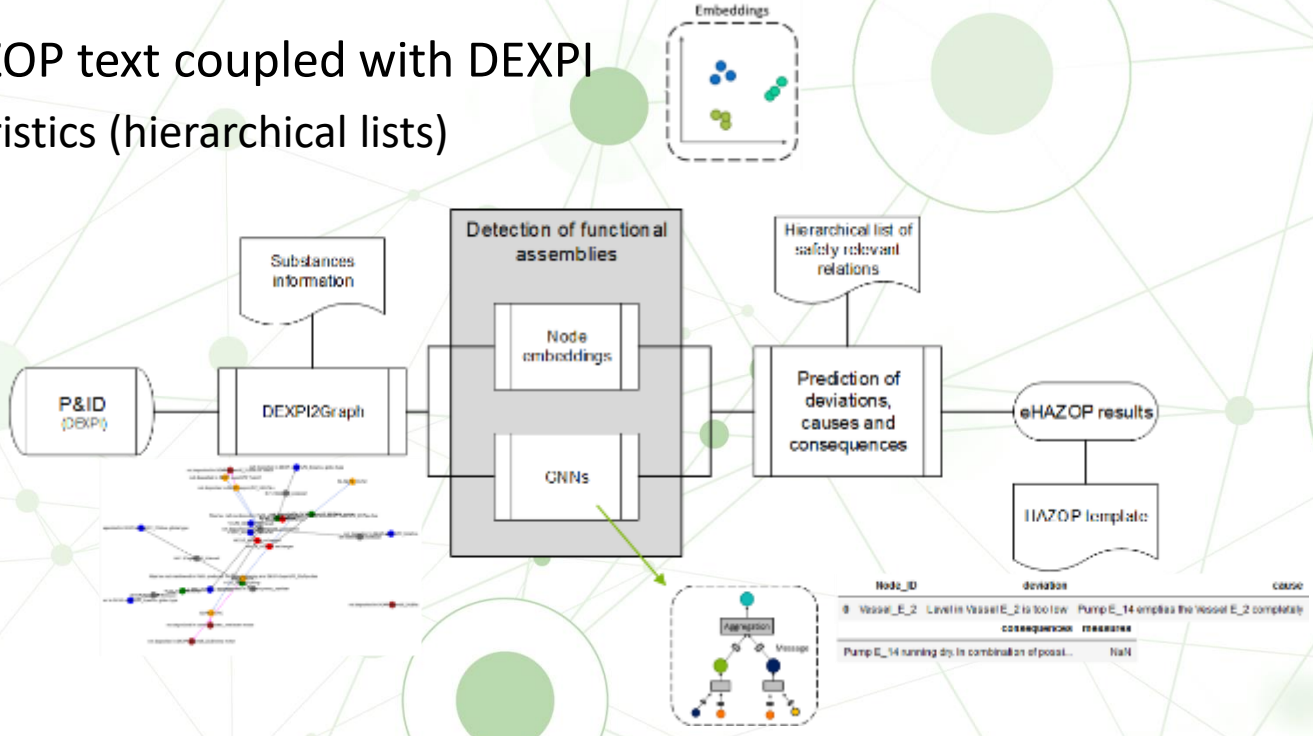
Normalization workflow



eHAZOP & DEXPI

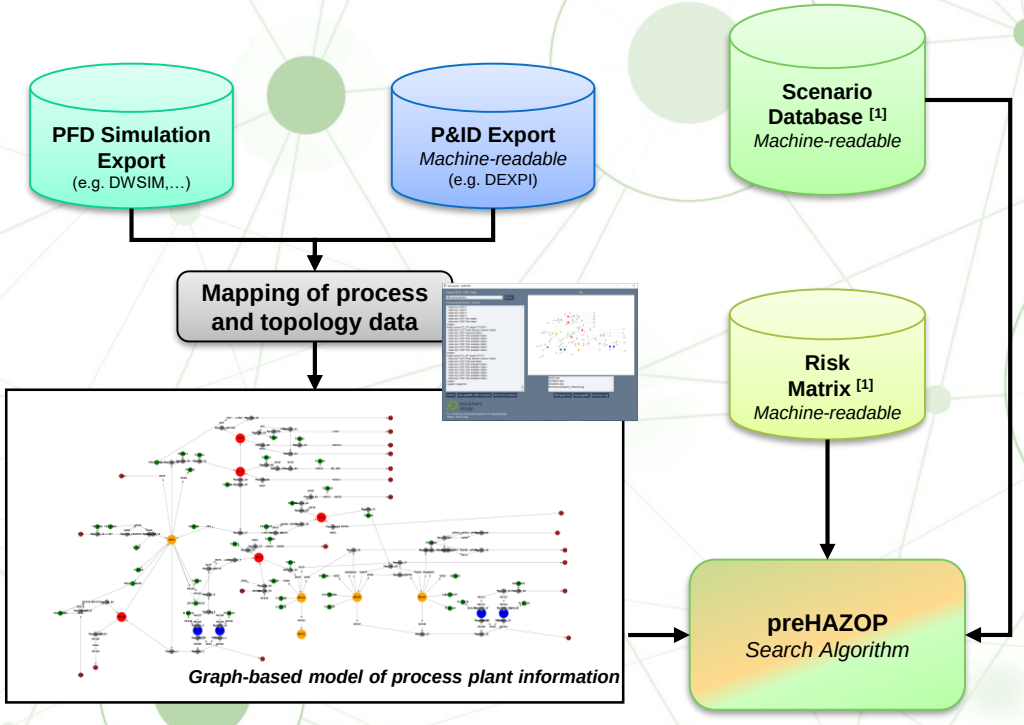
- next approach: HAZOP text coupled with DEXPI
  - application of heuristics (hierarchical lists) to DEXPI P&IDs (machine-readable asset topology)

→direct derivation of safety functions from the P&ID



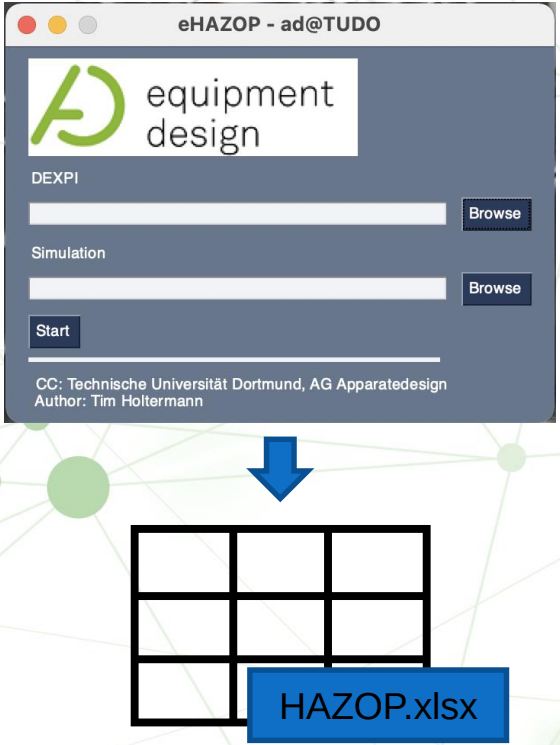
modular preHAZOP <-> DEXPI

- workflow:
  - mapping a scenario to locations in the P&ID by iterating through a graph-based plant and process data
  - risk assessment by comparison of data in the graph and the scenario database via a risk matrix
- advantages:
  - first safety assessment in an early development stage (while drawing a P&ID)
  - fast safety assessment in multipurpose plants (change simulation)



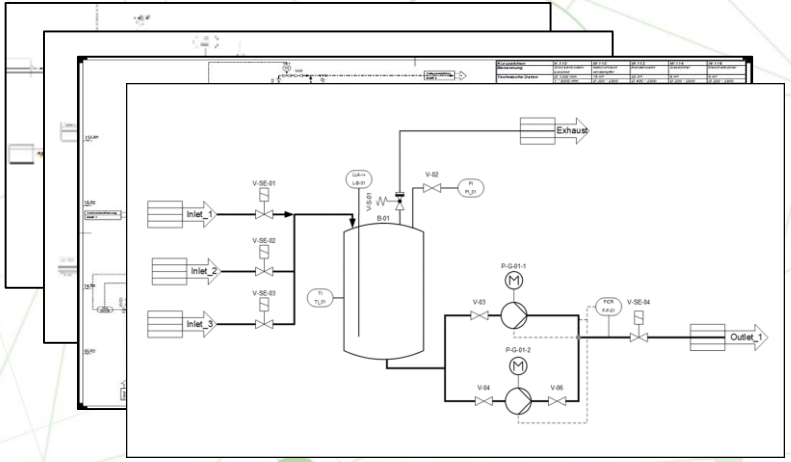
results preHAZOP

- application by user interface:
  - DEXPI – P&ID import
  - DWSIM - simulation import
- example P&ID from textbooks (destillation plant, water/ethanol)
- safety relevant scenarios → Excel file
  - systematic detection of scenarios
  - risk assessment based on the simulation process data via a risk matrix provides good results for initial evaluation
  - automatic detection of pressure spaces



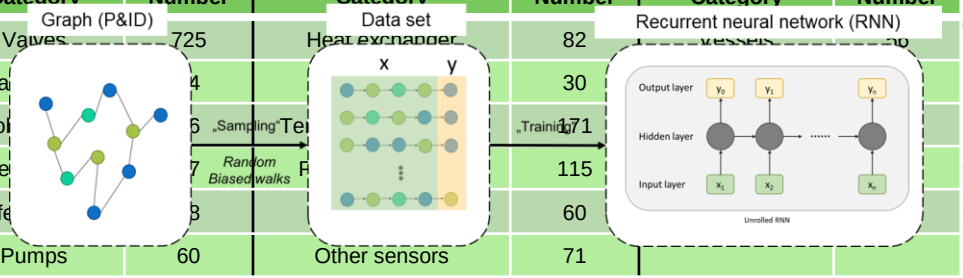
P&ID engineering with DEXPI

- 25 P&IDs (DEXPI) from textbook and lab
- Directed graphs (GraphML)
  - 2504 nodes
  - 2842 edges (directed)
- Categories
  - 16 categories with unbalanced distribution



Category	Number	Category	Number	Category	Number
Valves	725	Heat exchanger	82	Vessels	50
Ba	4		30		
Glob	6	„Sampling" Te	„Training" 171		
Che	7	Random Biased walks P	115		
Safe	8		60		
Pumps	60	Other sensors	71		

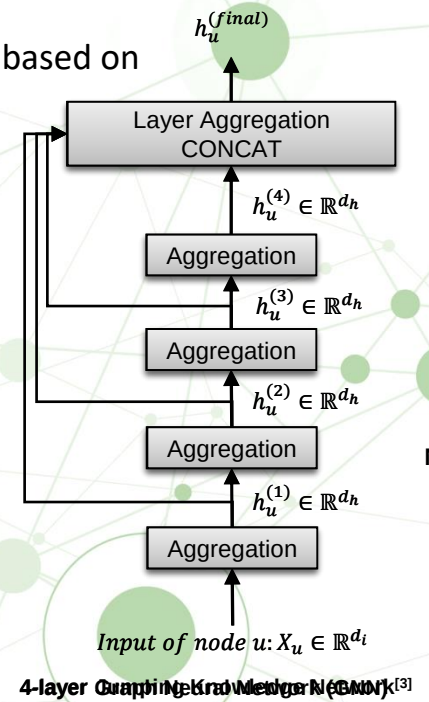
- Modelling –
  Recurrent Neural Networks (RNN)
  - Prediction of following equipment using the trained RNN



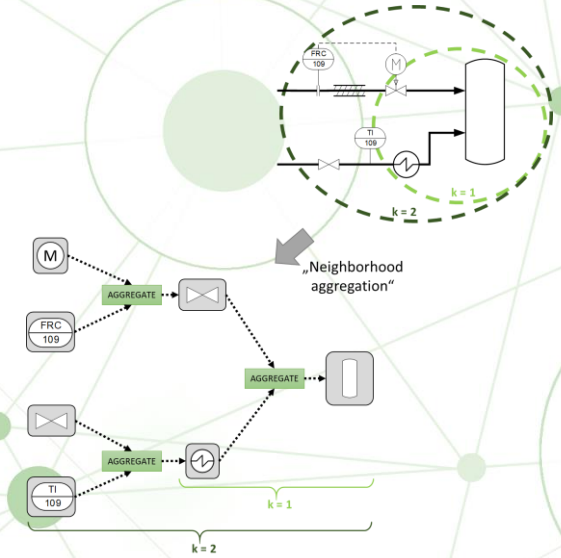
P&ID engineering & modeling

- modeling with GNN
  - k-layer GNN‘s generate embeddings h_u of node u based on their neighborhood structure[1]
  - nodes features of one layer used for calculation of features of next layer

- modeling with JKG
  - save features of all layers and use it again at the end
  - concatenation of all hidden feature vectors as input of last layer
  - nodes only receive information from neighbours



4-layer Graph Neural Network (GNN)[3]

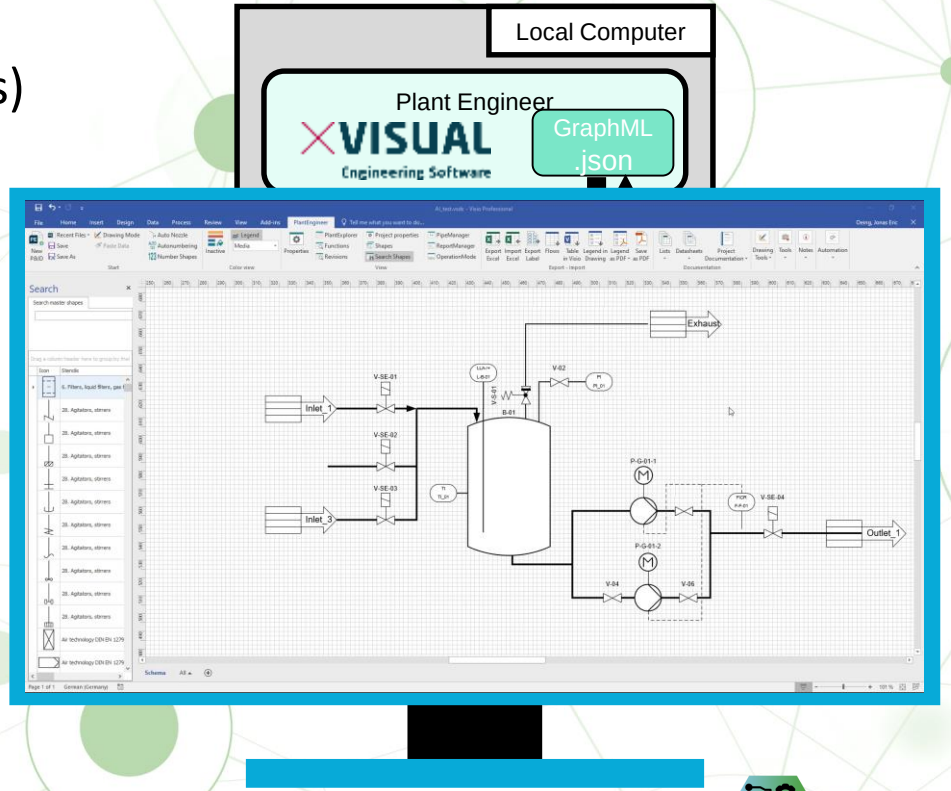


Neighborhood aggregation of a P&ID - GNN[2]

[1] Leskovec, J., Inductive Representation Learning on Large Graphs, 2017
[2] Oeing, J. et al., Dig. Chem. Eng., 2022
[3] K. Xu et al., 2018

Implementation of smart engineering

- Plant Engineer (X-Visual Technologies)
  - Data Exchange via exchange directory
  - Data Exchange using GraphML / .json
- Docker Container (TU Dortmund AD)
  - Python 3.9
  - GNN (pytorch) – consistency checks
    → Output: Inconsistent nodes/edge
  - RNN (tensorflow) – auto-completion
    → Output: Prediction of suitable equipment
- Graphical User Interface

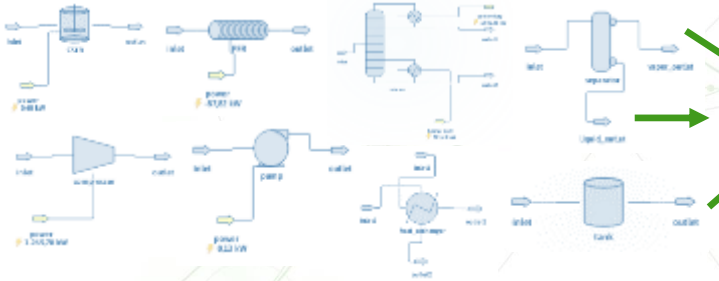


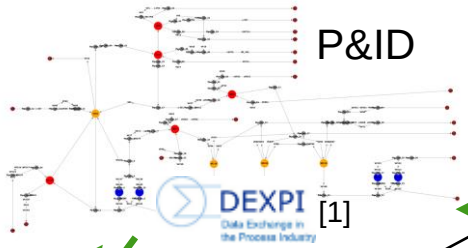
[1] Oeing, J. et al., CIT, 2023

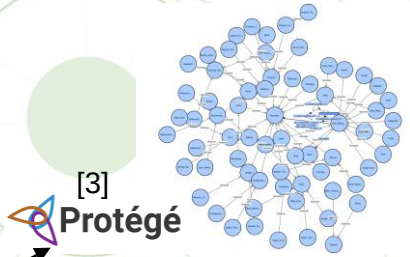
Outlook: Process Simulation <-> PFD <-> P&ID

- first results and link to NFDI4Cat
  - process ontology with data -> knowledge grap
- DWSIM[2] and Protégé [3]

➢ data landscape for process engineering







[3] Protégé

Knowledge graph(s)

Metadata structure(s)

FAIR Data

python

PFD

DWSIM Chemical Process Simulator [2]

Outlet conditions:
pressure, temperature,
concentration(s),
mass stream(s) …

Inlet conditions:
pressure, temperature,
concentration(s),
mass stream(s) …

[1] https://dexpi.org
[2] https://dwsim.org
[3] https://protege.stanford.edu

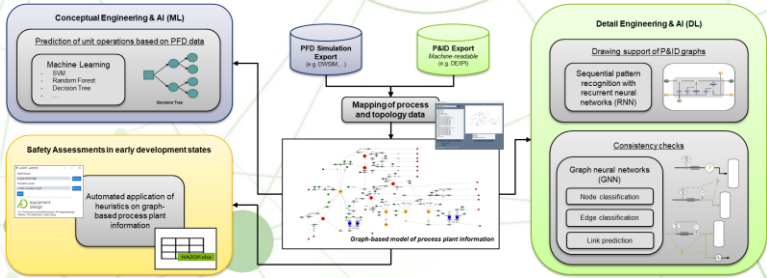
KEEN-Smart Engineering in Industry

- X-Visual: helpful in the engineering process
  - ➢ further (research&customer) projects are planned
  - ➢ combination with automation
  - ➢ high interest from industrial partners

- CGC: coupling to DWSIM, …

- Bayer: contact to INVITE research group

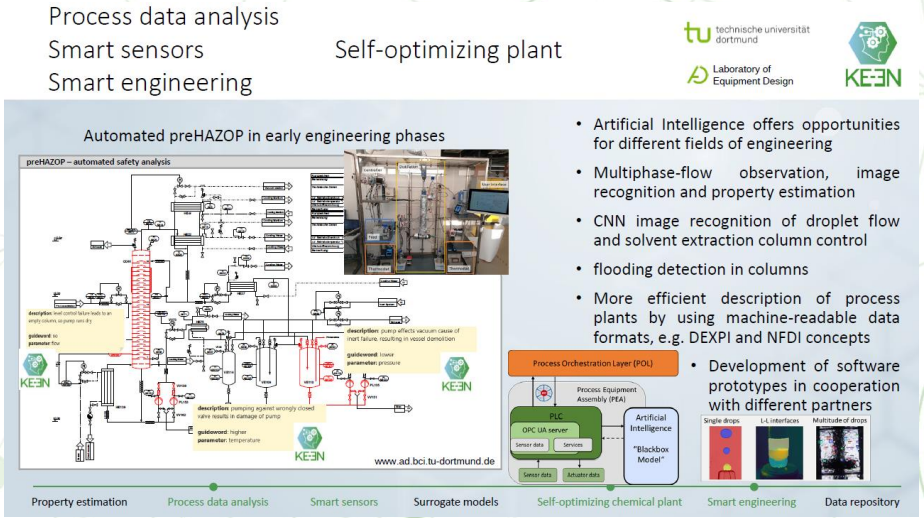
- others in the incubator lab TUDO-AD



TUDO Incubator lab

- Research projects
- Teaching and student theses
- Competence center for digital production technologies @ TU Dortmund concept GmbH

  https://tu-concept.com/



tu | concept.

cet Centrum für Entrepreneurship & Transfer.

tu | capital.

Acknowledgements

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Capital Gain Consultants

EVONIK Leading Beyond Chemistry

BAYER

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