

## Master Thesis Project

### Knowledge Graphs to Model Chemical Engineering Knowledge and Data

Together with Bilfinger Digital Next GmbH

Engineering knowledge is still largely restricted to textbooks and some databases. With the rise of the semantic web knowledge graphs have become popular to encode knowledge in many other fields. This is of great interest in chemical engineering, where knowledge and data exist in many different types and forms and are at the moment largely unavailable for automatic processing.

Within this master thesis project, several questions should be explored:

- How can we encode and link both engineering knowledge and numerical data in the form of knowledge graphs?
- Is a suitable data model already available for heterogenous engineering data or can we extend existing ones?
- What is a suitable format to store the obtained knowledge graphs?
- Which techniques can be used to mine hence encoded knowledge and linked data?
- Can we combine OntoCAPE with modern knowledge graph approaches?
- Can the attribution described in the DEXPI standard be used as, e.g., reference namespace?

Within a small case study a binary flash and its auxiliary equipment is to be modeled using a knowledge graph. This shall include: attributes of equipment, data on fluids, phases, and compound properties, physical location and 3D geometrical information on equipment and piping. A direct connection to a physico-chemical model should be drawn by including model equations from MOSAICmodeling (XML/MathML). Also, the connection to real-life measurement data should be envisioned.

A first software prototype is to be implemented in python and used to (1) construct the knowledge graph and (2) perform queries to obtain data. If possible, the Wikipedia API should be used to gather additional, publicly available information on compounds etc.

#### Resources for introductory reading:

<https://towardsdatascience.com/knowledge-graphs-at-a-glance-c9119130a9f0>  
<https://www.ontotext.com/knowledgehub/fundamentals/what-is-a-knowledge-graph/>  
<https://towardsdatascience.com/auto-generated-knowledge-graphs-92ca99a81121>  
<https://www.avt.rwth-aachen.de/cms/AVT/Wirtschaft/SoftwareSimulation/~jpts/OntoCape/?lidx=1>

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