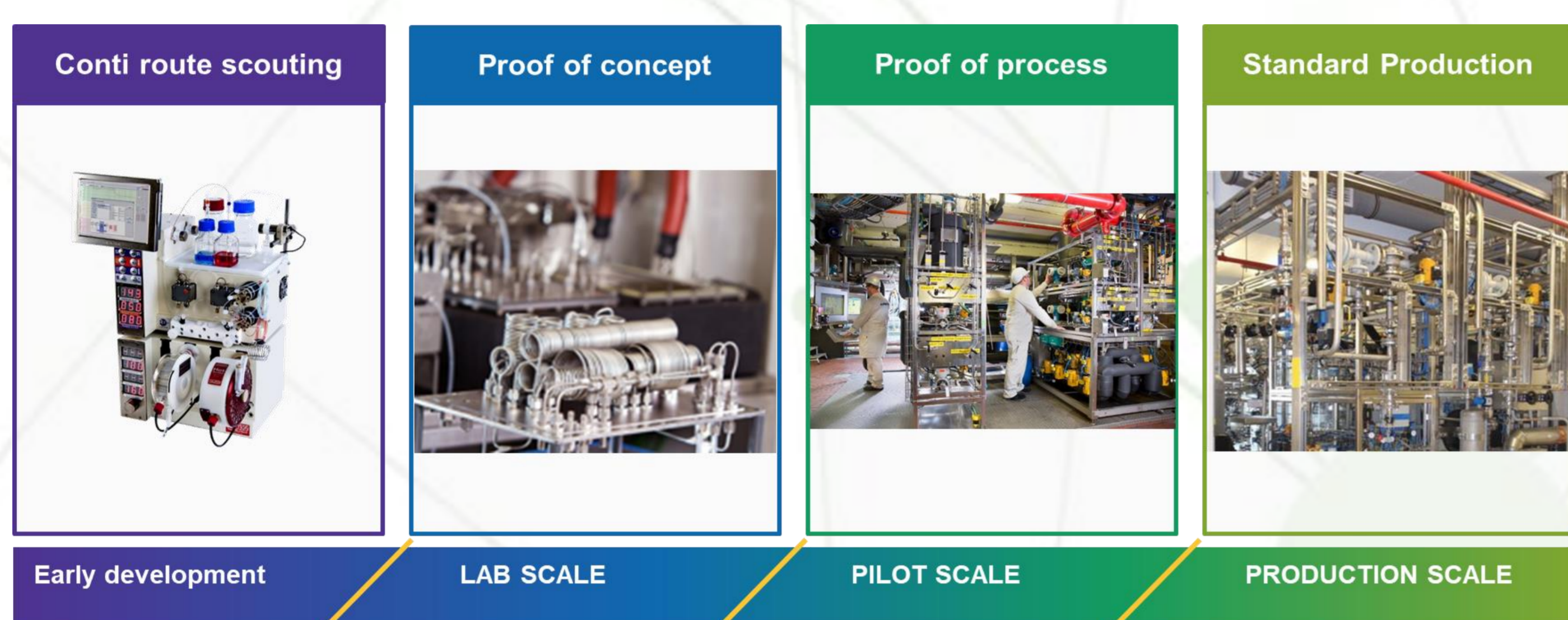


Operating window exploration of continuous reaction plant

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Continuous reaction plant

- Work package 5.3 – Focus on production scale

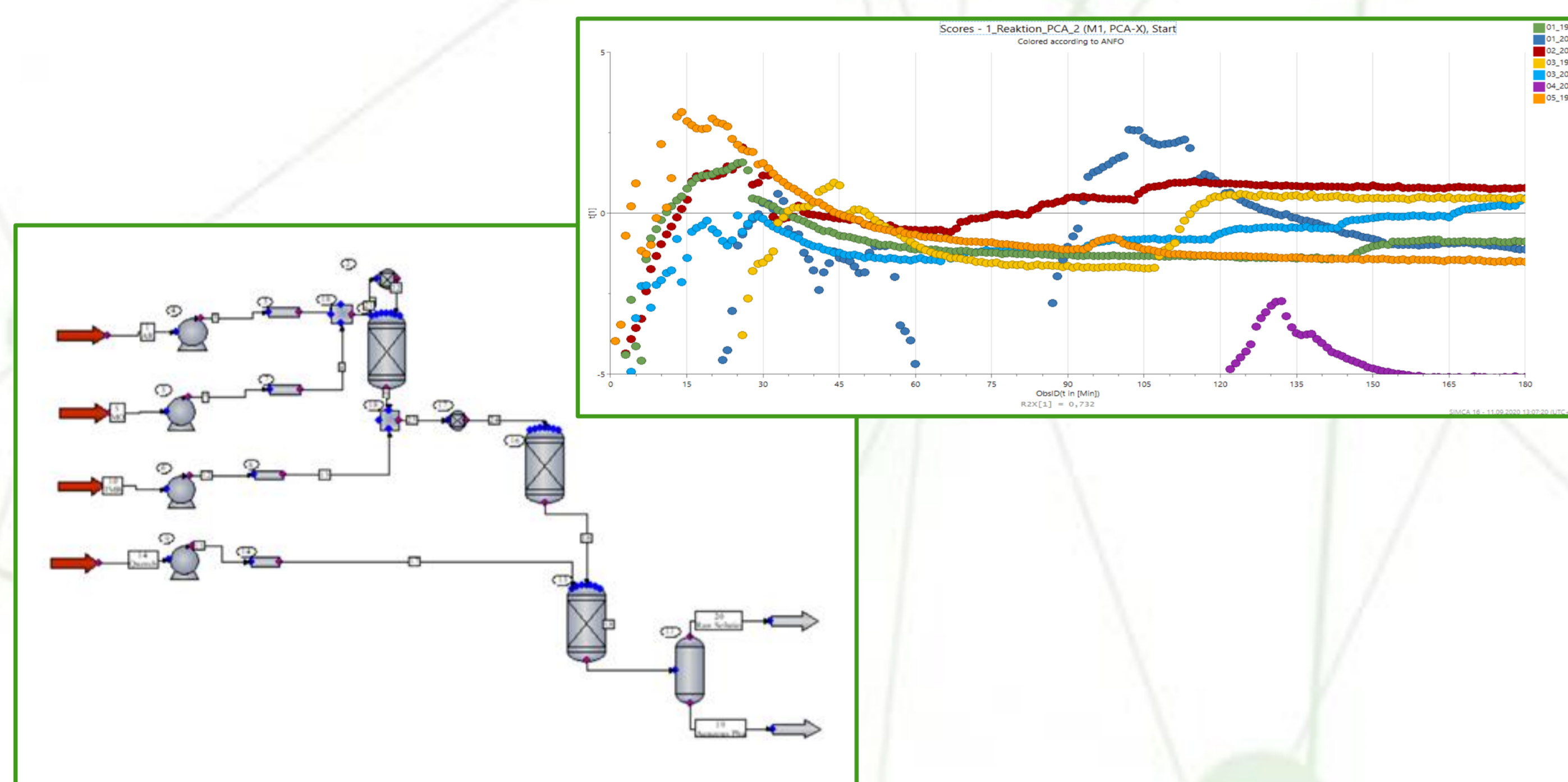


Use case description

- Title: Continuous reaction plant MERCK
- Goal: Increase of process efficiency and stability by finding a suitable operating window
- Description:
 - Plug flow reactor (continuous, steady state process) with two reaction steps in a tube reactor and hydrolysis step
 - Multipurpose plant in production scale
 - During a production run detrimental shut-downs occur due to exceeding of critical values (e.g. pressure)

Proprietary Tools

- CHEMCAD and SIMCA

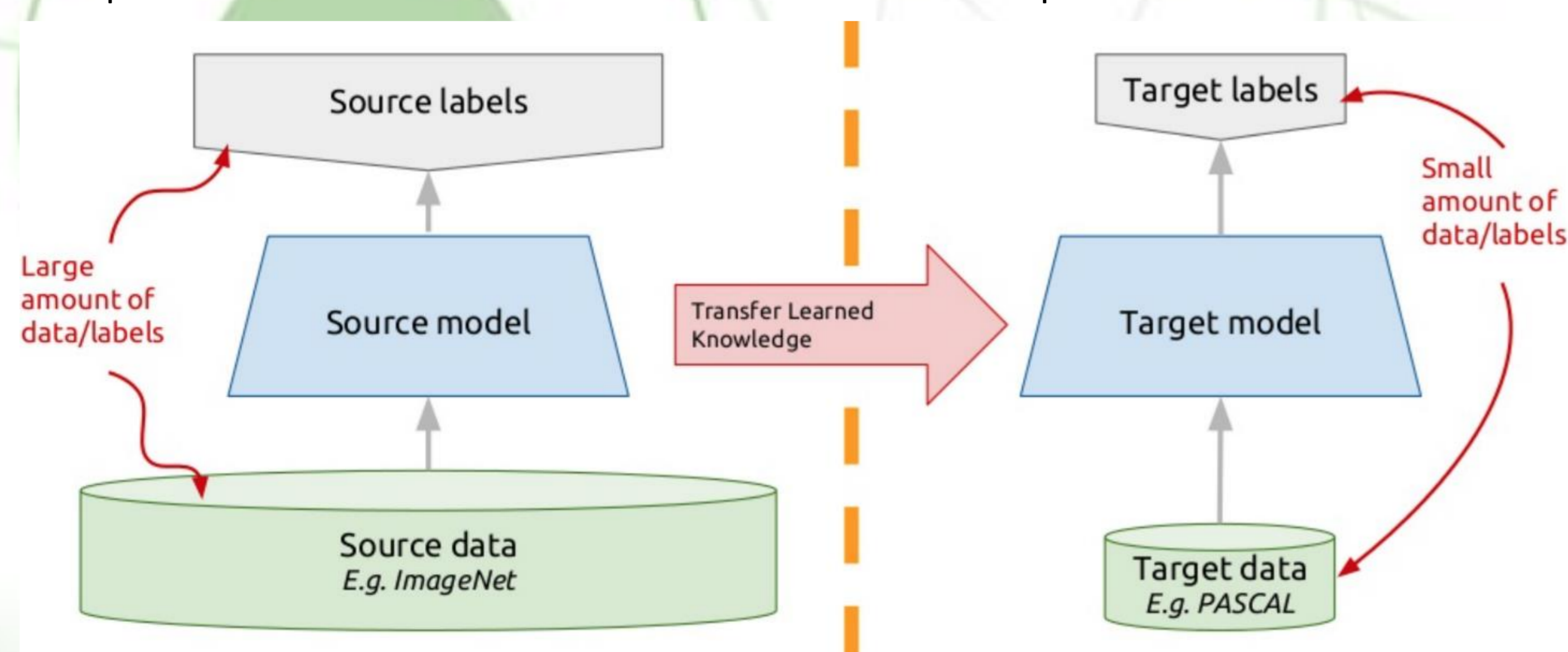


Data characteristics and methods

- Data characteristics:
 - Design data (P&IDs)
 - Process data (temperature, pressure, flow rate,...)
 - Product data (concentration and yield)
- Methods:
 - Multivariate data analysis, Multivariate sensitivity analysis
 - SIMCA: Multivariate data analysis
 - Process modelling with the depth required
 - CHEMCAD: Process modelling and simulation

Transfer learning ^[1]

- Motivation: usage of existing knowledge gained from simulation models from engineering phase or data gathered from lower scaled plants in order to reduce amount of data required for model



Approach

- Based on historical process data, the operating range will be investigated to increase process efficiency and stability.
- A multivariate data analysis will be conducted to identify the influence of coupled parameters and to understand correlations between different parameters.
- A comprehensive process simulation will be set up to take process phenomena like pressure drop, hot spots, residence time, heat transfer, etc. into account.
- Based on this prework, a sensitivity analysis will be conducted.
- Combining these insights will facilitate to reduce the amount of false alarms, to warn earlier and more focused and to integrate maintenance steps in a more efficient in the operation procedure.

[1] Kevin McGuinness - Transfer Learning (D2L4 Insight@DCU Machine Learning Workshop 2017)

Contact