Master's Project: Online Kinetic Model Building for Continuous Chemical Reactions, toward Model-Based Control

In a collaboration with the Institute of Chemistry at the University of Graz, TU Graz are looking for a master's student to work as part of an interdisciplinary team, investigating new approaches to rapidly construct controllers for lab-scale continuous chemical processes.

Background:

Due to the high complexity of pharmaceutical molecules, the processes to manufacturing them are unique in each case and can often require numerous (>10) different reaction steps. Bespoke models to describe each individual reaction step are generally not known and need to be constructed. The pharmaceutical industry is also currently undergoing a paradigm shift from traditional batch manufacturing to continuously-operated processes. Continuous processes can offer many supply chain, economic and environmental advantages, but are often more complex to develop.

To build model-based control strategies for novel chemical processes, kinetic models are a valuable tool. These models link the reaction conditions (e.g. reactor temperature, feed flow rates, pressure) to the reaction output (e.g. reaction yield, impurities), in a time-resolved manner. Although defined equations describing standard chemical kinetics exist, most notably the Arrhenius equation, parameterizing these equations for each new reaction is a laborious task using standard workflows and is often not performed, even in the case of pharmaceutical manufacturing processes.

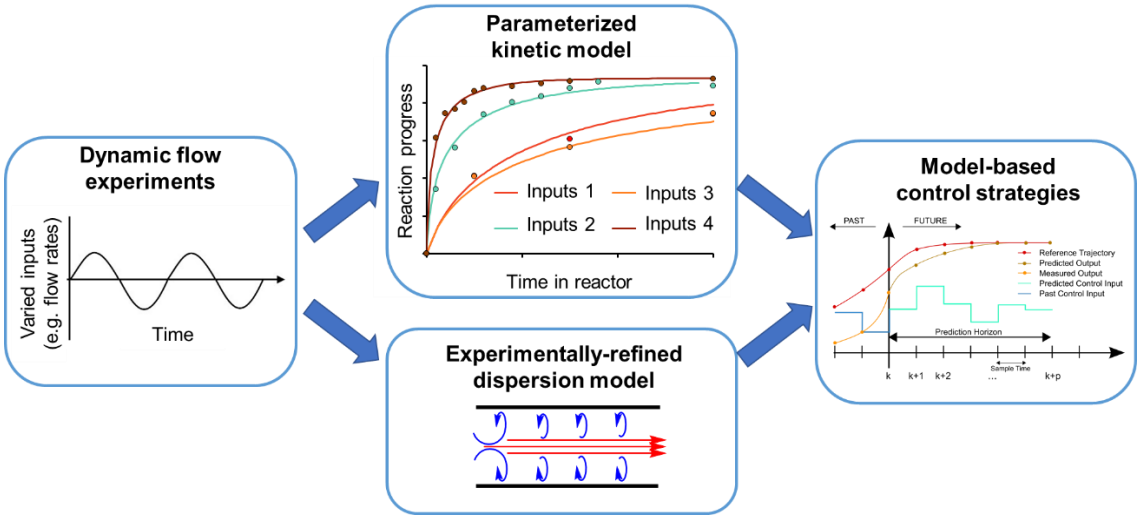

Figure 1. *The proposed approach, using dynamic flow experiments to parameterize models for control strategies.*

Project aims:

- Develop and demonstrate a workflow which uses non-steady state (dynamic) data from flow reactors to build a kinetic model, reactor dispersion model
- Apply the developed models in control strategies for the chemical synthesis reactor