UniSysCat - Colloquium

Prof. Lorenz T. Biegler

Carnegie Mellon University, Pittsburgh

Start Time: Wednesday, July 13, 2022 05:00 pm

End Time: Wednesday, July 13, 2022 06:00 pm

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or via Zoom

An Optimization-based Approach for Kinetic Parameter Estimation from Spectral Data

Prof. Lorenz T. Biegler

Carnegie Mellon University, Pittsburgh

Determination of accurate reaction kinetics is imperative in many industries to ensure safe, controllable, and scalable processes. In research-based chemical industries, particularly the pharmaceutical industry during the early development phase, little is known about the reaction being studied in advance and it is difficult to determine the chemical species present, reaction mechanisms, and kinetic parameters involved from obtained experimental datasets. Since many of the experiments are costly to run, it is important to develop tools that are able to maximize the information obtained from each experiment. Typical data types that are collected during experiments include spectroscopic data (infrared, near-infrared, ultraviolet- visible, Raman etc.), as well as high-performance liquid chromatography, ultra-performance liquid chromatography and calorimetric data. The determination of kinetic parameters and discriminating among kinetic models is enabled by a unified optimization framework based on maximum likelihood principles and large-scale nonlinear programming strategies, which solve estimation problems that involve systems of nonlinear differential algebraic equations (DAEs). The resulting solution strategy includes tools for data preprocessing, estimability analysis, and determination of parameter confidence levels for a variety of problem types. Several case studies will be presented to demonstrate the effectiveness of this approach.

Prof. Dr. Jens-Uwe Repke

Organizer