# PSTC 2016 Publications – Michael Baldea

1. Pattison, R.C., C. Tsay, and M. Baldea, "Pseudo-Transient Models for Multiscale, Multiresolution Simulation and Optimization of Intensified Reaction/Separation/Recycle Processes," *Computers & Chemical Engineering, submitted.*

   A unified multiscale framework was presented for including "non-standard" unit operations, such as intensified equipment or unconventional reactor designs, in equation-oriented process flowsheet modeling, simulation, and optimization. The approach allows detailed, distributed-parameter representations of reacting systems and rigorous models of (intensified) separation units to be embedded in and optimized simultaneously with process flowsheet models. A dimethyl ether production process case study showed that the optimal process design is highly dependent on the level of detailed included in the flowsheet model.

2. Pattison, R.C., Touretzky, C.R., Harjunkoski, I., and Baldea, M., "Moving horizon scheduling of process operations under dynamic constraints," *AIChE Journal*, 49(7), 681-686 (2016).

   To maximize operating profit under highly variable economic conditions in modern markets, changes in production rate and product grade must be scheduled with increased frequency. To do so, process dynamics must be considered in production scheduling calculations, and schedules should be recomputed when updated economic information becomes available. In this article, this need is addressed by introducing a novel moving horizon closed-loop scheduling approach. Process dynamics are represented explicitly in the scheduling calculation via low-order models of the closed-loop dynamics of scheduling-relevant variables, and a feedback connection is built based on these variables using an observer structure to update model states. The theoretical developments are demonstrated on the model of an industrial-scale air separation unit.

3. Tsay, C., R.C. Pattison, and M. Baldea, "Equation-Oriented Simulation and Optimization of Process Flowsheets Containing Detailed Multistream Heat Exchanger Models," *AIChE Journal, submitted*.

   An equation-oriented model for multistream heat exchangers (MHEXs) using industry-accepted heat transfer and pressure drop correlations for single- and multi-phase streams was developed. A framework was presented that allows simultaneous optimization of the MHEX design and the process flowsheet, and the approach was demonstrated on the PRICO® natural gas liquefaction process as a case study.