Texas Tech University
Department of Chemical Engineering
Seminar Series

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Advancing chemical process development using theoretical modeling and machine learning

Abstract
Computational modeling is an important tool to aid chemical process development. Theoretical and data-driven models can be applied both for the optimization of specific processes, and for the initial screening of potential process chemistries. I will talk about my research in advancing both of these areas. First, I will introduce the development of an efficient kinetic Monte Carlo simulation to facilitate property optimization of polymer materials. The algorithm predicts the explicit sequence distribution of the polymer chains and can be used to design reaction recipe for desired molecular weight and sequence properties of synthetic polymers. Second, I will discuss the use of machine learning in the context of organic synthesis planning. Specifically, I developed an algorithm capable of efficiently and accurately recommending reaction conditions, including catalysts, solvents, reagents and temperature, for organic synthesis development. I will also demonstrate how we can leverage this information to optimize synthesis plans for individual molecules or molecular libraries.

Bio
Hanyu Gao is a postdoctoral associate at Massachusetts Institute of Technology, working with Prof. Klavs Jensen since May 2017. Hanyu obtained his Bachelor's degree in chemical engineering in Tsinghua University, China, where he was *Magna Cum Laude*. He then came to the U.S. and completed his Ph. D. in the Department of Chemical and Biological Engineering at Northwestern University with Prof. Linda Broadbelt. Hanyu's research interest lies in using modeling techniques, including simulation, optimization and machine learning, to solve chemical engineering problems ranging from polymer reaction engineering to organic synthesis design.

Tuesday, Jan 21st
Petroleum Engr 110
2:00 pm