

**Texas Tech University**  
**Department of Chemical Engineering**  
**Seminar Series**



**Yachao Dong**  
Postdoctoral fellow  
Department of Chemical and Biological Engineering  
Tufts University

## **Data-Driven Modeling & Optimization in Chemical Engineering**

### **Abstract**

Data-driven modeling and optimization have ubiquitous applications in Chemical Engineering, leading to performance improvements in terms of product quality, process robustness, environmental sustainability, and capital and operational cost. In this talk, we will focus on two examples: pharmaceutical reaction modeling and inventory routing.

First, we discuss how advances in reaction automation technologies (e.g., high-throughput platforms and auto-samplers) result in richer experimental datasets in the pharmaceutical industry. These datasets can then be used in a variety of ways, including process characterization, unknown stoichiometry identification, and operating window optimization. We present the development of a Dynamic Response Surface Methodology (DRSM) to address the necessity of modeling time-dependent profiles of organic reactions.

Second, we introduce the Inventory Routing (IR), a distribution optimization problem that arises in a wide range of manufacturing sectors, including industrial gases and petrochemicals. We discuss how implementing advanced IR methods can lead to significant improvements in the overall efficiency of manufacturing supply chains, and then propose a novel optimization approach for solving large-scale IR problems. We close with the discussion of an advanced solution method and its application to real-world instances.

### **Bio**

Yachao Dong is currently a postdoctoral fellow in the Department of Chemical and Biological Engineering at Tufts University. Yachao obtained his bachelor's degree in Zhejiang University in China. He completed his Ph.D. in Chemical Engineering in University of Wisconsin-Madison in 2017. His research interests lie in the area of process system engineering, ranging from process optimization to machine learning and data-driven modeling. He has studied problems in the areas of production scheduling, chemical supply chain, and pharmaceutical reaction modeling. Through these projects, he has collaborated extensively with researchers not only in academia, but also in industry (e.g., Praxair, BP, Pfizer and Merck). He has received multiple student scholarship awards.

**Friday, Jan 24<sup>th</sup>**  
**Livermore 101**  
**3:00 pm**