CHEN E4580 ***Artificial Intelligence in Chemical Engineering***

Instructor: Venkat Venkatasubramanian

Credits and Meeting Times: 3 credits; Mon-Wed 1:10 – 2:25 pm

Prerequisite/Co-Requisite: Background in chemical engineering and Python/MATLAB programming, or instructor permission.

Background: The practice of chemical engineering routinely involves decision-making to solve challenging problems that often arise in process/product design, fault diagnosis and control, optimization, and process operations and safety. To accomplish this, historically, chemical engineers have adapted modeling concepts and techniques from different disciplines such as applied mathematics and operations research over the decades. To this, Artificial Intelligence (AI) methods have increasingly been incorporated in the last three decades. Contrary to common impression, AI in chemical engineering is not new – it has a 35-year-long history and a body of literature comprising of a few thousand papers in chemical engineering[1-2]. It has become clear that AI-based approaches need to be part of the modeling arsenal of well-educated chemical engineers. This course is offered to address this important need.

Description: This course is aimed at chemical engineering students to teach them how to incorporate AI-based modeling in combination with first-principles-based models derived from the understanding of the physics and chemistry (and biology) of our products, processes, and systems. To accomplish this, this course will combine the traditional symbolic AI with the more recent data-driven AI. In this regard, this course is different from the standard data science course which typically focuses only on the data-driven aspect.

Topics would include: Chemical engineering modeling approaches, knowledge representation, symbolic reasoning and inference, knowledge-based systems, statistical data analysis, and machine learning methods such as clustering, neural networks, random forests, Bayesian networks, and directed evolution. All these will be discussed using chemical engineering case studies in process monitoring, diagnosis, and control, process/product design, scheduling, optimization, and process hazards analysis. In particular, the course will address the development of hybrid models that combine first-principles knowledge of the underlying physics & chemistry with data-driven techniques and the development of causal mechanism-based models, in contrast with typical AI courses taught in computer science departments.

Grading: Homework 40% and Project 60% (using MATLAB, Python, TensorFlow and/or Keras)

Textbook: There is no textbook. Several papers from the literature will be made accessible during the course.

1. Venkatasubramanian, V., Artificial Intelligence in Process Engineering: Experiences from a Graduate Course. *Chem. Eng. Educ*., Fall Issue, 188–192, 1986.

2. Venkatasubramanian, V., The promise of artificial intelligence in chemical engineering: Is it here, finally?. *AIChE J*., 65: 466-478, 2019.