

# Introductory Numerical Methods for Simulating Batch Reactors

## Instructor

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*Bio:* Joshua is a post-doc at CMU working with Profs. Carl Laird and Ignacio Grossmann, and he specializes in developing methods in optimization under uncertainty and data science to solve problems pertaining to sustainability, energy, and the environment. He completed his Ph.D. at UW-Madison under the direction of Prof. Victor Zavala and obtained his B.Sc. at BYU, both in chemical engineering.

## Course Summary

In this lecture, we will address how to simulate a multi-component reaction system in a batch reactor using common numerical methods. In particular, we will explore the use of explicit Euler methods for approximating ordinary differential equations (ODEs) which are a critical consideration in modeling batch reactors. This will feature hands-on activities designed around applying these techniques to simulate batch reactors with a system of reactions. Finally, we will highlight more advanced methods/tools commonly used to simulate these systems.

## Learning Outcomes

Attendees of this lecture will learn:

- The relative advantages/disadvantages of using explicit Euler methods
- How to implement explicit Euler to simulate ODEs using common computation environments (e.g., Python)
- How to simulate batch reactors using numerical methods
- A familiarity of other numerical methods/tools for simulating batch reactors

## Required Materials/Background

- Personal laptop or tablet that can connect to the internet
- Familiarity with basic Python syntax
- Familiarity with transient material balances and ordinary differential equations
- A positive learning mindset