

Lecture #01

Finite Difference-based Numerical Methods in Chemical Engineering

Recommended Books:

- 1) Numerical Methods for Engineers (Gupta)
- 2) Numerical Methods for Engineering Application (Ferziger)
- 3) Linear Algebra (Strang)

Objective: Learn a few basic numerical techniques (Finite Difference) to solve simple ODEs/PDEs/algebraic equations derived from a variety of heat and mass transfer related conservation equations.

- Analytical methods yield exact solutions, often in infinite series, use mathematical functions.
- Numerical methods yield approximate solutions, use numbers, computations, results are dependent on the method accuracies and limited by computers machine errors.

Course focuses on

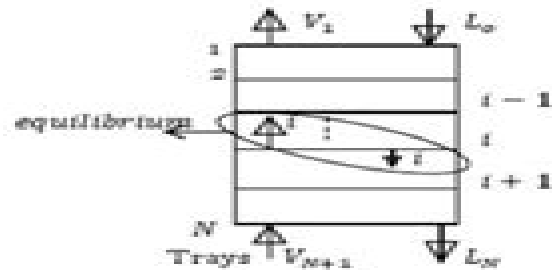
- Algebra (Matrix Operation)
- Methods (Finite Difference)

Requires knowledge of

- Computer Programming (because large # of iterations)
(there are engineering software, e.g., Matlab, NAG, IMSL, Polymath)
- No numerical analysis in this course!

Examples: (Applications in chemical engineering)

1. Distillation



Assume: Constant molar flowrates of vapor & liquid

Binary components: A , B

A (more volatile)

Species balance on i^{th} plate:

Numerical Methods In Chemistry

Michael Seilmaier



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