COMPUTATIONS IN CHEMICAL ENGINEERING: MONTE CARLO SIMULATIONS

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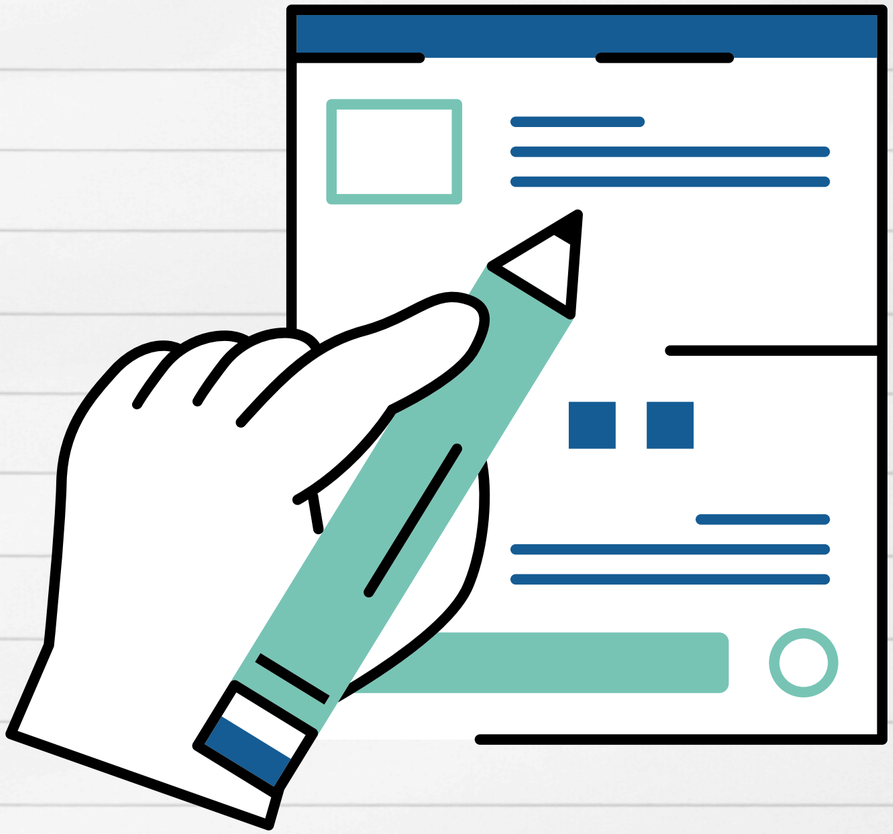
INTRODUCTION: OVERALL PROJECT OBJECTIVE

- Develop strong computational and analytical skills among students
- Enhance their understanding of advanced programming concepts and statistical methods.
- Equip them with practical tools and techniques for solving real-world engineering and scientific problems.
- Foster an appreciation for the interdisciplinary applications of Monte Carlo simulations, particularly in chemical engineering.



OBJECTIVES

MAIN OBJECTIVE

- Introducing application of Monte Carlo simulations, a stochastic approach, to teach mass transfer unit operations.
- Simulating a multi-component batch distillation problems using Monte Carlo.
- Improving Monte Carlo simulations using a SLMC Model.

SECONDARY OBJECTIVES

- Recursion : Unraveling Loops of Logic
- STL Basics: Unveiling C++ Power Tools
- Data Structures & Algorithms: Fundamentals
- What are Graphs?
- Chemical Graph Theory: The Molecules of Connectivity
- Beautiful Djikstras Algorithm

CONTEXT: BACKGROUND AND JUSTIFICATION

1.**Probabilistic Nature of Chemical Phenomena**: Many chemical phenomena follow probabilistic laws, which can be challenging to address using traditional deterministic methods.

2.Deterministic Method: Traditionally, chemical problems are solved using deterministic methods based on differential equations, such as ordinary differential equations (ODEs) according to the mass action law.

3.Complexity and Limitations: Solving these equations can be difficult, especially with coupled mechanisms that result in complex rate laws. Simplifications might be necessary but can lead to inaccuracies.

4. Conceptual Understanding: Deterministic equations may not always help students fully understand the underlying chemical phenomena.

5. Stochastic Approaches: Monte Carlo simulations and other stochastic approaches have been successfully applied to these chemical problems, offering a more intuitive and sometimes more accurate way to conceptualize and solve them.

TIMELINE: KEY DATES AND PHASES

Week 01

- Problems on Recursion
- Stacks
- Queues
- Basic STL(for C++)

Week 02

- Introduction to Linked Lists
- Implementation of Stacks using Queues and vice-versa
- Introduction to Binary Tree & its trvaersal algorithms.

Week 03

- Introduction to Graphs
- Heaps
- Dijkstra’s Algorithms
- Topological Sorting(BFS)

Week 04

- Random Variables
- Expectation, Variance & Standard Deviation of Random Variable
- Different Statistical Distributions

Week 05

- Introduction to Monte Carlo
- Inverse Transform Method
- Discrete Accept-Reject

Week 06

- Continuous Accept-Reject
- Solving the Case-Study

WEEK 01

- Problems on Recursion:-
  - The project started up with standard problems on recursion. The difficulty of the problems varied from reversing a string to Tower of Hanoi and other problems.
- Implementation of Stacks & Queues:-
  - Stacks and Queues were implemented not just by the virtue of each other but also with the help of arrays.

WEEK 01

- Basic STL(for C++):-
  - Many other data structures and important C++ library functions were taught which can be accessed through the C++ STL. This enhanced the programming efficiency of the mentees and also helped them develop more optimized solutions for different problems.

WEEK 02

- Introduction to Linked Lists:-
  - Moving towards some advanced data structures, we were familiarized with Linked Lists and their applications.
  - Starting off with the basic implementation of the data structure we moved forward with different problems based on it.
  - The problems varied from finding the length of the linked list to actual competitive programming level questions.

WEEK 02

- Introduction to Binary Tree:-
  - After Linked Lists we headed towards Binary tree.
  - Initially, we understood the process of developing a binary tree from scratch (using Linked Lists).
  - The problems varied from finding the size & diameter of the binary tree to different interview-standard questions.

WEEK 03

- Introduction to Graphs:-
  - After covering Binary Tree & Linked Lists in the previous week. We started off with Graphs.
  - Initially, we understood the adjacency matrix and list representation of a graph to develop a basic structure.
  - Then we started working on different traversal algorithms:-
    - DFS(Depth First Search)
    - BFS(Breadth First Search)

WEEK 03

- Topological Sort-
  - After Covering the basics of Graph we understood and implemented the Topological Sorting Algorithm and understood its applications in real-life situations.

WEEK 03

- Dijkstra’s Algorithms :-
  - After dwelling on the basics, we understood the Dijkstra’s Algorithms and it’s implementation.
  - After working on the implementation, we solved questions of different variety based on it, starting right from the basics to advanced level questions.

WEEK 04

- Introduction to Probability and Random Variables :-
  - Post- Data Structures and Algorithms, we headed towards Probability and Statistics, which is an important pre-requisite for our project.
  - We started off with random variables and Studying Different Statistical Distributions.
  - Also, we discovered different real-life situations where the distributions are applied.

WEEK 04 & 5

- Random Variables (Expectations, Variance & Standard Deviation) :-
  - After understanding the concept of random variables, there was a need of defining quantities which could summarize the random variable in a number and would tell about the nature of it’s distributions hence, three different quantities were introduced:-
    - Expectation E[X]
    - Variance Var(X)
    - Standard Deviation

WEEK 05

- Introduction To Monte Carlo :-
  - In continuation to previous week, we started off with Monte Carlo, we dwelled upon understanding that why it is needed in the first place.
  - Then we understood it’s different real-life applications and how it has affected the field of probability.

- **Discrete Inverse Transform:-**
  - After covering the above we understood different methods to transform a uniform distribution to the desired distribution of our choice.

WEEK 05 & 6

- **Discrete and Continuous Accept Reject :-**
  - Since the Inverse Transform Method is not computationally efficient in every case, we needed a different method, hence we studied about The Accept-Reject method in detail for both (Discrete and Continuous Distributions).
- **Case Study:-**
  - Since all the pre-requisites are covered for the project, we headed towards solving the case study.

CASE STUDY

USING STOCHASTIC APPROACHES FOR MASS TRANSFER UNIT OPERATIONS:THE MONTE CARLO METHOD

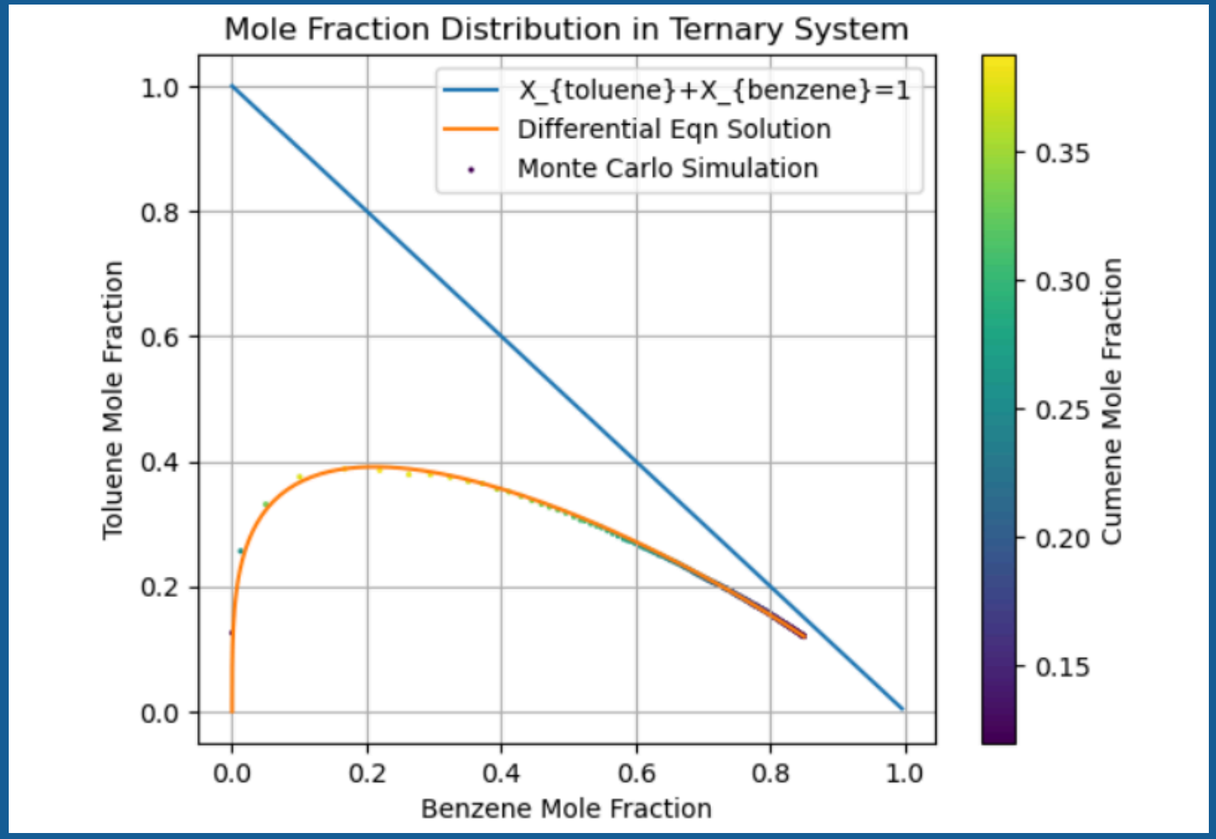
- Many chemical phenomena follow probabilistic laws, which can be challenging to address using traditional deterministic methods like differential equations.
- Typically, chemical reaction problems are modeled with ordinary differential equations (ODEs) according to the mass action law. However, these methods can be difficult to solve, especially with complex coupled mechanisms, often requiring simplifications that may lead to inaccuracies.
- Moreover, deterministic equations may not fully help students understand the underlying phenomena.
- To overcome these limitations, stochastic approaches such as Monte Carlo simulations have been successfully applied, providing a more intuitive and accurate way to conceptualize and solve chemical problems.

APPROACH?

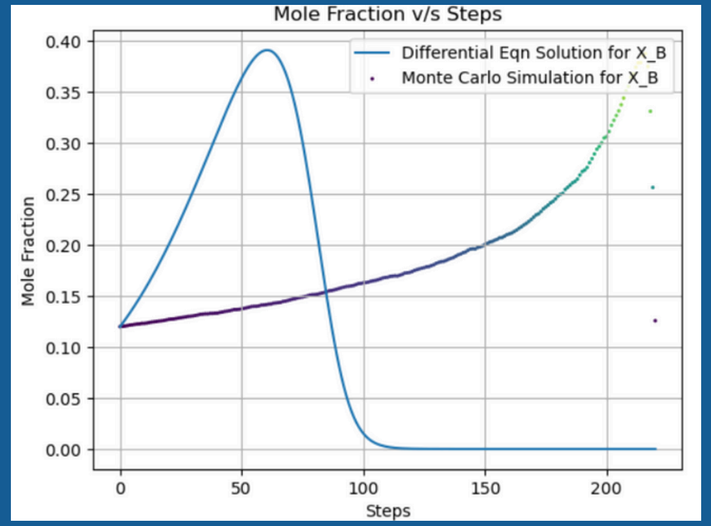
DEVELOPING THE MONTE CARLO SIMULATION AND EULER INTEGRATION

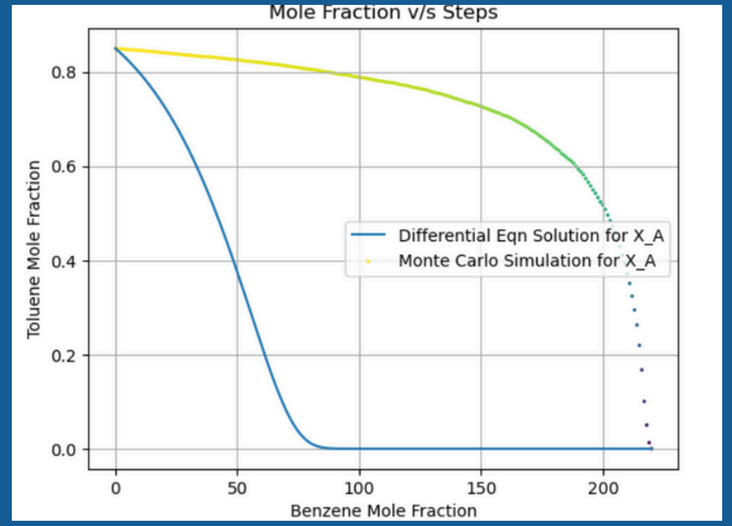
- We consider a sample of 10000 molecules, which consist of 3 different components:-
  - Benzene
  - Toluene
  - Cumene
- Each of them have different relative volatilities and initial molecules in the monte-carlo environment.
- We simulate the environment by using a uniform distribution, through which we iterate through the whole process.
- Finally we plot the graph and analyse the results.

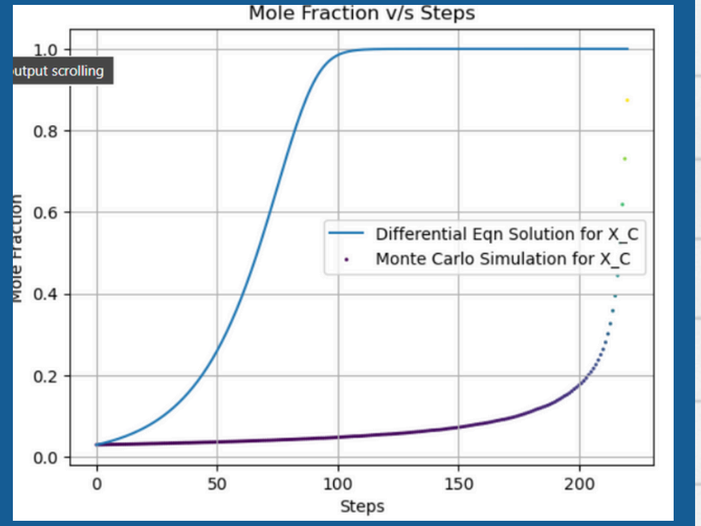
TERNARY DIAGRAM



MOLE FRACTION PER STEP







FOR BENZENE

FOR TOLUENE

FOR CUMENE

THANK YOU VERY MUCH!