MOD510: Project4

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Exercise 1: Stochastic modeling of mixing tanks

Introduction

Mixing tanks are fundamental components in chemical and environmental engineering. They are often used to model processes such as chemical reactions, heat transfer, and pollutant dispersion. In this exercise, we will model a system of interconnected mixing tanks using a **stochastic modeling approach** based on **Monte Carlo methods**. Beginning with a single tank, you will progressively model a three-tank system, incorporating uncertainty estimation and validating results against ordinary differential equation (ODE) solutions.

Learning Outcomes

By the end of this exercise, students will:

1. Understand the principles of Monte Carlo methods and their application in stochastic modeling.
2. Develop skills in formulating and solving mass balance equations for single and interconnected systems.
3. Quantify uncertainties in simulation results and interpret their implications for system behavior.
4. Compare stochastic simulation outcomes to deterministic ODE solutions, critically analyzing their performance and limitations.
5. Gain hands-on experience with computational tools for solving engineering problems.

Part 1. Single Mixing Tank with Parameter Uncertainty

Description: Explore the effect of parameter uncertainty on contaminant concentration in a single mixing tank using Monte Carlo simulations. Assume that the tank volume remains constant throughout all simulations, even when inflow and outflow rates vary.

Tasks:

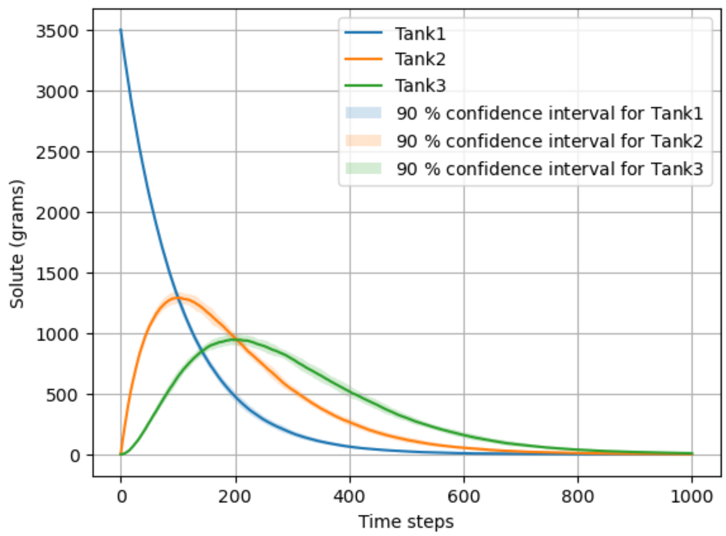

Figure 1: Montecarlo solution to the three mixing tanks problem

1. Derive and solve the governing equation for the solute concentration over time:

$$\frac{dC}{dt} = \frac{Q_{\text{in}}}{V} C_{\text{in}} - \frac{Q_{\text{out}}}{V} C, \tag{1}$$

   where C is the solute concentration in the tank, C_{in} is the solute concentration of the inflow, Q_{in} and Q_{out} are the inflow and outflow rates, and V is the tank volume (constant).

2. **Analytical Solution with Average Parameters:** Compute the analytical solution of the single-tank problem using the *average values* of the parameters:

   - $\bar{V} = 1000\,\text{liters}$
   - $\bar{Q}_{\text{out}} = 100\,\text{L/s}$
   - $\bar{Q}_{\text{in}} = 100\,\text{L/s}$
   - $\bar{C}_{\text{in}} = 0.25\,\text{g/L}$
   - $\bar{C}(0) = 3.5\,\text{g/L}$

   Derive the concentration as a function of time using these average parameters.

3. Assume that the probability of a gram of fluid to leave the tank over a given time interval Δt is

$$p = 1 - e^{-\frac{Q_{\text{out}}}{V}\Delta t}. \tag{2}$$

4. **Monte Carlo Simulation – Option 1 (Fixed Parameters per Run):** Perform a Monte Carlo simulation where parameters are sampled *once at the beginning of each run and remain constant throughout the run.* Use the following uniform distributions:

   - $V \sim \text{Uniform}(950, 1050)$ liters
   - $Q_{\text{out}} = Q_{\text{in}} \sim \text{Uniform}(95, 105)\,\text{L/s}$
   - $C_{\text{in}} = 0\,\text{g/L}$
   - $C(0) \sim \text{Uniform}(3.4, 3.6)\,\text{g/L}$

   Simulate 1000 time steps for each run and perform 100 independent runs. Compute:

   - Mean concentration across runs
   - Standard deviation
   - 95% confidence intervals

5. **Monte Carlo Simulation – Option 2 (Parameters Vary at Each Time Step):** Repeat the simulation, but now allow parameters to fluctuate at every time step to represent dynamic variability. For each time step, resample:

   - $Q_{\text{in}} = Q_{\text{out}} \sim \text{Uniform}(95, 105)\,\text{L/s}$
   - $C_{\text{in}} = 0\,\text{g/L}$

   Keep V and $C(0)$ fixed per run. Compare the uncertainty in concentration between Option 1 and Option 2.

Part 2. Three Interconnected Tanks with Parameter Uncertainty

Description: Extend the model to a system of three interconnected tanks with inflows, outflows, and interconnecting flow between tanks. Assume that the volume of each tank remains constant throughout all simulations.

Tasks:

1. **Formulate the System of Equations:** Write the governing equations for the solute concentrations in all three tanks:

$$\frac{dC_1}{dt} = \frac{Q_{\text{in}}}{V} C_{\text{in}} - \frac{Q_{\text{out}}}{V} C_1, \tag{3}$$

$$\frac{dC_2}{dt} = \frac{Q_{\text{in}}}{V} C_1 - \frac{Q_{\text{out}}}{V} C_2, \tag{4}$$

$$\frac{dC_3}{dt} = \frac{Q_{\text{in}}}{V} C_2 - \frac{Q_{\text{out}}}{V} C_3. \tag{5}$$

2. **Monte Carlo Simulation (Fixed Parameters per Run):** Perform a Monte Carlo simulation where parameters are sampled once at the beginning of each run and remain constant throughout the run:

   - $V \sim \text{Uniform}(950, 1050)$ liters
   - $Q_{\text{in}} = Q_{\text{out}} \sim \text{Uniform}(95, 105)\,\text{L/s}$
   - $C_{\text{in}} = 0\,\text{g/L}$
   - Initial concentrations:

   $$C_1(0) \sim \text{Uniform}(3.4, 3.6)\,\text{g/L},$$
   $$C_2(0), C_3(0) \sim \text{Uniform}(0, 0.1)\,\text{g/L}.$$

   Simulate 1000 time steps for each run and perform 100 independent runs. Compute mean, standard deviation, and confidence intervals for all three tanks.

Part 3. Validation Against ODE Solutions

Description: Solve the system of ODEs analytically (if possible) or numerically using the *average values* of the parameters:

- $\bar{V} = 1000\,\text{liters}$, $\bar{Q}_{\text{in}} = \bar{Q}_{\text{out}} = 100\,\text{L/s}$
- $\bar{C}_{\text{in}} = 0.25\,\text{g/L}$, $\bar{C}_1(0) = 3.5\,\text{g/L}$, $\bar{C}_2(0) = \bar{C}_3(0) = 0\,\text{g/L}$

Tasks:

1. Compare the Monte Carlo simulation results to the deterministic ODE solution.
2. Evaluate accuracy, consistency, and computational efficiency of the stochastic approach.
3. Discuss advantages and limitations of Monte Carlo methods versus deterministic ODE solutions.

Exercise 2: Spreading of contaminants in underground aquifers using random walk

Introduction

The spreading of contaminants in underground aquifers can be modeled as a diffusion process. Such a model, however, does not incorporate spatial variations in porosity within the aquifer. As an alternative to the diffusion model, here we will construct a 2D random walk model of contaminant transport in aquifers.

A random walk is a mathematical concept used to describe a sequence of steps, each determined by chance, within a given space. It serves as a model for

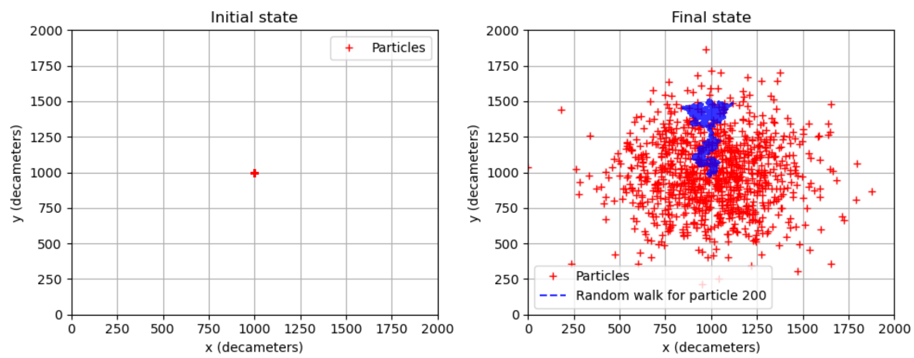

Figure 2: 2D random walk

processes where the outcome is influenced by randomness, such as the movement of particles, stock prices, or biological processes.

In its simplest form, a random walk takes place on a 1D line where a particle moves one step forward or backward at each interval, with equal probability. This idea can be extended to higher dimensions, such as a 2D plane or 3D space, making it a powerful tool for modeling various physical and natural phenomena.

Random walks are widely used in fields like physics, finance, and environmental science. For example, they help simulate diffusion processes in fluids, contaminant transport in aquifers, and even search optimization algorithms in computer science. By analyzing patterns and statistical properties, random walks provide insight into the behavior of systems influenced by randomness.

Learning Outcomes

By the end of this exercise, students will be able to:

1. **Model Contaminant Spread Using Random Walks**
   - Simulate contaminant transport from a central source using a random walk approach.
2. **Calculate Key Metrics in Contaminant Transport**
   - Estimate the time required for contaminants to reach a specific distance under both typical and worst-case scenarios.
3. **Incorporate Directional Bias in Random Walks**
   - Modify the movement probabilities to simulate directional transport effects, such as groundwater flow.
4. **Compare Risk Scenarios in Contaminant Spread**

- Assess and quantify relative contamination risk at different locations by comparing arrival times under various scenarios.

5. **Link Theoretical Models to Practical Applications**
   - Relate random walk diffusion models to real-world challenges in aquifer contamination and environmental risk assessment.

Part 1. 2D Random Walk Model

Description: Construct and analyze a random walk model of diffusion in a 2D environment.

Tasks:

1. **Basic Model:**
   - Initialize 1000 particles positioned on a square grid centered at $(1000, 1000)$ (Figure 2).
   - At each time step, move (or don't move) each particle one integer step in the x and y directions. No diagonal walking should be allowed.
   - Ensure that if a particle's movement takes it beyond the predefined boundary of the space ($0 \leq x \leq 2000$, $0 \leq y \leq 2000$; Figure 2), the simulation stops.

2. **Probability-Weighted Movement:**
   - Modify the program to define different probabilities for a particle moving (or not) in the x and y directions. In 2D, there should be a total of nine possible movement directions, including staying in place. Each movement is associated with a defined probability.
   - Verify that the sum of all movement probabilities equals 1.

Part 2. 2D Random Walk Model of Contaminant Transport in Aquifers

Description: Simulate the spread of contaminants in an aquifer using a random walk model and assess contamination risk at varying distances from the source.

Tasks:

1. **Define Contaminant Source:** The contaminant source is located at the central grid point:
   $$x = 1000,\ y = 1000$$
   (See Figure 2). Each grid unit represents **10 meters**.

2. **Worst-Case Scenario:** A worst-case scenario is defined as the contaminant moving in a straight line toward the target distance without any random deviation, at the maximum possible average migration rate of 10 m/year. Calculate the **minimum time** required for the contaminant to reach a distance of 10 km from the source under this assumption.

3. **Simulate Contaminant Spread:** Implement a **2D random walk** where each step moves the contaminant by one grid unit in one of four directions (North, South, East, West) with equal probability. Simulate the spatial distribution after a fixed number of steps and visualize the concentration map.

4. **Time to Reach 10 km (Unbiased Random Walk):** Assume the contaminant moves randomly at an average of 10 m/year.

    - Run at least 10 independent simulations and record the time (in years) when the contaminant first reaches a distance of 10 km from the source.
    - Plot a histogram of these arrival times.
    - Determine whether the arrival times approximate a normal distribution.

5. **Introduce Net Transport (Biased Random Walk):** Modify the movement probabilities so that the probability of moving South is twice the probability of moving North, while East and West remain equal. Then:

    - Simulate 100 runs and plot a histogram of arrival times for reaching 10 km South.
    - Determine whether the arrival times approximate a normal distribution.
    - Compare contamination risk for unbiased vs biased cases by computing the ratio of their most likely arrival times for reaching 10 km South.