A logo with text and a circle

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**Bolu Abant Izzet Baysal University  
Faculty of Engineering  
Department of Chemical Engineering**  
  
**Final Exam Report  
Chemical Engineering Modelling and Simulation**

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A diagram of a mathematical equation

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# Abstract

This report presents the modeling, simulation, and analysis of dynamic chemical engineering systems using MATLAB and Simulink. Three problems were addressed: (1) the first-order decay of a reactant, (2) the numerical solution of a first-order linear ODE representing a damp system, and (3) the concentration profiles in a batch reactor undergoing a series reaction A → B → C. Each system was modeled mathematically, simulated using both MATLAB scripts and Simulink blocks, and analyzed in terms of behavior and performance. The results demonstrated expected trends such as exponential decay, damp oscillation, and product accumulation. The models were validated using function-based and gain-based Simulink architecture. This report provides a strong foundation in simulation-based process modeling, relevant to reactor design and control.

# Introduction

Modeling and simulation play a fundamental role in understanding and predicting the behavior of chemical processes. In this report, we explore three key engineering problems using MATLAB and Simulink to demonstrate their practical applications. These include the decay of a chemical species in a batch system, solving a first-order ODE with an oscillatory input, and tracking concentration changes in a batch reactor with sequential reactions. The objective is to translate physical phenomena into mathematical models, implement them computationally, and extract meaningful engineering insights.

# Part 1: MATLAB Plot of Concentration vs. Time

The following reaction data has been obtained from a simple decay reaction:

A **🡪** B

Use MATLAB to plot the concentration of component A in mol/L against the reaction time, t, in minutes. With titled plot, labeled axes, and obtain elementary statistics for the data.

## Mathematical Model

Assuming this is a **first-order decay reaction**, the model is:

Where:

* CA is the concentration of A (mol/L)
* k is the first-order rate constant (min−1)

This type of equation has the solution:

It models how a substance like a reactant decay over time in a batch reactor or closed system.

|  |  |
| --- | --- |
| Time (minutes) | Concentration (moles/liter) |
| 0 | 100 |
| 1 | 80 |
| 3 | 65 |
| 6 | 55 |
| 9 | 49 |
| 12 | 45 |
| 15 | 42 |
| 18 | 41 |
| 21 | 38 |

MATLAB Visualization

* **X-axis**: Reaction Time (minutes)
* **Y-axis**: Concentration of A (mol/L)
* **Title**: Concentration of A vs Time for a First-Order Decay Reaction

## MATLAB Code

clc;

clear all;

%{

Question1

To plot the concentration of A(mol/L) vs reaction time t (min).

Title the plot, label the axes, and obtain advanced statistics for the data.

%}

concentration\_A = [100, 80, 65, 55, 49, 45, 42, 41, 38];

Time = [0, 1, 3, 6, 9, 12, 15, 18, 21];

% Create the plot

figure('Name', 'Concentration of A vs Time for a First-Order Decay Reaction', 'NumberTitle','off');

plot(Time, concentration\_A, 'g\*-', 'LineWidth', 2);

title('Concentration of A vs Time for a First-Order Decay Reaction');

xlabel('Reaction Time (minutes)');

ylabel('Concentration of A(mol/L)');

grid on;

% Elementary statistics

mean\_A = mean(concentration\_A);

median\_A = median(concentration\_A);

std\_A = std(concentration\_A);

min\_A = min(concentration\_A);

max\_A = max(concentration\_A);

% Display results

fprintf('\*\*\*\*\* Statistics for Concentration of A \*\*\*\*\n');

fprintf('Mean: %.2f mol/L\n', mean\_A);

fprintf('Median: %.2f mol/L\n', median\_A);

fprintf('Standard Deviation: %.2f mol/L\n', std\_A);

fprintf('Minimum: %.2f mol/L\n', min\_A);

fprintf('Maximum: %.2f mol/L\n', max\_A);

The script provided for Q1 decay plotting and statistical output.

## A screenshot of a computer screen AI-generated content may be incorrect.Results

## Statistics for Concentration of A

Mean: 57.22 mol/L  
Median: 49.00 mol/L  
Standard Deviation: 20.90 mol/L  
Minimum: 38.00 mol/L  
Maximum: 100.00 mol/L

## Discussion

The trend confirms expected first-order behavior.

* The curve shape matched **exponential decay**, supporting the first-order assumption.
* The stats helped summarize the concentration trend.
* The data could later be used to estimate **k** by fitting CA(t) vs. time.

# Part 2: Solving the First-Order ODE

## Mathematical Model

The given differential equation is:

This is a nonhomogeneous linear ODE representing a damp driven system.

## MATLAB Code

ode45 implementation to solve and plot the ODE.

clc;

clear;

tspan = [0 10]; % Time interval for the solution

x0 = 0; % Initial condition

% Define the differential equation dx/dt = 2\*sin(3t) - 4\*x

f = @(t, x) 2\*sin(3\*t) - 4\*x;

% Solve the differential equation using ode45

[t, x] = ode45(f, tspan, x0);

% Plot the solution

figure('Name', 'Numerical Solution of dx/dt = 2sin(3t) - 4x', 'NumberTitle','off');

plot(t, x, 'LineWidth', 2);

title('Numerical Solution of dx/dt = 2sin(3t) - 4x');

xlabel('Time (seconds)');

ylabel('x(t)');

grid on;

## Simulink Model:

### Approach 1 – Standard Simulink Blocks

Block Setup:

#### 🔹 Simulink Block Solution – Sine + Gain + Sum + Integrator

* **Sine Block**: Amplitude = 2, Frequency = 3 rad/s
* **Gain Block**: -4 applied to feedback x(t)
* **Sum Block**: combines the inputs
* **Integrator**: solves for x(t)
* **Scope**: visualizes result
* **X-axis**: Time (s)
* **Y-axis**: x(t)
* A diagram of a function

  AI-generated content may be incorrect.**Title**: Numerical Solution of dx/dt = 2sin(3t) - 4x

It describes a system with an oscillatory input (2sin(3t)) and a damping term (−4x)..

|  |  |  |
| --- | --- | --- |
| Block Type | Name | Description |
| Sine Wave | Sin\_2sin3t | Input signal 2sin(3t) |
| Gain | Gain\_-4x | Multiplies feedback x(t) by −4 |
| Sum | Sum\_inputTerms | Adds 2sin(3t) and −4x |
| Integrator | Integrator\_x | Integrates RHS to get x(t) |
| Scope | Scope\_x) | Plots the result |

Expected Output:

The output x(t) starts with high oscillations and gradually decays as the damping effect dominates.

### Approach 2 – MATLAB Function Block in Simulink

Instead of using separate Sine and Gain blocks, the entire RHS is computed inside a MATLAB Function block.

MATLAB Function Block Code:

function dx = Compute\_dx(t, x)

dx = 2 \* sin(3 \* t) - 4 \* x;

end

Block Setup:

|  |  |  |
| --- | --- | --- |
| Block Type | Name | Description |
| Clock | Simulation\_Time | Multiplies feedback x(t) by −4 |
| MATLAB Function | Copute\_dX | Evaluates RHS of the equation |
| Integrator | Integrator(x) | Integrates RHS to get x(t) |
| Scope | Scope(x) | Plots or displays the result |

Simulation Settings

* Time range: 0 to 10 seconds
* A diagram of a computer program

  AI-generated content may be incorrect.Solver: ode45 (or auto)

## Discussion

Both methods solve the same ODE. The block-by-block approach makes each operation visible, while the MATLAB Function block method is more compact and flexible, especially useful for more complex models.

The output curve exhibits **damp oscillatory behavior**, consistent with physical systems that involve periodic forcing and resistive damping (like electrical circuits or mechanical vibrations).

# Part 3: Batch Reactor Simulation – A → B → C

Reactions Scheme:

The decomposition of reactant A to the desired product B is occurring and the flow rate of the feed-containing A is 50 liter/min. The initial concentrations of A, B, and C are CA0 = 5 mol/liter, CB0 = CC0 = 0. The reaction rate constants are k1 = 0.4 min−1, k2 = 0.2 min−1 Assume isothermal conditions

I. Determine the maximum concentration of B and the time when the concentration of B reaches the maximum value.

II. Find the volume when CB is at maximum concentration for the above problem develop a mathematical model and simulate this model by using MATLAB Simulink. (Sketch a flow diagram for the reactor, write down the equations for the mathematical model, and build a model in MATLAB Simulink.

## Mathematical Model

With Initial conditions:

* CA0 =5, CB0 = 0, CC0 ​= 0
* k1= 0.4, k2​ = 0.2

## Flow Diagram:

 No continuous feed or outlet during the reaction.

 All reactants (A) are added at time **t = 0**

 Products (B and C) accumulate inside the reactor and are removed **after** the batch is complete.

A diagram of a cylinder

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## MATLAB Code & Result

See full script for system of equations solved using ode45.

clc;

clear;

% Rate constants

k1 = 0.4; % 1/min

k2 = 0.2; % 1/min

% Initial concentrations [CA0, CB0, CC0]

C0 = [5, 0, 0];

% Time span minutes

tspan = [0 50];

% ODE system

reactionODE = @(t, C) [-k1\*C(1);

k1\*C(1) - k2\*C(2);

k2\*C(2)];

% Solve ODEs

[t, C] = ode45(reactionODE, tspan, C0);

% Extract concentrations

CA = C(:,1);

CB = C(:,2);

CC = C(:,3);

% Find maximum of CB and corresponding time

[max\_CB, idx\_max\_CB] = max(CB);

t\_max\_CB = t(idx\_max\_CB);

% Calculate volume when CB is max

flow\_rate = 50; % L/min

V\_at\_max\_CB = flow\_rate \* t\_max\_CB;

% Plot

figure('Name','Batch Reactor - Concentration Profiles','NumberTitle','off');

plot(t, CA, 'r', t, CB, 'b', t, CC, 'g', 'LineWidth', 2);

xlabel('Time (min)');

ylabel('Concentration (mol/L)');

title('Concentration Profiles in Batch Reactor');

legend('C\_A', 'C\_B', 'C\_C');

grid on;

% Output

fprintf('Maximum CB: %.3f mol/L at t = %.2f min\n', max\_CB, t\_max\_CB);

fprintf('Volume at max CB: %.2f L\n', V\_at\_max\_CB);

used ode45 to solve the equations and plot:

* CA(t) decreasing
* CB(t) increasing to a max, then decreasing
* CC(t) rising and plateauing
* Time range: 0 to 50 minutes.

A graph of a function

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MATLAB Code Results

Max C\_B: = 2.5 mol/L at = 3.39 min  
Volume at max: = 169.67 L

## Simulink

### Approach 1 – Standard Simulink Blocks

Gain + Sum + Integrator Blocks

 Used basic blocks to visually represent kinetics:

* Gain -k1, gain k1, Gain -k2, Gain k2
* Sum block for B’s production and loss
* A diagram of a computer

  AI-generated content may be incorrect.3 Integrators (CA, CB, CC)

Function-Based Model

### Approach 2 – MATLAB Function Blocks

Each rate equation is coded as a separate function:

Functions are concentration rate of A, B, C respectively.

Functions code

function dCA = dCA\_func(CA)

k1 = 0.4;

dCA = -k1 \* CA;

end

function dCB = dCB\_func(CA, CB)

k1 = 0.4;

k2 = 0.2;

dCB = k1 \* CA - k2 \* CB;

end

function dCC = dCC\_func(CB)

k2 = 0.2;

dCC = k2 \* CB;

end

A diagram of a computer

AI-generated content may be incorrect.Each function connects to an Integrator and Scope.

Screenshot of Function Block Model

Results Summary

Scope Plot Labels

* **Scope CA**: Title: Concentration of A, X: Time (min), Y: mol/L
* **Scope CB**: Title: Concentration of B, X: Time (min), Y: mol/L
* **Scope CC**: Title: Concentration of C, X: Time (min), Y: mol/L

### A screen shot of a computer AI-generated content may be incorrect.Results of Simulink model

A screen shot of a graph

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A screen shot of a graph

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## Discussion

* This model shows how **intermediate products like B** peak and then depletes.
* B peaks early and then decays as it forms C.
* Final conversion confirms reaction completion.
* Function and Gain methods match, validating model.
* Useful for reactor design, especially batch operations aiming to isolate intermediates.
* Function-based modeling supports modularity and system clarity.

# ****Conclusion:****

This report has demonstrated key concepts of chemical process modeling using both numerical methods and block-based simulation tools. The ability to translate physical behavior into solvable equations and interpret their results is essential in reactor design and chemical system optimization. From simple decay to more complex reaction networks, MATLAB and Simulink have proven to be powerful and complementary tools for modern chemical engineers.

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