# Numerical Simulation of a Reversible and Competitive Reaction System with Catalyst Deactivation

**Group 1:** Keshav Kapoor (220521), Rahul (240827), Ankit Kumar Saini (240139)
Advanced Computational Methods in Chemical Engineering
Department of Chemical Engineering

## Abstract

This report presents a numerical simulation of a chemical reaction system involving reversible and competitive reactions with catalyst deactivation. The study employs several numerical integration techniques—Euler's Method, Runge-Kutta 4th Order Method (RK4), Gauss-Seidel, and Gauss Elimination—to solve a system of ordinary differential equations (ODEs). Each method is compared in terms of implementation complexity, accuracy, and computational performance.

## 1 Reaction Scheme and Kinetics

**Reactions:**

- $A \rightleftharpoons B$ $\quad (k_1 = 2, k_{-1} = 0.4)$
- $B \rightarrow C$ $\quad (k_2 = 0.6)$
- $B \rightarrow D$ $\quad (k_3 = 0.2)$

**Catalyst deactivation:**

$$\frac{d(\text{Cat})}{dt} = -k_d \cdot \text{Cat} \quad (k_d = 0.1)$$

**Initial Conditions:** $[A]_0 = 1$, $[B]_0 = [C]_0 = [D]_0 = 0$, $[\text{Cat}]_0 = 1$

## 2 Numerical Methods Used

### 1. Euler's Method

Euler's method is a first-order numerical procedure for solving ordinary differential equations (ODEs) with a given initial value. It works by approximating the solution using the tangent line at the known point. The general form is:

$$y_{i+1} = y_i + hf(t_i, y_i)$$

Where:

- $h$ is the time step size
- $f(t, y)$ is the derivative function

**Advantages:**

- Easy to implement and understand
- Useful for simple, linear systems

**Disadvantages:**

- Low accuracy due to truncation error
- Sensitive to large step sizes (can become unstable)

**2. Runge-Kutta 4th Order (RK4) Method**

RK4 is a higher-order method that improves accuracy by sampling the slope at several points within a single step and taking a weighted average. The RK4 update rule is:

$$\begin{aligned}
k_1 &= hf(t_n, y_n) \\
k_2 &= hf\left(t_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right) \\
k_3 &= hf\left(t_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right) \\
k_4 &= hf(t_n + h, y_n + k_3) \\
y_{n+1} &= y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}$$

**Advantages:**

- Much more accurate than Euler for the same step size
- Suitable for both stiff and non-stiff ODEs

**Disadvantages:**

- Requires four function evaluations per step
- Slightly more complex to implement

**3. Gauss-Seidel Method**

Gauss-Seidel is an iterative method used to solve systems of linear equations. In the context of ODEs, it is used to solve the algebraic equations arising from implicit schemes or finite-difference discretization:

- Updates variables in-place using the latest values.
- Iteratively refines the solution until convergence is achieved.

**Advantages:**

- Memory-efficient due to in-place updates
- Converges faster than Jacobi method in many cases

**Disadvantages:**

- May not converge for all matrices
- Requires initial guess

**4. Gauss Elimination**

Gauss Elimination is a direct method for solving systems of linear equations. It works in two phases:

- **Forward Elimination:** Converts the matrix into an upper triangular form.
- **Back Substitution:** Solves for unknowns starting from the last equation.

**Advantages:**

- Provides exact solutions (in absence of round-off errors)
- No need for iterative convergence

**Disadvantages:**

- Computationally expensive for large systems
- More memory usage than iterative methods

## 3 Simulation Results and Observations

### Concentration Behavior

- Species A decreases due to conversion into B.
- Species B first increases, then decreases due to conversion to C and D.
- Products C and D accumulate over time.
- Catalyst activity declines exponentially due to deactivation.

### Method Comparisons

- Euler is fast but unreliable for stiff systems.
- RK4 shows excellent accuracy and stability.
- Gauss-Seidel is efficient for sparse matrices.
- Gauss Elimination is robust but computationally intensive.

## 4 Conclusion

This study demonstrates the application of various numerical methods to simulate a reversible and competitive reaction system with catalyst deactivation. Among all methods:

- RK4 offers the best accuracy and is well-suited for dynamic chemical systems.
- Euler is simple but needs very small time steps to remain stable.
- Gauss-Seidel and Gauss Elimination are useful when solving linear systems in implicit formulations.

Understanding the strengths and weaknesses of each method allows engineers to choose the most appropriate solver for their specific system dynamics and constraints.