CAPE Laboratory Assignment-5

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Problem Statement

Consider a catalytic reactor of length L = 1 where a first-order reaction A → B takes place. The reactor model that describes the concentration of A in the reactor (C_A) and concentration of A on catalyst surface (C_{As}) can be described as follows:

$$u\frac{dC_A}{dz} = -k_g\underline{a}\left(C_A - C_{As}\right)$$

$$0 = k_g\left(C_A - C_{As}\right) - kC_{As}$$

Model parameter values: u = 1, k_g = 0.02, k = 0.01, a = 200, C_A (0) = 1

Determine the axial profiles of concentration C_A and C_{As} in the reactor.

a) Solve the DAE using ODE solver (like *ode45*) and algebraic solver (like *fsolve*).
b) Analytical solution is also possible here. Compare numerical and analytical solution.

MATLAB Code

```
clear all;

global u a kg k; % Model Given Parameters
u = 1;
a = 200;
kg = 0.02;
k = 0.01;
CAi = 1; % Initial Condition on CA
length = [0,1];
```

```
[z,sol] = ode45(@(z,y) reactor_func(z, y),length,CAi); %
Solving ode
plot(z,sol,'-o','LineWidth',2); % Plotting CA vs z
hold on;
plot(z,(kg/(k+kg))*sol,'-.','LineWidth',2); % Plotting
CAs vs z
legend('CA','CAs');

function func = reactor_func(z,y) % Defining function for
ODE
global u a kg k;
CA = y;
CAs_initial_guess = CA;
CAs = fsolve(@(Cas) Alg_Eqn(CA,Cas),CAs_initial_guess); %
Solving Algebraic part
func = -(kg*a/u)*(CA - CAs);
end

function y = Alg_Eqn(CA,CAs) % Defining function for
Algebraic Equation
global u a kg k;
y = kg*(CA-CAs) - k*CAs;
end
```

Analytical Solution

$$u\frac{dC_A}{dz} = -k_g a (C_A - C_{As}) \quad \cdots (1)$$

$$0 = k_g (C_A - C_{As}) - kC_{As} \quad \cdots (2)$$

$u=1$, $a=200$, $k_g=0.02$, $k=0.01$

$C_A(0)=1$.

From eqn. (2) :-

$$\Rightarrow C_{As} = \frac{k_g C_A}{k_g + k}$$

putting this into (1) :-

$$\frac{dC_A}{dz} = \frac{-k_g a}{u}\left(C_A - \frac{k_g C_A}{k_g + k}\right)$$

$$\int_1^{C_A} \frac{dC_A}{C_A} = \int_0^z \frac{-a}{u}\left(\frac{k k_g}{k_g + k}\right) dz$$

$$\ln C_A = -\frac{a}{u}\cdot\left(\frac{k k_g}{k_g + k}\right) z.$$

putting parameter values :-

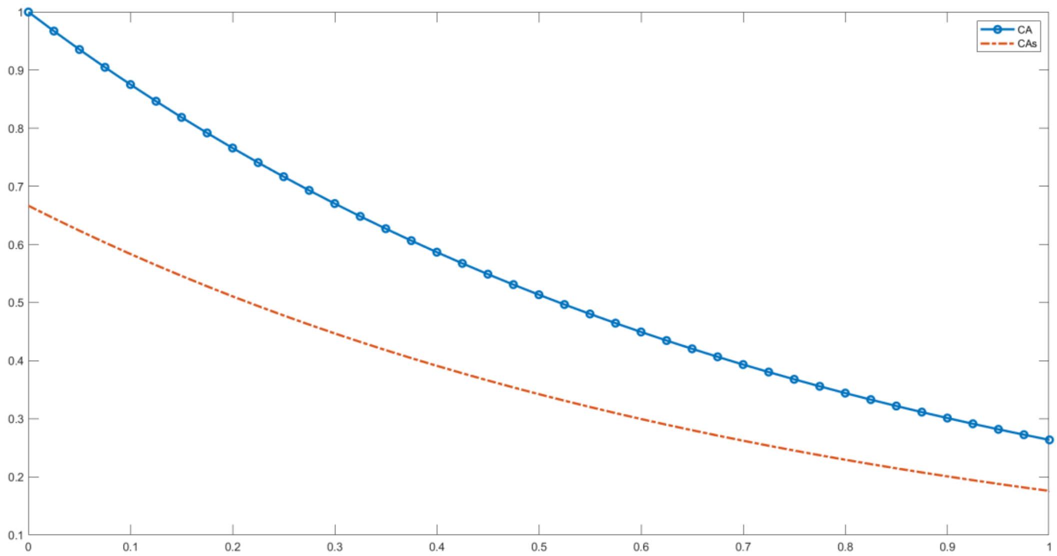
$$\ln C_A = -\frac{4}{3} z$$

$$C_A = \exp\left(-\frac{4z}{3}\right)$$

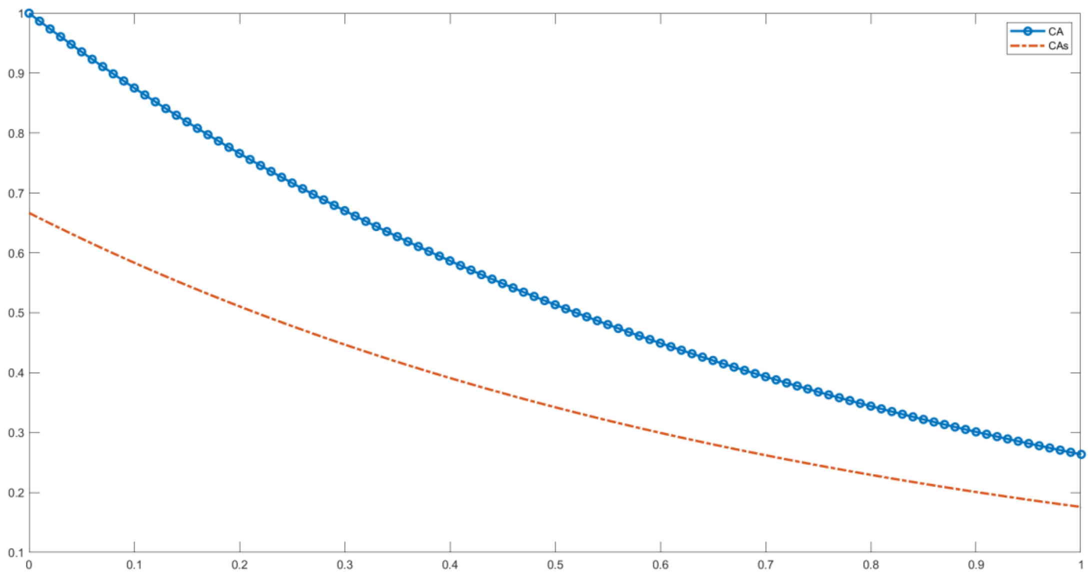
$$C_{A_S} = \frac{k_g}{k_g + k} C_A = \frac{2}{3} \exp\left(-\frac{4z}{3}\right).$$

Results

MATLAB



Analytical solution



Conclusion

The analytical solution and the numerical solution obtained using *ode45* and *fsolve* come out to be very similar. The plots are mostly same for both C_A and C_{As} using both methods. For increasing the precision further, the span could have been divided into a greater number of points but there are risks of overfitting. The given system was non stiff and linear too thus, a very simple system and thus, returned similar results. If we had stiff or non-linear or both together in a system, then systems could've returned different results by using these solvers. Non-linearity would have required convergence and thus, choosing an appropriate initial guess would've become important. There would've been additional error in the numerical methods owing to the truncation error involved in the methods. This kind of systems can also exist in process control systems, where we need to linearize the system systems by considering steady state which results in a DAE. For DAE systems with higher index, the computational complexity would have been higher.