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18CH30030

ASSIGNMENT-5

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 the catalyst surface (C_{As}) can be described as follows.

$$u\frac{dC_A}{dz} = -k_g a(C_A - C_{AS})$$

$$0 = k_g(C_A - C_{AS}) - kC_{AS}$$

Model parameters are given as: *u* = 1, *kg* = 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 above DAE using an ODE solver (say ode45) and algebraic equation solver (sat fsolve).

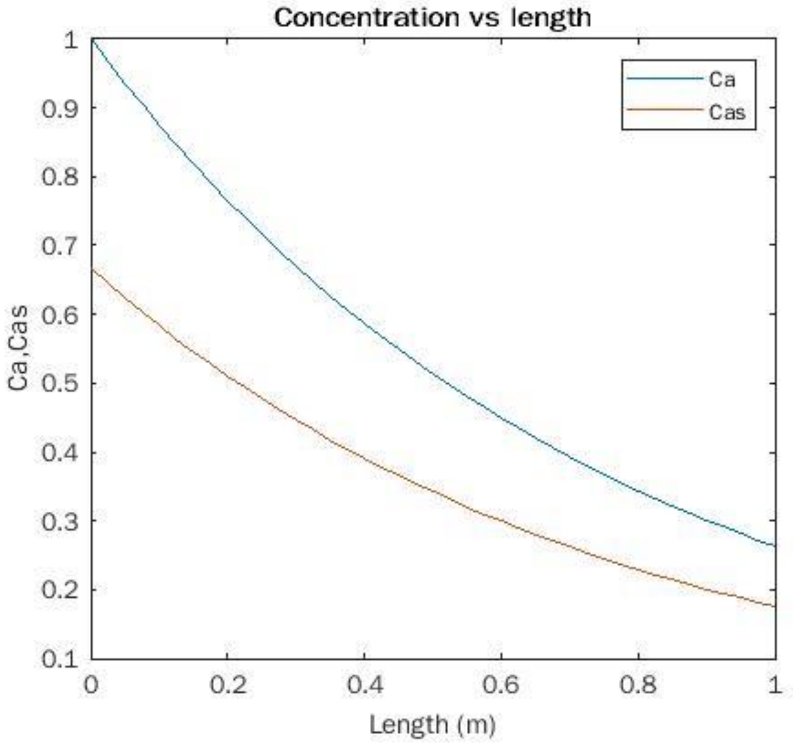
(b) Analytical solution is possible here. Compare your numerical solution with analytical solution.

SOLUTION

MATLAB Code

```
global u kg k a
u = 1;              % Parameters
kg = 0.02;
k = 0.01;
a = 200;
Ca0=1;
zspan = [0,1];

[z,y] = ode45(@(z,y) PFR(z, y), zspan,Ca0 );    % ODE Solver

plot(z,y);
hold on;
plot(z,(kg/(k+kg))*y);

function dCadz = PFR(z,y)   % Differential Equation
global u kg k a
 Ca = y;
 Cas_guess = Ca;
 Cas = fsolve(@(Cas) SurfaceReaction(Ca,Cas), Cas_guess); % Algebraic Equation Solver
 dCadz = -(kg*a/u)*(Ca - Cas);
end

function y = SurfaceReaction(Ca,Cas)     % Algebraic Equation
global u kg k a
y = kg*(Ca-Cas) - k*Cas;
end
```

PLOT (For Numerical Solution)



ANALYTICAL SOLUTION

Rearranging second equation, we get

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

Substituting this value in first equation and integrating

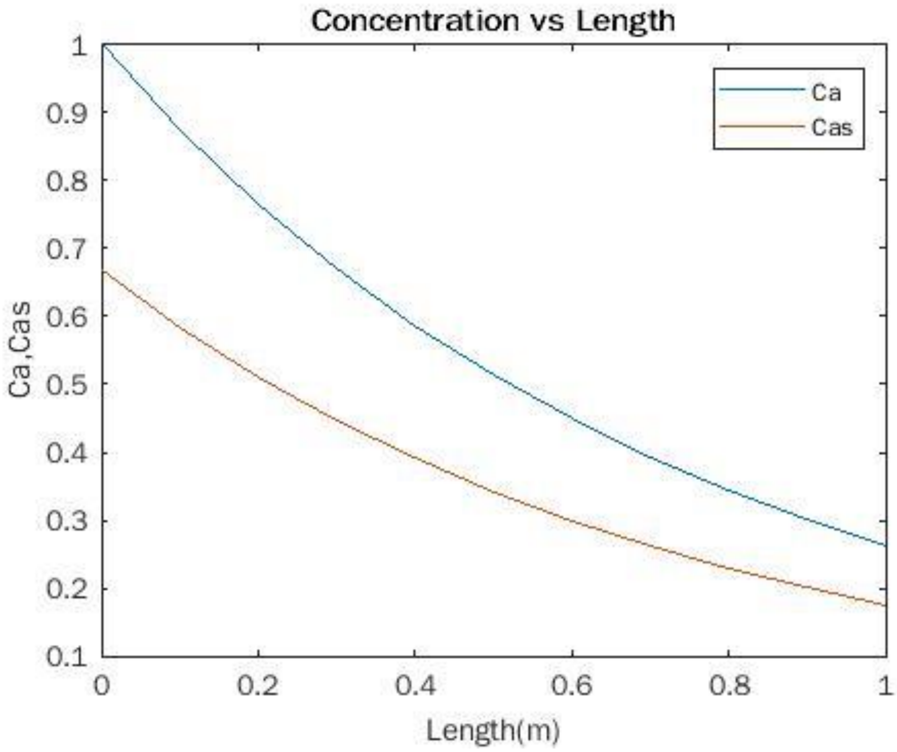
$$\int_1^{C_A} \frac{dC_A}{C_A} = -\int_0^z \frac{k k_g a\, dz}{(k_g + k)u}$$

$$lnC_A = -\frac{k k_g a}{(k_g + k)u} z$$

$$C_A = \boldsymbol{e}^{-\frac{4}{3}z} \text{ mol/L}$$

$$C_{As} = \frac{k_g\ \boldsymbol{e}^{-\frac{4}{3}z}\ \text{mol/L}}{k_g + k} = \frac{2}{3}\ \boldsymbol{e}^{-\frac{4}{3}z}\ \text{mol/L}$$

PLOT (For Analytical Solution)



CONCLUSION