Question 7 Harikrishnan R N, 18CHE147

Here I have shown how to solve the second order ordinary differential equation with two boundary conditions.

The physical phenomena is Diffusion with Chemical Reaction in one dimensional slab

Contents

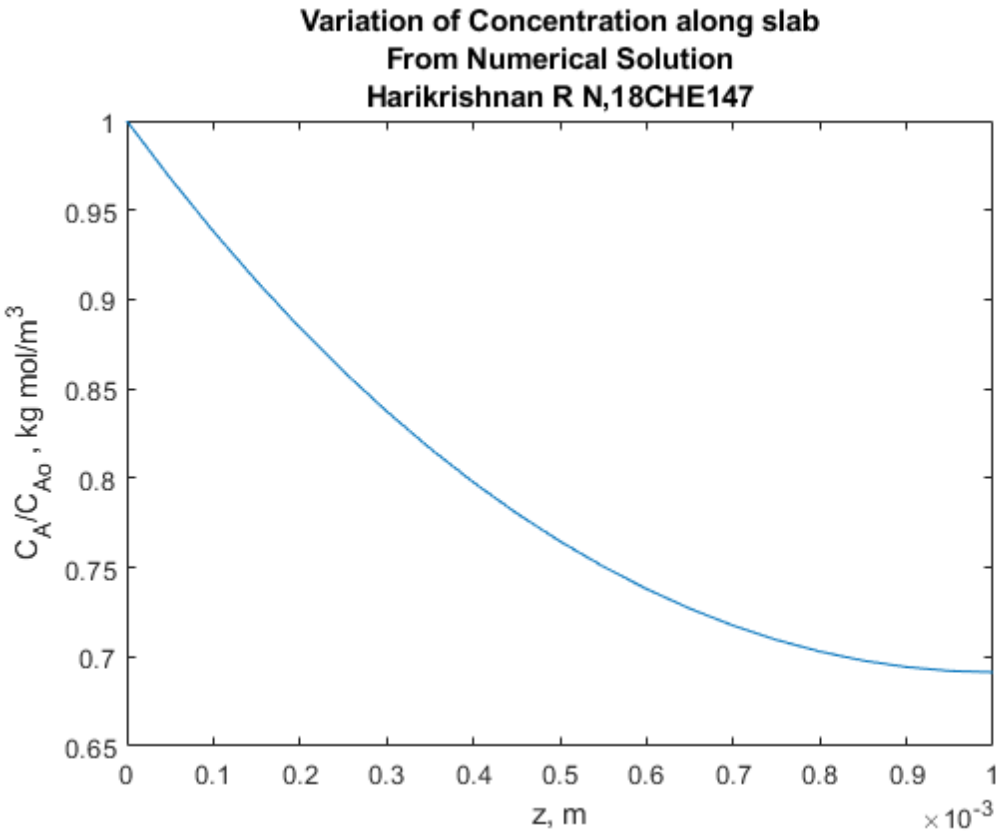
Defining Constants :

```
ca0 = 0.2 ;          % kg mol/m^3, constant concentration at surface
k = 1e-3 ;           % s^-1, homogeneous reaction rate constant
m = 1 ;              % Order of reaction
Dab = 1.2e-9 ;       % m^2/s, binary diffusion coefficient
L = 1e-3 ;           % m, distance from catalyst surface to reaction site
phi = L*(k/Dab)^0.5; % Thiele Modulus
```

Solving the Boundary Value Problem :

Here I have shown how to solve the boundary value problem

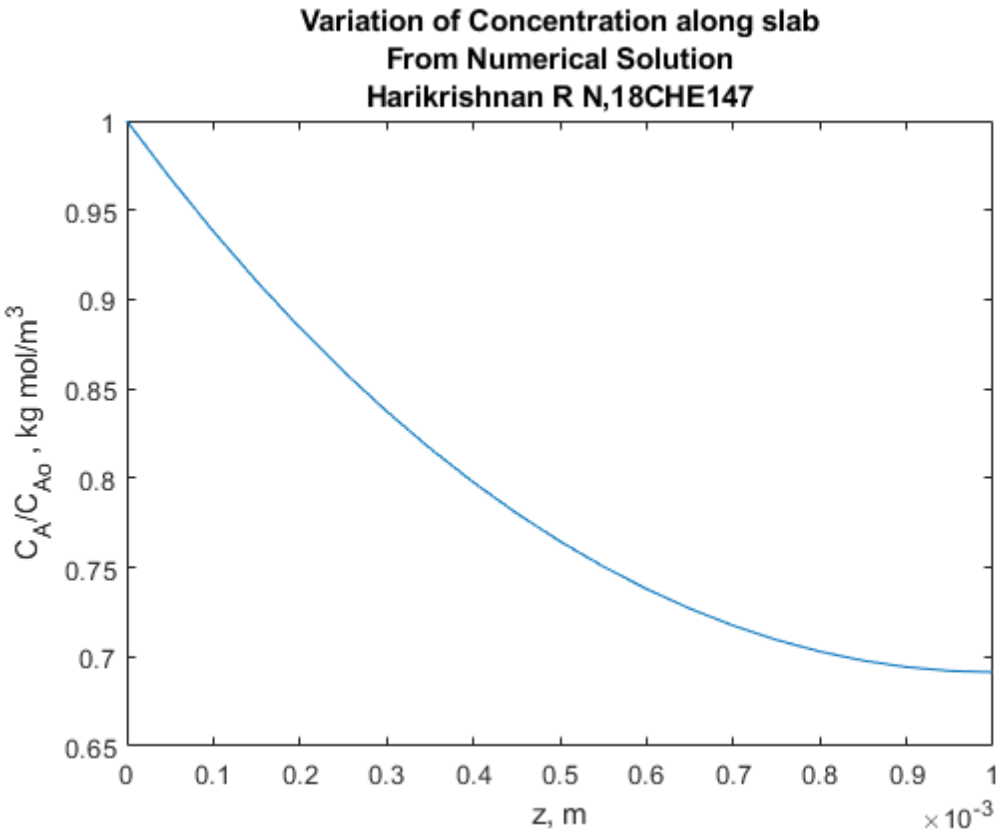
```
%First we define the scale along which we are solving the equation
n_step = 21 ;
x = linspace(0,1,n_step) ;
%Defining a function that provides initial guess for BVP :
guess = @(x) [ exp(-phi*x)
               0.*exp(-phi*x) ];
%Defining a function that provides the boundary conditions :
bcs = @(ya,yb) [ ya(1)-1
                 yb(2) ] ;
%Defining a function that provides the ODE :
odes = @(x,y) [ y(2)
                (phi^2)*y(1)^m ] ;
%Solving the BVP :
solinit = bvpinit(x ,@(x) guess(x)); % Trail solution given by guess function
sol = bvp4c(@(x,y) odes(x,y),@(ya,yb) bcs(ya,yb),solinit); % bvp solved
y = deval(sol,x) ; % Evaluating the solution to the BVP
figure
plot(x*L,y(1,:))
title({'Variation of Concentration along slab';'From Numerical Solution';'Harikrishnan R N,18CHE147'});
xlabel('z, m') ; ylabel('C_{A}/C_{Ao} , kg mol/m^{3}');
```

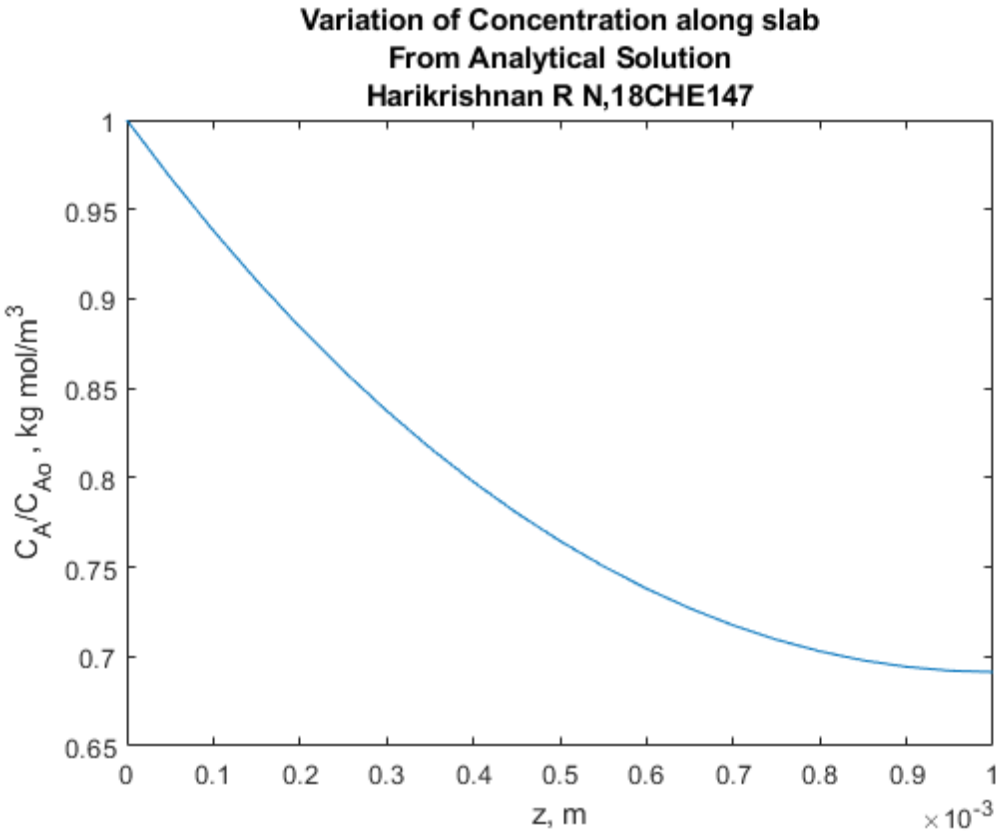


Comparing with the Analytical Solution :

Here we will compare the above obtained numerical solution with the analytical solution.

```
Ca =  cosh(phi*(1-x))/cosh(phi) ;
figure
plot(x*L,Ca)
title({'Variation of Concentration along slab';'From Analytical Solution';'Harikrishnan R N,18CHE147'});
xlabel('z, m') ; ylabel('C_{A}/C_{Ao} , kg mol/m^{3}');
```





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