Solution of Multi-System Advection-Diffusion Partial Differential Equations using Danckwerts Boundary Conditions

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Abstract

The study presents a numerical solution for a system of multi-species advection-diffusion partial differential equations subjected to Danckwerts boundary conditions. The advection-diffusion equation governs the transport of chemical species in fluid systems, incorporating both convection and diffusion effects. A three-equation system is discretized using the finite difference approximation (FDA) and solved in MATLAB to analyze species concentration profiles over time in an axial flow reactor. The numerical results are visualized through contour plots, illustrating the spatial and temporal evolution of species concentrations. The findings highlight the interaction between advection-dominated transport and diffusion-driven dispersion, with reaction kinetics influencing the transformation of species. The approach demonstrates the effectiveness of computational methods in modeling coupled transport-reaction systems and provides insights into the role of boundary conditions in maintaining realistic species distributions.

1 Introduction

The convection–diffusion equation is a parabolic partial differential equation that combines the diffusion and convection, also referred to as advection equations. It describes physical phenomena where particles, energy, or other physical quantities are transferred inside a physical system due to two processes: diffusion and convection [1]. Generally, the same equation can be called the advection–diffusion equation, drift–diffusion equation, or scalar transport equation. The general form of Advection-Diffusion equation in conservative form is given as:

$$\frac{\partial c}{\partial t} = \nabla.(D\nabla c - vc) + R \tag{1}$$

Where

- c is the variable of interest (species concentration for mass transfer, temperature for heat transfer)

- D is the diffusivity (also called diffusion coefficient), such as mass diffusivity for particle motion or thermal diffusivity for heat transport
- v is the velocity field that the quantity is moving with. It is a function of time and space. For example, in advection, c might be the concentration of salt in a river, and then v would be the velocity of the water flow as a function of time and location. Another example, c might be the concentration of small bubbles in a calm lake, and then v would be the velocity of bubbles rising towards the surface by buoyancy (see below) depending on time and location of the bubble. For multiphase flows and flows in porous media, v is the (hypothetical) superficial velocity.
- R describes sources or sinks of the quantity c, i.e. the creation or destruction of the quantity. For example, for a chemical species, R $R > 0$ 0 means that a chemical reaction is creating more of the species, and $R < 0$ means that a chemical reaction is destroying the species. For heat transport, $R > 0$ might occur if thermal energy is being generated by friction.
- ∇ represents gradient and $\nabla\cdot$ represents divergence. In this equation, ∇c represents concentration gradient [2, 3].

2 Three-Equation Advection-Diffusion Equation System (Axial Dispersion)

The system of equations can be written as:

$$\frac{\partial C_A}{\partial t} = D_A \frac{\partial^2 C_A}{\partial x^2} - U\frac{\partial C_A}{\partial x} - k_1 C_A \tag{2}$$

$$\frac{\partial C_B}{\partial t} = D_B \frac{\partial^2 C_B}{\partial x^2} - U\frac{\partial C_B}{\partial x} + k_1 C_A - k_2 C_B \tag{3}$$

$$\frac{\partial C_C}{\partial t} = D_C \frac{\partial^2 C_B}{\partial x^2} - U\frac{\partial C_C}{\partial x} + k_2 C_B \tag{4}$$

The above system is subjected to Danckwerts boundary conditions at x=0 aer defined as:

$$C_{A0} = \frac{-D_A}{U}(\frac{\partial C_A}{\partial x})_{x=0} + C_A(1); C_B(1) = 0; C_C(1) = 0 \tag{5}$$

The boundary conditions at x=L are defined as:

$$(\frac{\partial C_A}{\partial x})_{x=L} = (\frac{\partial C_B}{\partial x})_{x=L} = (\frac{\partial C_C}{\partial x})_{x=L} = 0 \tag{6}$$

The system of advection-diffusion equations can be subjected to discretization using Finite Difference Approximation (FDA) of first and second order in centered configuration.

$$\frac{\partial C_A}{\partial t} = D_A \frac{C_A(i+1) - 2C_A(i) + C_A(i-1)}{\Delta x^2} - U\frac{C_A(i+1) - C_A(i-1)}{2\Delta x} - k_1 C_A(i) \tag{7}$$

$$\frac{\partial C_B}{\partial t} = D_A \frac{C_B(i+1) - 2C_B(i) + C_B(i-1)}{\Delta x^2} - U \frac{C_B(i+1) - C_B(i-1)}{2\Delta x} + k_1 C_A(i) - k_2 C_B(i) \tag{8}$$

$$\frac{\partial C_C}{\partial t} = D_C \frac{C_C(i+1) - 2C_C(i) + C_C(i-1)}{\Delta x^2} - U \frac{C_C(i+1) - C_C(i-1)}{2\Delta x} + k_2 C_B(i) \tag{9}$$

Applying Second order FDA in forward configuration on boundary conditions at x=0, result in:

$$C_A(1) = \frac{D_A}{U}\left(\frac{-3C_A(3) + 4C_A(2) - 3C_A(1)}{2\Delta x}\right) + C_{A,in} = \frac{C_{A,in} - C_A(3)\frac{D_A}{2\Delta x U} + C_A(2)\frac{4D_A}{2\Delta x U}}{\left(1 + \frac{3D_A}{2\Delta x U}\right)} \tag{10}$$

$$C_B(1) = C_C(1) = 0 \tag{11}$$

Applying Second order FDA in reverse configuration on boundary conditions at x=L, result in:

$$\left(\frac{\partial C_A}{\partial x}\right)_{x=L} = \frac{3C_A(end) - 4C_A(end-1) + C_A(end-2)}{2\Delta x} = 0 \tag{12}$$

$$C_A(end) = \frac{4C_A(end-1) - C_A(end-2)}{3} \tag{13}$$

$$C_B(end) = \frac{4C_B(end-1) - C_B(end-2)}{3} \tag{14}$$

$$C_C(end) = \frac{4C_C(end-1) - C_C(end-2)}{3} \tag{15}$$

Table 1: Constant Term Values

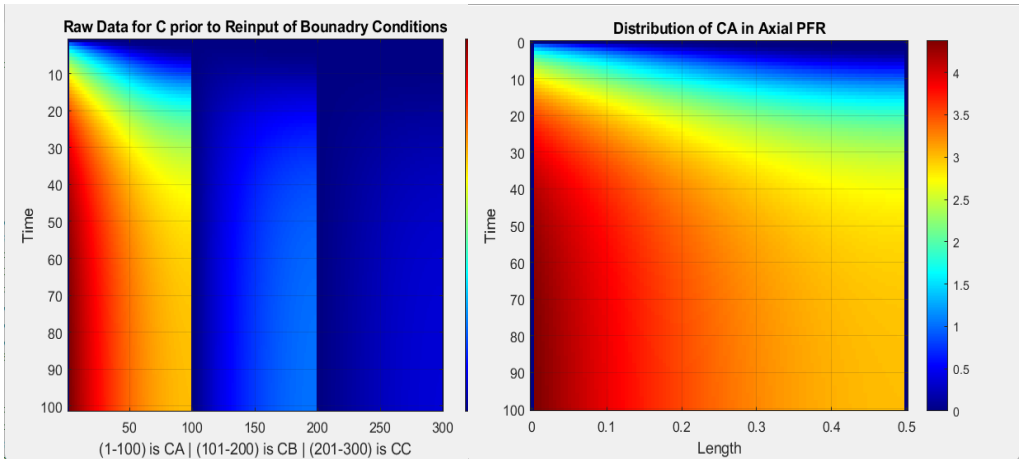
$D=D_A=D_B=D_C$	0.01 m^2/min
U	0.01 m^2/min
L	0.5 m
k_1	0.04 L/min
k_2	0.02 L/min
$C_{a,in}$	10 mol/L

```
clc
clear
close all
%Required Data
D=0.01;
U=0.01;
L=0.5;
k1=0.04;
k2=0.04;
```

```
CAin=10;
%Defining of Step Size for Position
Nx=100;
x=linspace(0,L,Nx);
dx=x(2)-x(1);
%Time Trajectory
t=0:100; %100 minutes worth of time
%Initial Condition
IC_A=zeros(1,Nx); %For CA
IC_B=zeros(1,Nx); %For CB
IC_C=zeros(1,Nx); %For CC
IC=[IC_A,IC_B,IC_C];
%ODE Solver
[t,c]=ode15s (@f,t,IC,[],CAin,D,U,k1,k2,dx,Nx);
%Redifining of Values
%Defination of each value
CA=c(:,1:Nx); %For CA
CB=c(:,Nx+1:2*Nx); %For CB
CC=c(:,2*Nx+1:3*Nx);%For CC
%Input of Boundary Conditions at x=0
CA(:,1)=(CAin-D/(2*U*dx)*CA(3)+4*D*CA(2)/2/dx/U)./(1+3*D/2/U/dx);
CB(:,1)=0;
CC(:,1)=0;
%Bounadry conditions for x=L
CA(:,end)=(4*CA(end-1)-CA(end-2))./3;
CB(:,end)=(4*CB(end-1)-CB(end-2))./3;
CC(:,end)=(4*CC(end-1)-CC(end-2))./3;
figure(1) %For Raw Data
imagesc(c)
colormap jet
colorbar
grid on
title('Raw Data for C prior to Reinput of Bounadry Conditions')
xlabel('(1-100) is CA | (101-200) is CB | (201-300) is CC')
ylabel('Time')
figure (2) %For CA
imagesc(x,t,CA)
colormap jet
colorbar
grid on
title('Distribution of CA in Axial PFR')
xlabel('Length')
ylabel('Time')
figure (3)
imagesc(x,t,CB)
colormap jet
colorbar
grid on
title('Distribution of CB in Axial PFR')
xlabel('Length')
ylabel('Time')
figure (4)
imagesc(x,t,CC)
colormap jet
colorbar
grid on
title('Distribution of CC in Axial PFR')
```

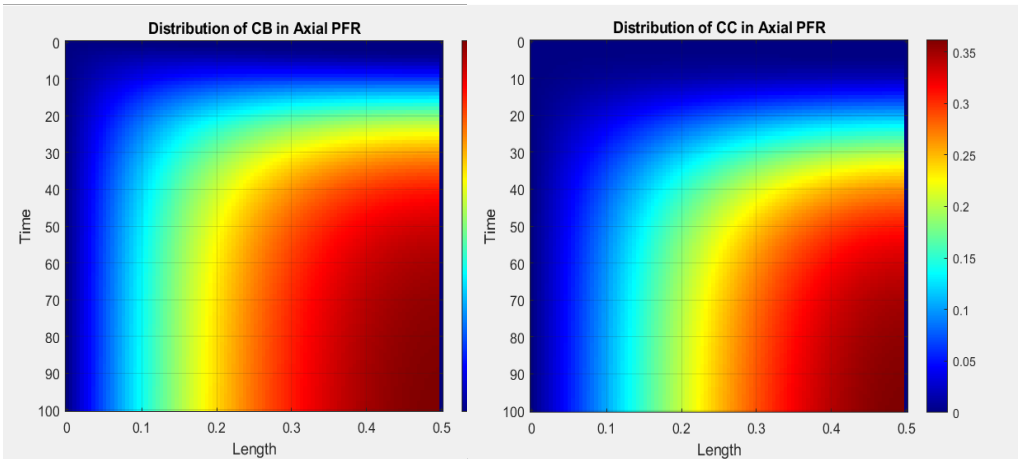
```
xlabel('Length')
ylabel('Time')
function dcdt=f(t,c,CAin,D,U,k1,k2,dx,Nx)
dcdt=zeros(length(c),1);
dCAdt=zeros(Nx,1);
dCBdt=zeros(Nx,1);
dCCdt=zeros(Nx,1);
%Defination of each value
CA=c(1:Nx); %For CA
CB=c(Nx+1:2*Nx); %For CB
CC=c(2*Nx+1:3*Nx);%For CC
%Input of Boundary Conditions at x=0
CA(1)=(CAin-D/(2*U*dx)*CA(3)+4*D*CA(2)/2/dx/U)./(1+3*D/2/U/dx);
CB(1)=0;
CC(1)=0;
%Bounadry conditions for x=L
CA(end)=(4*CA(end-1)-CA(end-2))./3;
CB(end)=(4*CB(end-1)-CB(end-2))./3;
CC(end)=(4*CC(end-1)-CC(end-2))./3;
%Interior Operation
for i=2:Nx-1
    dCAdt(i)=D*(CA(i+1)-2*CA(i)+CA(i-1))./dx^2-U*(CA(i+1)-CA(i-1))
    ./2/dx-k1*CA(i);
    dCBdt(i)=D*(CB(i+1)-2*CB(i)+CB(i-1))./dx^2-U*(CB(i+1)-CB(i-1))
    ./2/dx-k2*CB(i)+k1*CA(i);
    dCCdt(i)=D*(CC(i+1)-2*CC(i)+CC(i-1))./dx^2-U*(CC(i+1)-CC(i-1))
    ./2/dx+k2*CB(i);
end
dcdt=[dCAdt;dCBdt;dCCdt];
end
```

Listing 1: Three-Equation Advection-Diffusion System



(a) Raw Data for Concentrations (b) Distribution of C_A in Axial PFR

Figure 1: Concentration Profile Contours



(a) Distribution of C_B in Axial PFR (b) Distribution of C_C in Axial PFR

Figure 2: Concentration Contours

3 Conclusion

The study explores the numerical solution of a multi-system advection-diffusion partial differential equation subjected to Danckwerts boundary conditions. The advection-diffusion equation governs the transport of species in fluid media, where the combined effects of diffusion and convection dictate the concentration profile of reacting species. A system of three coupled equations representing the concentration evolution of different species is solved using the finite difference approximation (FDA). The discretized form of the governing equations is implemented in MATLAB, incorporating both first-order and second-order finite difference schemes for spatial derivatives. The study provides visualizations of species concentrations along the axial direction of a packed flow reactor (PFR) over time, demonstrating the impact of reaction kinetics and transport phenomena on species distribution. The contour plots generated offer insights into concentration variations and highlight regions where diffusion or advection dominates, reinforcing the interplay of physical transport and chemical reaction mechanisms. The results obtained from the concentration contours indicate distinct transport behaviors for the three species. The distribution of species A demonstrates an initial steep decline, confirming its rapid consumption due to reaction kinetics. Species B exhibits a transient peak as it is formed from species A and subsequently consumed to generate species C. The final species, C, accumulates over time, following the expected reaction pathway. The contour plots effectively highlight the dominance of advection in the axial transport, where concentration profiles shift progressively along the reactor length. Diffusion effects, though present, contribute primarily to smoothing the concentration gradients rather than significantly altering the bulk transport characteristics. The implementation of Danckwerts boundary conditions ensures physically realistic

inflow and outflow behavior, preventing unphysical reflections at the domain boundaries. The study underscores the utility of numerical methods in solving coupled transport-reaction problems, providing a framework applicable to a wide range of engineering and environmental systems involving advection-diffusion processes.

References

[1] Chandrasekhar, S. Stochastic problems in physics and astronomy. *Rev. Mod. Phys. 15* (Jan 1943), 1–89.

[2] Jr., C. E. B., Gershtein, V., and Li, X. J. *Computational Fluid Dynamics in Industrial Combustion*. CRC Press, 2001.

[3] Wesseling, P. *Principles of Computational Fluid Dynamics*, 1 ed. Springer, 3 2009.