Solution of Multi-System Advection-Diffusion Partial Differential Equations

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Abstract

The advection-diffusion equation governs numerous transport phenomena, encompassing heat, mass, and momentum transfer in physical and engineering systems. This study examines a three-equation system of advection-diffusion partial differential equations , representing an axial dispersion process with reaction kinetics. The system is solved using the MATLAB ***pdepe*** function, involving Danckwerts-Dirichlet-Neumann boundary conditions to ensure physical realism. The numerical solution provides insights into species concentration evolution over time and space. The results are visualized using contour and mesh plots, highlighting important transport mechanisms and reaction-diffusion interactions. This work contributes to the computational modeling of multi-component transport systems, which are essential in chemical engineering, environmental studies, and biomedical applications.

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:

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

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

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

By the application of Danckwerts-Dirichlet-Neumann Boundary Conditions: The initial conditions are:

$$t = 0; x = x; c = 0 \tag{5}$$

Boundary conditions at x=0 can be written as:

$$C_A(1) = C_{Ain} + \frac{D_A}{U}(\frac{\partial C_A}{\partial x})_{x=0}; C_B(1) = 0; C_C(1) = 0 \tag{6}$$

Boundary conditions for x=L can be written as:

$$(\frac{\partial C_A}{\partial x})_{x=L} = (\frac{\partial C_B}{\partial x})_{x=L} = (\frac{\partial C_C}{\partial x})_{x=L} = 0 \tag{7}$$

The reference values to constant terms involved in the expression are given as:

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

3 Solution using pdepe MATLAB Library

The general form of pdepe MATLAB equation form is given as:

$$c(x,t,u,\frac{\partial u}{\partial x})\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}(x^m f(x,t,u,\frac{\partial u}{\partial x})) + s(x,t,u,\frac{\partial u}{\partial x}) \tag{8}$$

Here:

$$c = \frac{\partial C_A}{\partial t}, \frac{\partial C_B}{\partial t}, \frac{\partial C_C}{\partial t}$$

$$f = D_A, D_B.D_C$$

$$s = -U\frac{\partial C_A}{\partial t} - k_1 C_A, -U\frac{\partial C_B}{\partial t} + k_1 C_A - k_2 C_B, -U\frac{\partial C_C}{\partial t} + k_2 C_B$$

Here, the Danckwerts Boundary Condition is given as:

$$C_A(1) = C_{Ain} + \frac{D_A}{U}(\frac{\partial C_A}{\partial x})_{x=0} \tag{9}$$

The Dirichlet Boundary Conditions are given as:

$$C_B(1) = 0; C_C(1) = 0 \tag{10}$$

The Neumann Boundary Conditions are given as:

$$(\frac{\partial C_A}{\partial x})_{x=L} = (\frac{\partial C_B}{\partial x})_{x=L} = (\frac{\partial C_C}{\partial x})_{x=L} = 0 \tag{11}$$

```
    clc;
clear;
close all;
x=linspace(0,0.5,101); %Length
t=linspace(0,100,151); %Time in minutes
m=0;

sol=pdepe(m,@pdefun,@icfun,@bcfun,x,t);
CA=sol(:,:,1);
CB=sol(:,:,2);
CC=sol(:,:,3);

figure(1);
imagesc(x,t,CA);
```

```
colormap hot;
colorbar;
grid on
title('Profile for C_A in mol/m^3');
xlabel('Length (m)');
ylabel('Time (s)');

figure(2);
imagesc(x,t,CB);
colormap hot;
colorbar;
grid on
title('Profile for C_B in mol/m^3');
xlabel('Length (m)');
ylabel('Time (s)');

figure(3);
imagesc(x,t,CC);
colormap hot;
colorbar;
grid on
title('Profile for C_C in mol/m^3');
xlabel('Length (m)');
ylabel('Time (s)');

figure(4);
mesh(x,t,CA);
colormap hot;
colorbar;
grid on
title('Profile for C_A in mol/m^3');
xlabel('Length (m)');
ylabel('Time (s)');

figure(5);
mesh(x,t,CB);
colormap hot;
colorbar;
grid on
title('Profile for C_B in mol/m^3');
xlabel('Length (m)');
ylabel('Time (s)');

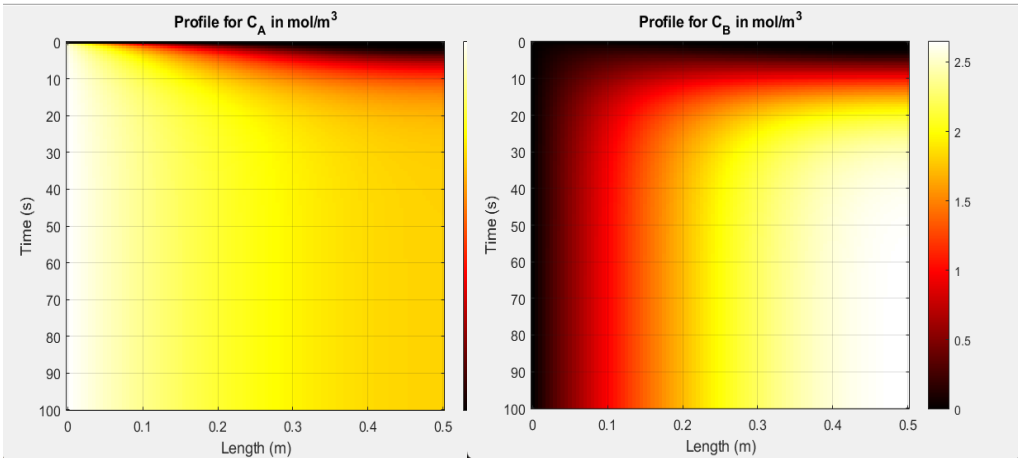
figure(6);
mesh(x,t,CC);
colormap hot;
colorbar;
grid on
title('Profile for C_C in mol/m^3');
xlabel('Length (m)');
ylabel('Time (s)');

%Building of functions for PDEs
function[c,f,s]=pdefun(x,t,u,dudx)
%Input of Data
D=0.01;
U=0.01;
```

```
k1=0.04;
k2=0.02;
CAin=10;
c=ones(3,1);
f=[D*dudx(1);
    D*dudx(2);
    D*dudx(3)];

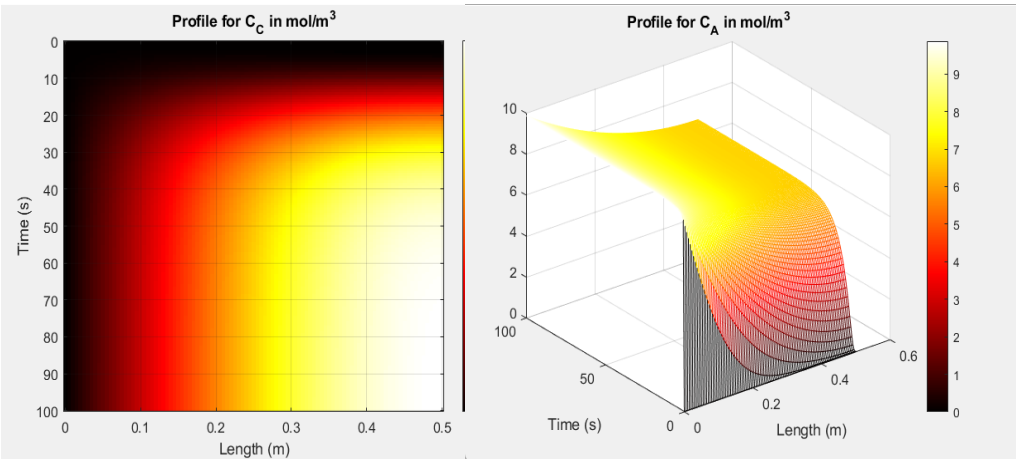
s=[-U*dudx(1)-k1*u(1);
    -U*dudx(2)+k1*u(1)-k2*u(2);
    -U*dudx(3)+k2*u(2)];
end
%Function building for Initial Condition
function u0=icfun(x)
u0=zeros(3,1);
end
%FUnction building for Boundary Conditions
function[p1,q1,pr,qr]=bcfun(x1,u1,kr,ur,t)
CAin=10;
D=0.01;
U=0.01;
p1=[u1(1)-CAin;u1(2);u1(3)];
q1=[-D/U;0;0];
pr=zeros(3,1);
qr=ones(3,1);
end
```

Listing 1: Three-Equation Advection-Diffusion System



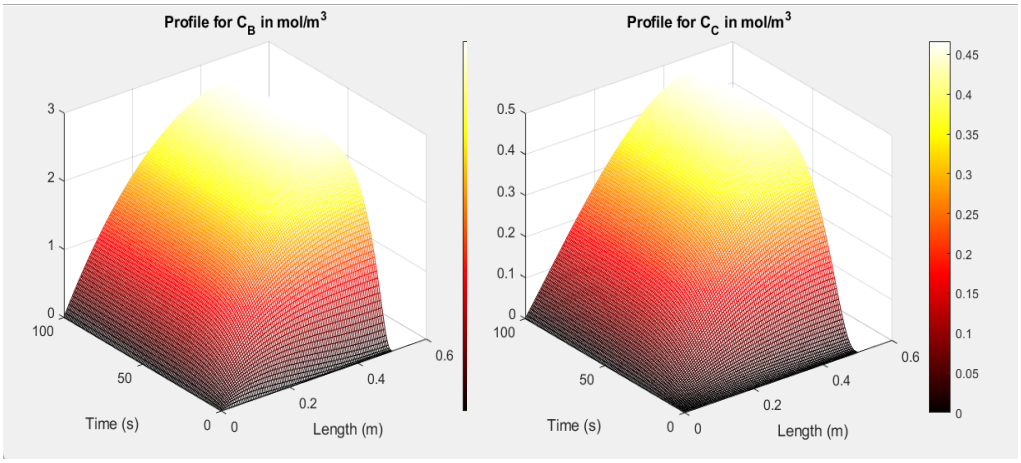
(a) Concentration Profile for C_A (b) Concentration Profile for C_B

Figure 1: Concentration Profile Contours



(a) Concentration Profile for C_C (b) Mesh Profile for C_A

Figure 2: Concentration Contour and Mesh Profiles



(a) Mesh Profile for C_B (b) Mesh Profile for C_C

Figure 3: Mesh Profiles for Concentration Contours

4 Conclusion

The numerical analysis of the multi-species advection-diffusion system provides valuable insights into the complex interplay of diffusion, convection, and reaction kinetics. The results demonstrate that species concentrations evolve dynamically under the influence of axial dispersion and reaction rate parameters. The transformation of species C_A into C_B and C_C highlights the impact of reaction kinetics, where the rate constants k_1 and k_2 governthe extent and

speed of conversion. The boundary conditions play a crucial role in shaping the concentration profiles, with the Danckwerts condition ensuring proper flux balance at the inlet and the Neumann conditions preventing artificial losses at the outlet. The MATLAB pdepe solver proves to be an effective computational tool for capturing spatial and temporal variations, preserving numerical stability while resolving steep concentration gradients. The concentration contour and mesh plots illustrate the transport mechanisms at play, showing the progressive diffusion of species and their reaction-driven transformations. These findings have practical implications in fields such as environmental engineering, where pollutant dispersion must be accurately modeled, and in chemical engineering, where reaction-diffusion systems govern catalytic processes and chromatographic separations. While the current model provides a robust framework for analyzing advection-diffusion systems, future research can explore non-linear reaction kinetics, variable diffusivity, and multi-phase interactions to extend its applicability to more complex real-world scenarios.

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.