Solution of Fix Bed Reactor Partial Differential Equation using Danckwerts Boundary Conditions

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Abstract

Fixed-bed reactors are widely used in industrial catalytic processes due to their efficiency in facilitating chemical reactions. The governing transport phenomena within these reactors can be described using partial differential equations (PDEs), which account for diffusion, convection, and reaction kinetics. This study focuses on solving the PDE governing the concentration profile in a fixed-bed reactor using the finite difference method with Danckwerts boundary conditions. The numerical approach implemented in MATLAB employs a discretized form of the PDE, allowing for an accurate representation of the concentration distribution over time and space. The results are visualized using concentration contour plots, providing insights into the impact of Peclet and Damköhler numbers on reactor performance. This approach enables a deeper understanding of mass transport in fixed-bed reactors, offering a valuable tool for optimizing reactor design and operation.

1 Introduction

A fixed bed reactor is a cylindrical tube filled with catalyst pellets with reactants flowing through the bed and being converted into products. The catalyst may have multiple configuration including: one large bed, several horizontal beds, several parallel packed tubes, multiple beds in their own shells. The various configurations may be adapted depending on the need to maintain temperature control within the system. Serial connection of two reactors with option to dose oxidant between the stages enable under optimal conditions to increase the product yield in oxidation catalysis.By dosing intermediates or products between the stages, valuable information could be found concerning the reaction pathways [1]. The catalyst pellets may be spherical, cylindrical, or randomly shaped pellets. They range from 0.25 cm to 1.0 cm in diameter. The flow of a fixed bed reactor is typically downward. The partial differential equation governing the concentration of reactant enclosed in a flat bed reactor with respect to time is given by following equation:

$$\frac{\partial C}{\partial t} = \frac{1}{Pe}\frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial x} - Da\frac{C}{C+v} \tag{1}$$

subjected to initial condition of:

$$C(x,0) = 0 \tag{2}$$

and boundary conditions as:

$$-\frac{1}{Pe}\frac{\partial C}{\partial x}(0,t) = 1 - C(0,t) \quad \frac{\partial C}{\partial x}(1,t) = 0 \tag{3}$$

Through finite difference approximation in centered configuration, the partial differentiation expressions of concentration with respect to displacement "x" are given as:

$$\frac{\partial^2 C}{\partial x^2} = \frac{C(i+1) - 2C(i) + C(i-1)}{\Delta x^2} \tag{4}$$

$$\frac{\partial C}{\partial x} = \frac{C(i+1) - C(i-1)}{2\Delta x} \tag{5}$$

$$\frac{\partial C}{\partial t} = \frac{1}{Pe}\frac{C(i+1) - 2C(i) + C(i-1)}{\Delta x^2} - \frac{C(i+1) - C(i-1)}{2\Delta x} - Da\frac{C(i)}{C(i) + v} \tag{6}$$

Applying forward scheme of finite difference approximation on boundary condition as x=0, the expression results in:

$$-\frac{1}{Pe}\frac{\partial C}{\partial x}(0,t) = 1 - C(0,t) \rightarrow -\frac{1}{Pe}\frac{C(2) - C(1)}{\Delta x} = 1 - C(1) \tag{7}$$

$$C(1) = \frac{Pe\Delta x + C(2)}{Pe\Delta x + 1} \tag{8}$$

By backward finite difference approximation on the other boundary condition at x=1, the expression becomes:

$$\frac{\partial C}{\partial x}(1,t) = 0 \rightarrow \frac{C(end) - C(end-1)}{\Delta x} = 0 \tag{9}$$

```
    clc;
clear;
close all;
%Dimensionless Number Values
Pe=200; %Peclet Number
Da=2; %Damkohler Number
v=2; %Kinematic viscosity

Nx=200; %Size
L=1; %Length

x=linspace(0,L,Nx);
dx=x(2)-x(1);
tf=2; %Time delay
Nt=101;
t=linspace(0,tf,101);

%Initial Condition
IC=zeros(1,Nx);

[t,C]=ode15s(@fpde,t,IC,[],Nx,dx,Pe,v,Da);
C(:,1)=(Pe.*dx+C(:,2))./(Pe.*dx+1);
C(:,end)=C(:,end-1);

figure(1)
imagesc(x,t,C)
colormap jet
colorbar
title('Concentration Profile at x and t');
xlabel('Length')
ylabel('Time')
grid on

function dCdt=fpde(t,C,Nx,dx,Pe,v,Da)
dCdt=zeros(Nx,1);
C(1)=(Pe.*dx+C(2))./(Pe.*dx+1);
C(end)=C(end-1);

for i=2:Nx-1
    dCdx(i)=(C(i+1)-C(i-1))./2./dx;

    d2Cdx2(i)=(C(i+1)-2*C(i)+C(i-1))./dx.^2;

    dCdt(i)=1./Pe.*d2Cdx2(i)-dCdx(i)-Da.*C(i)./(C(i)+v);

end
end

```

Listing 1: Flat Bed Reactor PDE Code using Danckworth Boundary Conditions

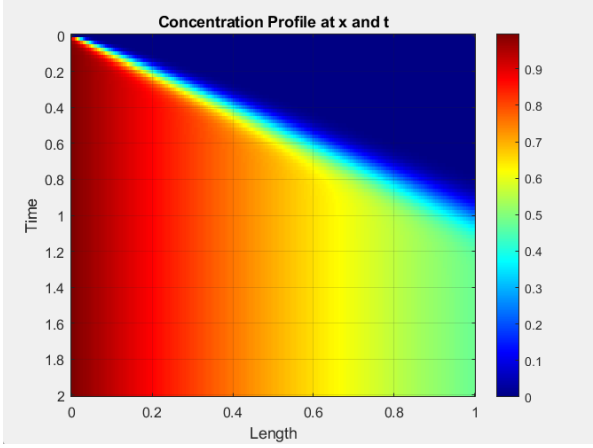


Figure 1: Concentration Contour

2 Conclusion

This study effectively implements a numerical solution to the partial differential equation governing concentration distribution in a fixed-bed reactor using the finite difference method under Danckwerts boundary conditions. The MATLAB-based approach accurately captures the effects of diffusion, convection, and reaction kinetics within the reactor, offering valuable insights into the transport phenomena at play. The results highlight the influence of Peclet and Damköhler numbers on concentration profiles, demonstrating how changes in these dimensionless parameters affect mass transfer and reaction efficiency.

The generated concentration contour plot provides a visual representation of how reactant concentration evolves along the reactor length over time. A steeper concentration gradient near the inlet suggests strong reactant consumption due to the chemical reaction, while the gradual decrease along the reactor length indicates the effect of diffusion and convection balancing out. The contour also reveals that for high Peclet numbers, advection dominates, leading to a sharper front of reactant depletion, whereas lower Peclet numbers result in smoother concentration variations due to increased dispersion. Similarly, higher Damköhler numbers indicate rapid reaction rates, reducing reactant concentration more significantly in the initial reactor section.

These findings underscore the importance of optimizing Peclet and Damköhler numbers to control reactor performance and ensure efficient reactant utilization. The developed numerical model serves as a foundation for further studies, potentially incorporating additional effects such as heat transfer, multi-species reactions, and catalyst deactivation.

References

[1] Csepei, L.-I. Kinetic studies of propane oxidation on mo and v based mixed oxide catalyst. Master's thesis, Technical University of Berlin, 2011.