Experiment and Simulation on Zr_2Fe Bed for Tritium Capturing

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```
function PDE1Dd_pdepe

% using pdepe()in MATLAB software to solve the one-dimension
differential equation

global D A B

global ua ub v Rp fi

D=1.63*10^-4;                    % dispersion coefficient/ m2/s

dp=150*10^-6;                    % mean Zr2Fe particle/ m

ua =1.12;                        %initial concentration/ mol/m3

ub = 0;                          % exhaust gas concentration/ mol/m3

m = 0;

a = 0;

b = 0.1;                         % bed length/ m

fi=0.014;                        % bed diameter/m

v=0.02;                           %gas velocity/  m/s

t0 = 0.1;

tf = 400;

x = linspace(a,b,100);

t = linspace(t0,tf,100);
```

```
k=0.85;                              % coefficiency constant of reaction

to=3000;                             % time at the 87.3% accounts

tao=1-(1-k*sqrt(t/to)).^3;

dtao=3*k/to*(1-k*(t/to).^(1/2)).^2 .*(t/to).^(-1/2);
                                     %the fitted kinetics equation

epslon=0.5;                          % the bed porosity

rou=6900;                            % applied Zr2Fe density/ kg/m3

Rp=dtao*rou*epslon.*v*3.14*(fi/2).^2/2;

sol = pdepe(m,@PDEfun,@ICfun,@BCfun,x,t);

% Extract the first solution component as u.  This is not necessary

% for a single equation, but makes a point about the form of the
output.

u = sol(:,:,1);

% surface plot of the solution

figure;

surf(x,t,u);

title('Numerical solution computed with mesh points.');

xlabel('Length x/m');

ylabel('Time t/day');


% solution profile at t=end

figure;

plot(x,u(20,:),x,u(40,:),x,u(55,:));

title('Solutions at different time.');
```

```
legend('concentration profile',0);

xlabel('Distance x/m');

ylabel('u(x,t)');

% solution profile at x=70

figure;

plot(t,u(:,80),'red*');

title('Solutions at different locations.');

legend('concentration profile',0);

xlabel('Distance t/day');

ylabel('u(t,0.08)');


% -----------------------------------------------------------------

function [c,f,s] = PDEfun(x,t,u,DuDx)

global D v Rp

c = 1/D;

f = DuDx;

s =-v/D*DuDx-1/D*Rp;


% -----------------------------------------------------------------

function u0 = ICfun(x)

u0 = 0;     % degree centigrade


% -----------------------------------------------------------------
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```
function [pl,ql,pr,qr] = BCfun(xl,ul,xr,ur,t)

global ua ub v D

pl = ul-ua;

ql =0;

pr = ur-ub;

qr = 0;
```