M A T L A B

Plate Theory Simulation

Introduction

- Liquid chromatography
  - Used in protein analysis and production.
- Ion exchange chromatography
  - Basic principle : distribution of solute between stationary phase and mobile phase by way of electrical interaction of resin and protein.

Plate model simulation

- Adsorbed protein concentration in stationary phase at equilibrium.

$$C_S = K(C, I) \cdot C$$

- Mass balance at n-step

$$\nu \cdot [C_{n-1} - C_n] = \frac{V_0}{N_P} \cdot \frac{dC_n}{dt} + \frac{V_t - V_0}{N_P} \cdot \frac{dC_{S,n}}{dt}$$

$$\theta = t \cdot \nu / V_0 , \quad H = (V_t - V_0)/V_0$$

$$C_{n-1} - C_n = \frac{1}{N_P} \cdot \frac{dC_n}{d\theta} + \frac{H}{N_P} \cdot \frac{dC_{S,n}}{d\theta}$$

- Concentration change at n-step

$$\frac{dC_n}{d\theta} = \frac{N_P \cdot (C_{n-1} - C_n) - H \cdot C_n \cdot (dK / dI)_N (dI / d\theta)}{1 + H \cdot (K + C_n (dK / dC)_n)}$$

- Ion strength

$$I = I_e \qquad \text{for} \quad \theta \langle (1 + HK')(n / N_P)$$

$$= I_e + (\Delta I / \Delta\theta)(\theta - (1 + HK')(n / N_P)) \qquad \text{for} \quad \theta \rangle (1 + HK')(n / N_P)$$

- Initial condition

  $C_1 = C_2 = \ldots\ldots = C_{Np} = 0 \qquad \theta = 0$

- Boundary condition

  $C_0 = C_0 \qquad$ for $\quad 0 < \theta < X_0$

  $C_0 = 0 \qquad$ for $\quad \theta > X_0$

- Distribute constant of protein

$$K = A \cdot I^B + K_C$$

MATLAB program list

```
clear all
global XKE XK XIE KK H nn c0 delit Kc t0 Np
KK=0.9;
nn=20;
c0=0.8;
H=1.5;
XIE=0.7;
delit=0.001;
Kc=0.44;
XKE=Kc+2.247*10^(-3)*XIE^(-3.1667);
t0=0.5;
Np=nn;
%initial value
c_0=zeros(20,1);
[t,c_dot]=ode45('plate',[0,10],c_0);
plot(t,c_dot);
title('plate modeling');
xlabel('Dimensionless time');
ylabel('Dimensionless consentration');
set(gca,'xlim',[0 5]);
set(gca,'ylim',[0 1]);
```

```
function c_dot_ok=plate(t,c)
global XKE XK XIE KK H nn c0 delit Kc t0 Np
for n=1:nn
        if ((t-t0)<=(1+H*KK)*n/Np)
            dKdt(n)=0;
            XIS(n)=XIE;
            XK(n)=Kc+2.247*10^(-3)*XIS(n)^(-3.1667);
        else
            XIS(n)=XIE+0.001*(t-t0-(1+H*KK)*n/Np);
            XK(n)=Kc+2.247*10^(-3)*XIS(n)^(-3.1667);
            dKdt(n)=delit*(2.247*10^(-3))*(-3.1667)*XIS(n)^(-4.1667);
        end
    end
%boundary condition
for n=1:nn
    if n==1
        if t<t0
            c_dot(n)=(20*(0.8-c(n))-1.5*c(n)*dKdt(n))/(1+1.5*XK(n));
        else t>t0
            c_dot(n)=(20*(0-c(n))-1.5*c(n)*dKdt(n))/(1+1.5*XK(n));
        end
    else
            c_dot(n)=(20*(c(n-1)-c(n))-1.5*c(n)*dKdt(n))/(1+1.5*XK(n));
    end
end
%return
for i=1:nn
    c_dot_ok(i,1)=c_dot(i);
end
```

Plate model simulation(t0=0.5.le=0.7)

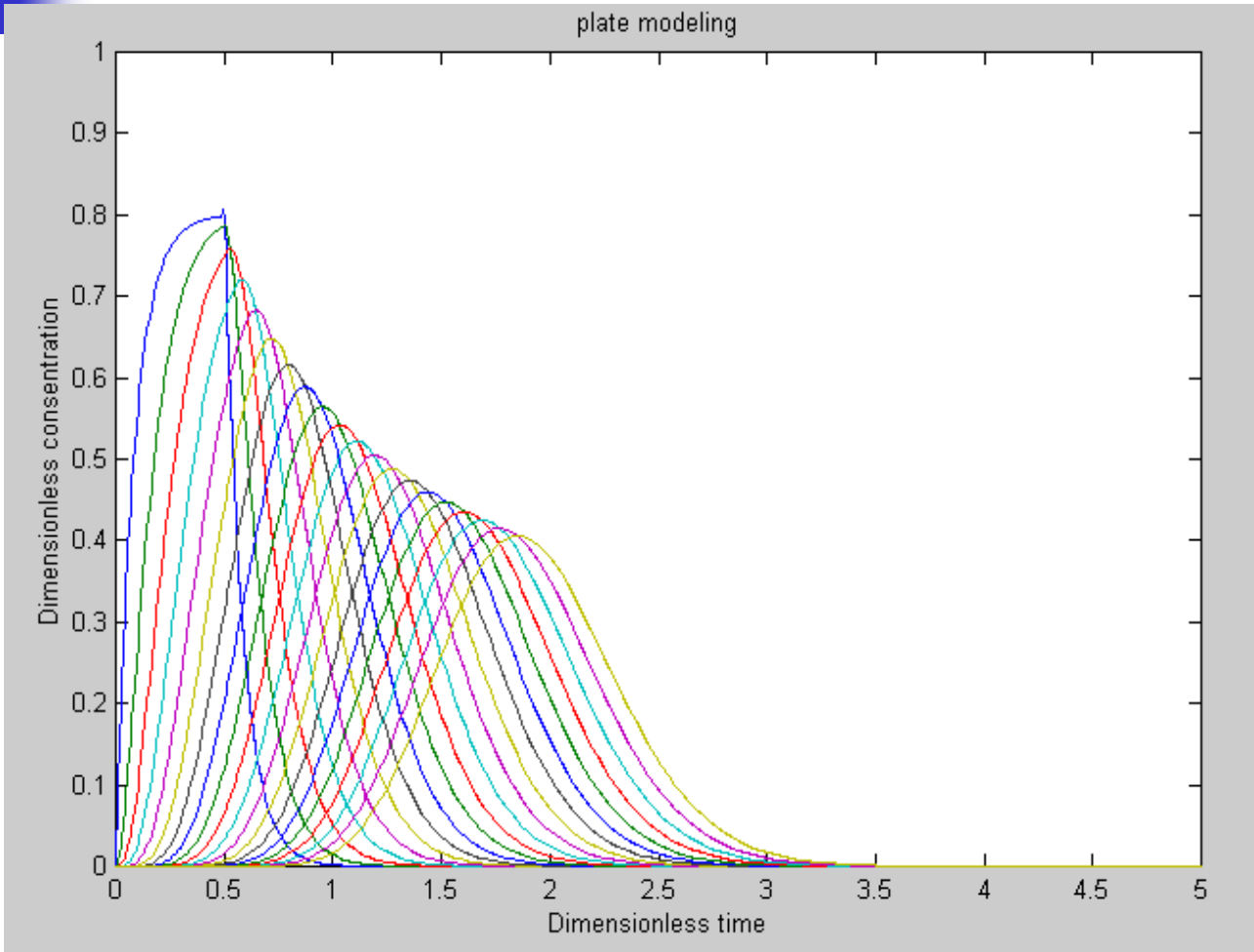

Fig. 1. Plot of the plate concentrations(t0=0.5,le=0.7).

```
clear all
global XKE XK XIE KK H nn c0 delit Kc t0 Np
KK=0.9;
nn=20;
c0=0.8;
H=1.5;
XIE=0.7;
delit=0.001;
Kc=0.44;
XKE=Kc+2.247*10^(-3)*XIE^(-3.1667);
t0=0.5;
Np=nn;
%initial value
c_0=zeros(20,1);
[t,c_dot]=ode45('plate',[0,10],c_0);
a=[t,c_dot];
b=a(:,2);c=a(:,11);,d=a(:,21);
plot(t,b,t,c,t,d);
title('plate modeling');
xlabel('Dimensionless time');
ylabel('Dimensionless consentration');
set(gca,'xlim',[0 5]);
set(gca,'ylim',[0 1]);
```

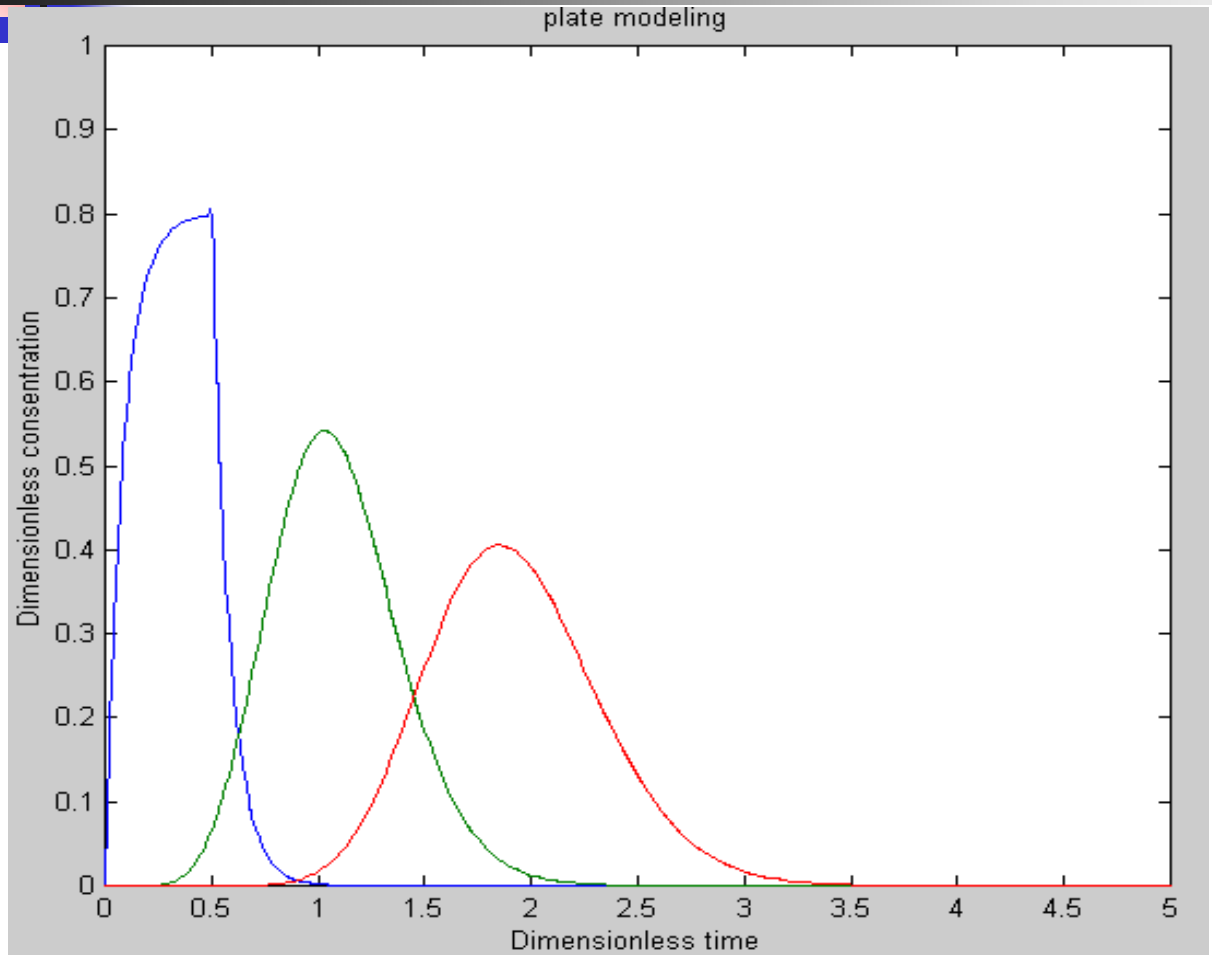

Fig. 2. Plot of the three plate concentrations (t0=0.5, le=0.7);

blue: inlet, green: middle, red: outlet of column.

Plate of model simulation (t0=0.1,le=0.7)

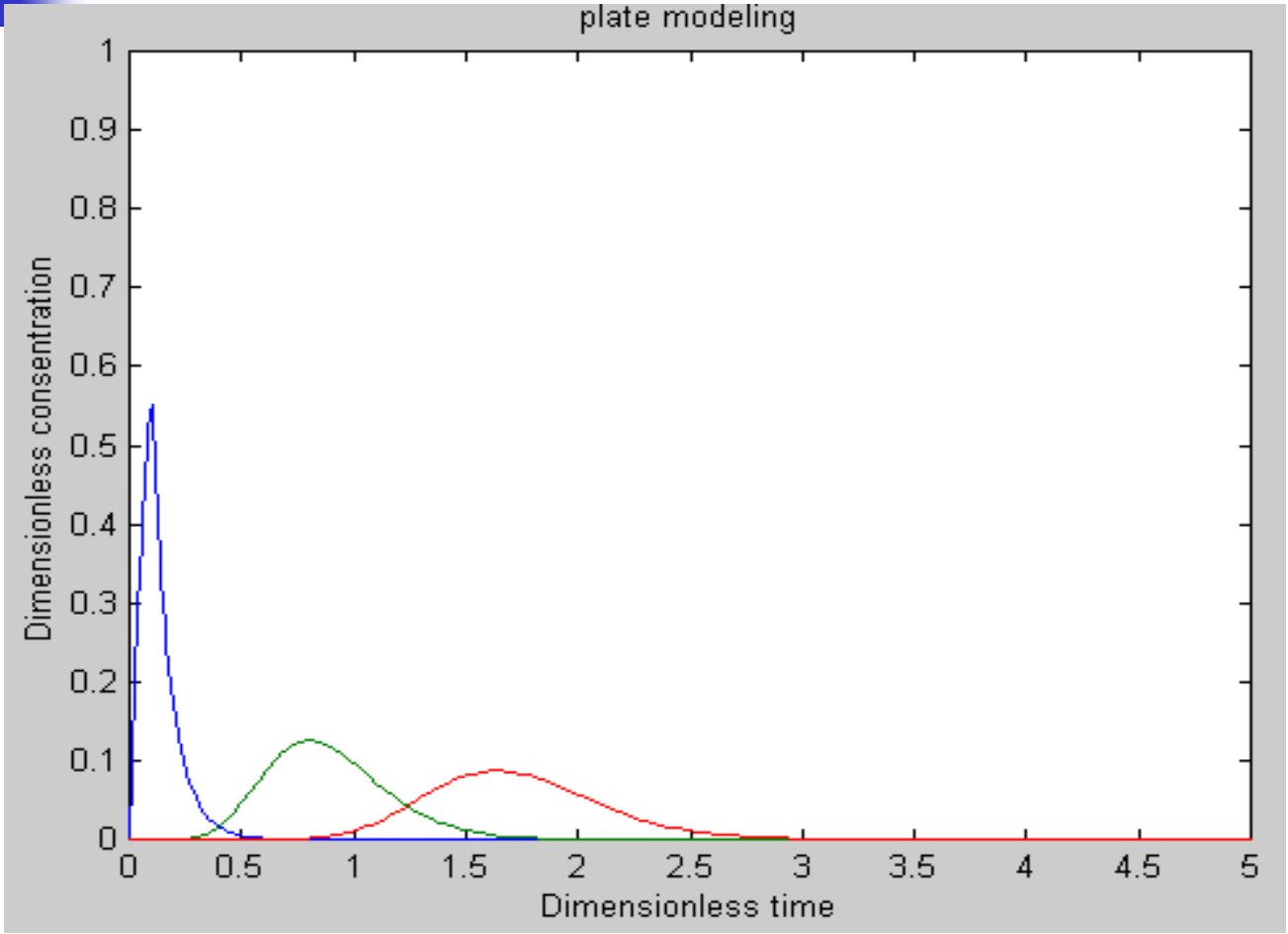

Fig. 3. Plot of the plate model (t0=0.1,le=0.7).

Plate of model simulation(t0=0.1,le=0.2)

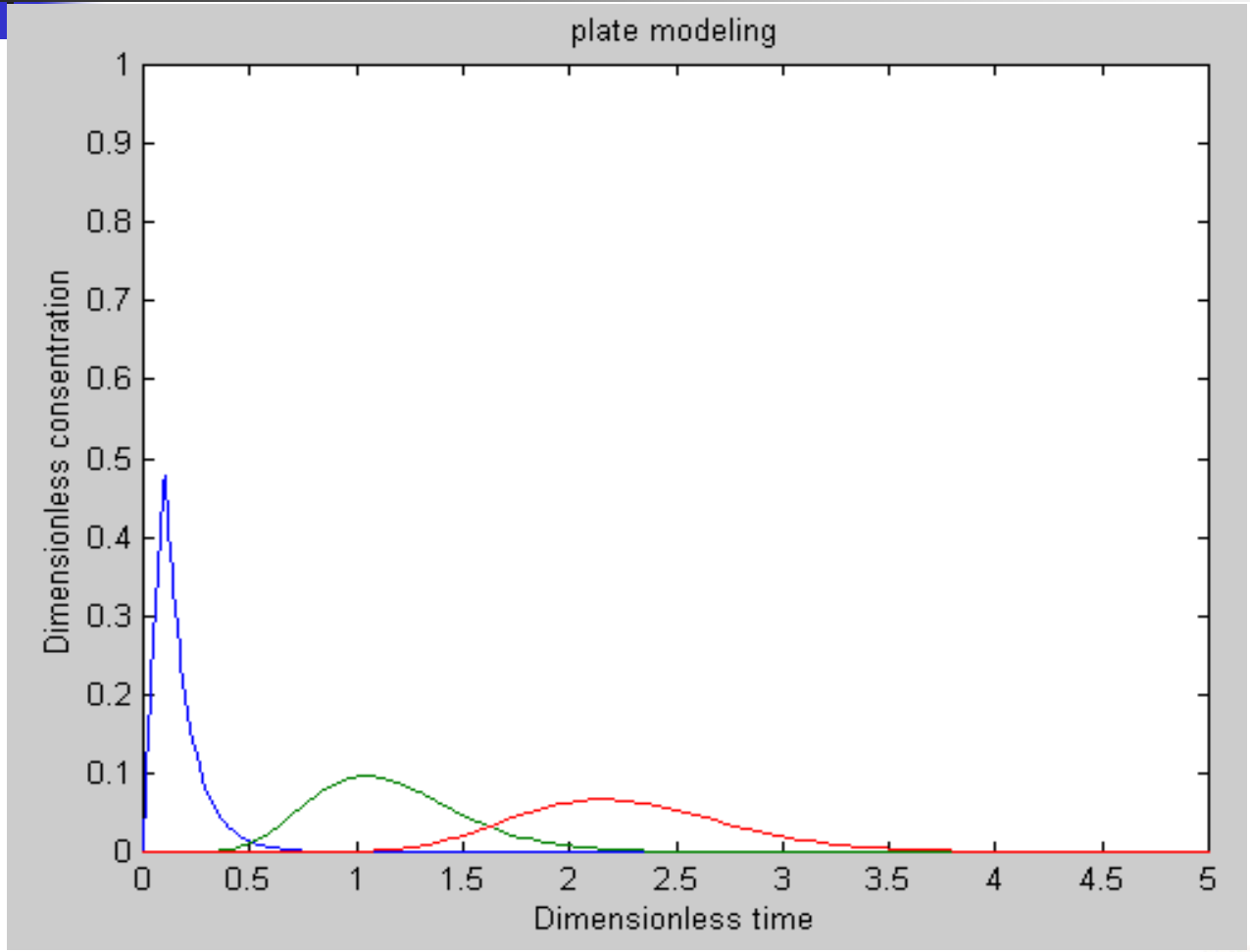

Fig. 4. Plot of the plate model (t0=0.1,le=0.2).