Ministry of Education and Science of the Republic of Kazakhstan
Al-Farabi Kazakh National University
Faculty: Mechanical Mathematics
Department: Mathematical and computer modeling

Project report

Theme: **Mathematical Modeling in Chemistry**

Done by: Kakibay A. K.

Checked by: Shakhan N.Sh.

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3. *Practical task №1:* Create the mathematical model for the given chemical process. Create the computer model with the implementation of Euler and Runge-Kutta numerical methods. Show the difference of two methods on separate plot. Make the computations till approximately end of the process. Take the time step and total number of iterations as you wish. Find the masses of final products in grams. Call the types of complex reactions which are participating in the mechanism of chemical reactions. Put the stoichiometric coefficients to the places where it is necessary. Draw on paper the structural and graphical form of all matters (moleculas) which are participating in the chemical process.

Process of the formation of calcium hydrocarbonate:

$$CaO + H_2O + CO_2 \xrightarrow{k_1} Ca(HCO_3)_2$$
$$Ca(HCO_3)_2 \xrightarrow{k_2} CaCO_3 + H_2O + CO_2$$
$$CaCO_3 \xrightarrow{k_3} CaO + CO_2$$
$$H_2O \xrightarrow{k_4} H_2 + O_2$$

Constants of the speeds of reactions:

$$k_1 = 0.4\ s^{-1}$$
$$k_2 = 0.5\ s^{-1}$$
$$k_3 = 0.25\ s^{-1}$$
$$k_4 = 0.3\ s^{-1}$$

Initial condition ($t = 0$) :

$$CaO = 2.1\text{ g}$$
$$H_2O = 1.5\text{ g}$$
$$CO_2 = 4\text{ g}$$

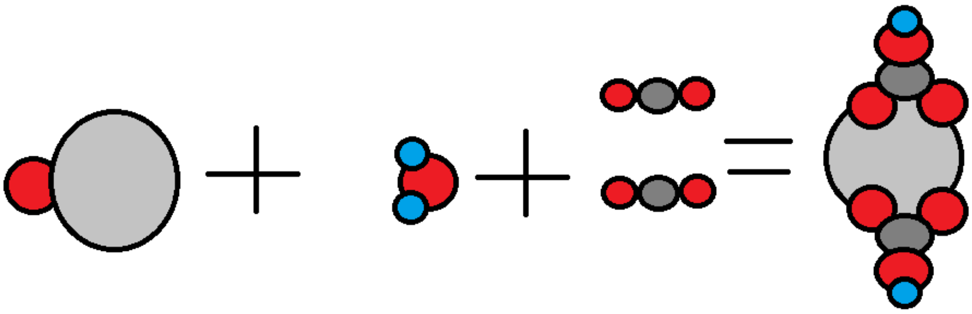
Volume of the reactor:

$$V = 0.6\text{ cm}^3$$

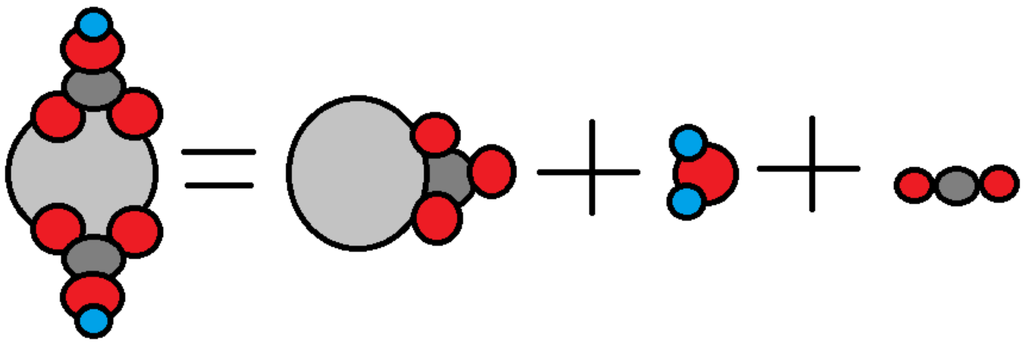
Solution:

First, we need to balance these reactions (in brackets we call the type of chemical reaction):

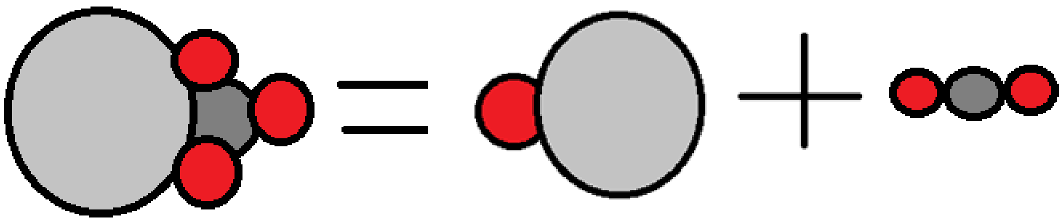
$$CaO + H_2O + 2CO_2 \xrightarrow{K_1} Ca(HCO_3)_2 \text{ (synthesis)}$$



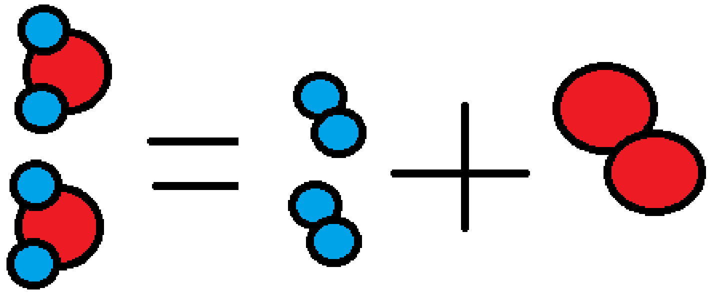
$$Ca(HCO_3)_2 \xrightarrow{K_2} CaCO_3 + H_2O + CO_2 \text{ (decomposition)}$$



$$CaCO_3 \xrightarrow{K_3} CaO + CO_2 \text{ (decomposition)}$$



$$2H_2O \xrightarrow{K_4} 2H_2 + O_2 \text{(decomposition)}$$



Let's denote as:

$$CaO - A$$
$$H_2O - B$$
$$CO_2 - C$$
$$Ca(HCO_3)_2 - D$$
$$CaCO_3 - E$$
$$H_2 - F$$
$$O_2 - G$$

Next, we need to write mathematical model of these chemical reactions:

$$\frac{dC_A}{dt} = -k_1 C_A C_B C_c^2 + k_3 C_E$$
$$\frac{dC_B}{dt} = -k_1 C_A C_B C_c^2 + k_2 C_D - 2k_4 C_B^2$$
$$\frac{dC_C}{dt} = -2k_1 C_A C_B C_c^2 + k_2 C_D + k_3 C_E$$
$$\frac{dC_D}{dt} = k_1 C_A C_B C_c^2 - k_2 C_D$$
$$\frac{dC_E}{dt} = k_2 C_D - k_3 C_E$$

$$\frac{dC_F}{dt} = 2k_4 C_B^2$$
$$\frac{dC_G}{dt} = k_4 C_B^2$$

So, after constructing mathematical model, we need to find concentration for all initial chemical reagents. Here the formula, by which we will find:

$$\nu = \frac{m}{M}, C = \frac{\nu}{\upsilon}$$

$$\nu_A = \frac{2.1}{56} = 0.0375\,mole\,, \nu_B = \frac{1.5}{18} = 0.0833\,mole\,, \nu_C = \frac{4}{44} = 0.09\,mole$$

$$C_A = \frac{0.0375}{0.6} = 0.0625\frac{mole}{cm^3}\,, C_B = \frac{0.0833}{0.6} = 0.138\frac{mole}{cm^3}, C_C = \frac{0.09}{0.6} = 0.15\frac{mole}{cm^3}$$

Let's find the mass of each chemical matters.

$\boldsymbol{CaO}$:

$$Ca: \begin{array}{ccc} 56 & - & 100\% \\ 40 & - & x \end{array},\; x = \frac{4000}{56} = 71.4\,\%,$$

$$\begin{array}{ccc} 2.1 & - & 100\% \\ x & - & 71.4\% \end{array},\quad x = \frac{71.4 * 2.1}{100} = 1.5\,g$$

$$O: \begin{array}{ccc} 2.1 & - & 100\% \\ x & - & 28.6\% \end{array},\quad x = \frac{28.6 * 2.1}{100} = 0.6\,g$$

$\boldsymbol{H_2O}$:

$$H_2: \begin{array}{ccc} 18 & - & 100\% \\ 2 & - & x \end{array},\quad x = 11.11\%, \begin{array}{ccc} 1.5 & - & 100\% \\ x & - & 11.11\% \end{array},\quad x = 0.16\,g$$

$O: x = 1.3\,g$

$\boldsymbol{CO_2}$:

$$C: \begin{array}{ccc} 44 & - & 100\% \\ 12 & - & x \end{array},\quad x = 27.27\%, \begin{array}{ccc} 4 & - & 100\% \\ x & - & 27.27\% \end{array},\quad x = 1.09\,g$$

$O_2: x = 2.91\,g$

After finding of all matters` masses we can find product masses by adding them properly as in reaction, then we can make sure that product masses are equal with the masses of addition of reagents.

Masses of final products:

$$2.1(CaO) + 1.5(H_2O) + 2 * 4(2CO_2) = 11.6(Ca(HCO_3)_2)$$
$$11.6(Ca(HCO_3)_2) - 1.5(H_2O) - 4(\boldsymbol{CO_2}) = 6.1(CaCO_3)$$
$$0.16(H_2) + 1.3(O) = 1.46(H_2O)$$
$$1.09(C) + 2.91(O_2) = 4(\boldsymbol{CO_2})$$
$$1.5(Ca) + 0.6(O) = 2.1(CaO)$$
$$2 * 0.16(H_2) = 0.32(2H_2)$$
$$1.3 * 2(O_2) = 2.6(O_2)$$

Code:

```
clear
clc
dt = 2.0;
k1 = 0.4;
k2 = 0.5;
k3 = 0.25;
k4 = 0.3;
for i=1:100
  C_A(i)=0.0;
  C_B(i)=0.0;
  C_C(i)=0.0;
  C_D(i)=0.0;
  C_E(i)=0.0;
  C_F(i)=0.0;
  C_G(i)=0.0;
  C_A_diff(i) = 0.0;
  C_B_diff(i) = 0.0;
  C_C_diff(i) = 0.0;
  C_D_diff(i) = 0.0;
  C_E_diff(i)=0.0;
  C_F_diff(i)=0.0;
  C_G_diff(i)=0.0;
end
C_A(1)=0.0625;
C_B(1)=0.138;
C_C(1)=0.15;
C_D(1)=0.0;
C_E(1)=0.0;
C_F(1)=0.0;
C_G(1)=0.0;
C_A_diff(1) = 0.0;
C_B_diff(1) = 0.0;
C_C_diff(1) = 0.0;
C_D_diff(1) = 0.0;
C_E_diff(1)=0.0;
C_F_diff(1)=0.0;
C_G_diff(1)=0.0;
for i = 1 : 99

 C_A(i+1) = C_A(i) + dt * (-k1 * C_A(i)*C_B(i)*(C_C(i)*C_C(i))+k3*C_E(i));
 C_B(i+1) = C_B(i) + dt * (-k1 * C_A(i)* C_B(i) *(C_C(i))^2 + k2* C_D(i)-
2*k4*C_B(i)*C_B(i));
 C_C(i+1) = C_C(i) + dt * (-2*k1 * C_A(i)*C_B(i) *(C_C(i))^2 + k2*C_D(i)+ k3*C_E(i));
 C_D(i+1) = C_D(i) + dt * (k1*C_A(i) * C_B(i) * (C_C(i))^2 - k2*C_D(i));
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```
    C_E(i+1) = C_E(i) + dt * (k2*C_D(i) - k3*C_E(i));
    C_F(i+1)=C_F(i)+dt*(2*k4*(C_B(i))^2);
    C_G(i+1)=C_G(i)+dt*(k4*(C_B(i))^2);
end
time = dt * (1:100);
fig = figure();
plot(time, C_A, 'b-.', 'LineWidth', 2)
hold on
plot(time, C_B, 'r', 'LineWidth', 2)
hold on
plot(time, C_C, 'y--', 'LineWidth', 2)
hold on
plot(time, C_D, 'g--', 'LineWidth', 2)
hold on
plot(time, C_E, 'b--.', 'LineWidth', 2)
hold on
plot(time, C_F, 'r--', 'LineWidth', 2)
hold on
plot(time, C_G, 'y-.', 'LineWidth', 2)
hold on

set(gca, 'FontSize', 18)
set(fig, 'color', 'white')
grid on
xlabel('time [sec]')
ylabel('Concentration [mole/cm^3]')
ylim([min(0.0) max(0.8)])
legend('C(A)','C(B)','C(C)','C(D)', 'C(E)', 'C(F)', 'C(G)');

%By Runge Kutta method:

dt = 2.0;
k1 = 0.4;
k2 = 0.5;
k3 = 0.25;
k4 = 0.3;
for i=1:100
    C_A2(i)=0.0;
    C_B2(i)=0.0;
    C_C2(i)=0.0;
    C_D2(i)=0.0;
    C_E2(i)=0.0;
    C_F2(i)=0.0;
    C_G2(i)=0.0;
end
C_A2(1)=0.0625;
C_B2(1)=0.138;
C_C2(1)=0.15;
C_D2(1)=0.0;
C_E2(1)=0.0;
C_F2(1)=0.0;
```

```
C_G2(1)=0.0;
for i = 1 : 99
% C_A
  k1_1 = -k1 * C_A2(i)*C_B2(i)*(C_C2(i))^2+k3*C_E2(i);
  k2_2 = -k1 * (C_A2(i) + dt * k1_1 / 2)*C_B2(i)*(C_C2(i))^2+k3*C_E2(i);
  k3_3 = -k1 * (C_A2(i) + dt * k2_2 / 2)*C_B2(i)*(C_C2(i))^2+k3*C_E2(i);
  k4_4 = -k1 * (C_A2(i) + dt * k3_3 / 2)*C_B2(i)*(C_C2(i))^2+k3*C_E2(i);
  deltaY1 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3 + k4_4);
  C_A2(i+1) = C_A2(i) + deltaY1;
% C_B
  k1_1 = (-k1 * C_A2(i)* C_B2(i) *(C_C2(i))^2 + k2* C_D2(i)-2*k4*C_B2(i)*C_B2(i));
  k2_2 = (-k1 * C_A2(i)* (C_B2(i) + dt * k1_1 / 2) *(C_C2(i))^2 + k2* C_D2(i)-2*k4*(C_B2(i)
+ dt * k1_1 / 2)*(C_B2(i) + dt * k1_1 / 2));
  k3_3 = (-k1 * C_A2(i)* (C_B2(i) + dt * k2_2 / 2) *(C_C2(i))^2 + k2* C_D2(i)-2*k4*(C_B2(i)
+ dt * k2_2 / 2)*(C_B2(i) + dt * k2_2 / 2));
  k4_4 = (-k1 * C_A2(i)* (C_B2(i) + dt * k3_3 / 2) *(C_C2(i))^2 + k2* C_D2(i)-2*k4*(C_B2(i)
+ dt * k3_3 / 2)*(C_B2(i) + dt * k3_3 / 2));
  deltaY2 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3  + k4_4);
  C_B2(i+1) = C_B2(i) + deltaY2;
% C_C
  k1_1 =  -2*k1 * C_A2(i)*C_B2(i) *(C_C2(i))^2 + k2*C_D2(i)+ k3*C_E2(i);
  k2_2 =  -2*k1 * C_A2(i)*C_B2(i) *((C_C2(i) + dt * k1_1 / 2))^2 + k2*C_D2(i)+ k3*C_E2(i);
  k3_3 =  -2*k1 * C_A2(i)*C_B2(i) *((C_C2(i) + dt * k2_2 / 2))^2 + k2*C_D2(i)+ k3*C_E2(i);
  k4_4 =  -2*k1 * C_A2(i)*C_B2(i) *((C_C2(i) + dt * k3_3 / 2))^2 + k2*C_D2(i)+ k3*C_E2(i);
  deltaY3 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3  + k4_4);
  C_C2(i+1) = C_C2(i) + deltaY3;
% C_D
  k1_1 = k1*C_A2(i) * C_B2(i) * (C_C2(i))^2 - k2*C_D2(i);
  k2_2 = k1*C_A2(i) * C_B2(i) * (C_C2(i))^2 - k2*(C_D2(i) + dt * k1_1 / 2);
  k3_3 = k1*C_A2(i) * C_B2(i) * (C_C2(i))^2 - k2* (C_D2(i) + dt * k2_2 / 2);
  k4_4 = k1*C_A2(i) * C_B2(i) * (C_C2(i))^2 - k2* (C_D2(i) + dt * k3_3 / 2);
  deltaY4 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3  + k4_4);
  C_D2(i+1) = C_D2(i) + deltaY4;
% C_E
  k1_1 = k2*C_D2(i) - k3*C_E2(i);
  k2_2 = k2*C_D2(i) - k3*(C_E2(i) + dt * k1_1 / 2);
  k3_3 = k2*C_D2(i) - k3*(C_E2(i) + dt * k2_2 / 2);
  k4_4 = k2*C_D2(i) - k3*(C_E2(i) + dt * k3_3 / 2);
  deltaY5 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3  + k4_4);
  C_E2(i+1) = C_E2(i) + deltaY5;

 % C_F
  k1_1 =(2*k4*(C_B2(i))^2);
  k2_2 = (2*k4*(C_B2(i))^2);
  k3_3 = (2*k4*(C_B2(i))^2);
  k4_4 = (2*k4*(C_B2(i))^2);
  deltaY6 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3  + k4_4);
  C_F2(i+1) = C_F2(i) + deltaY6;
 %C_G
  k1_1 =(k4*(C_B2(i))^2);
  k2_2 = (k4*(C_B2(i))^2);
  k3_3 = (k4*(C_B2(i))^2);
```

```
  k4_4 = (k4*(C_B2(i))^2);
  deltaY7 = dt / 6 * (k1_1 + 2 * k2_2 + 2 * k3_3  + k4_4);
  C_G2(i+1) = C_G2(i) + deltaY7;

  C_A_diff(i) = abs(C_A(i) - C_A2(i));
  C_B_diff(i) = abs(C_B(i) - C_B2(i));
  C_C_diff(i) = abs(C_C(i) - C_C2(i));

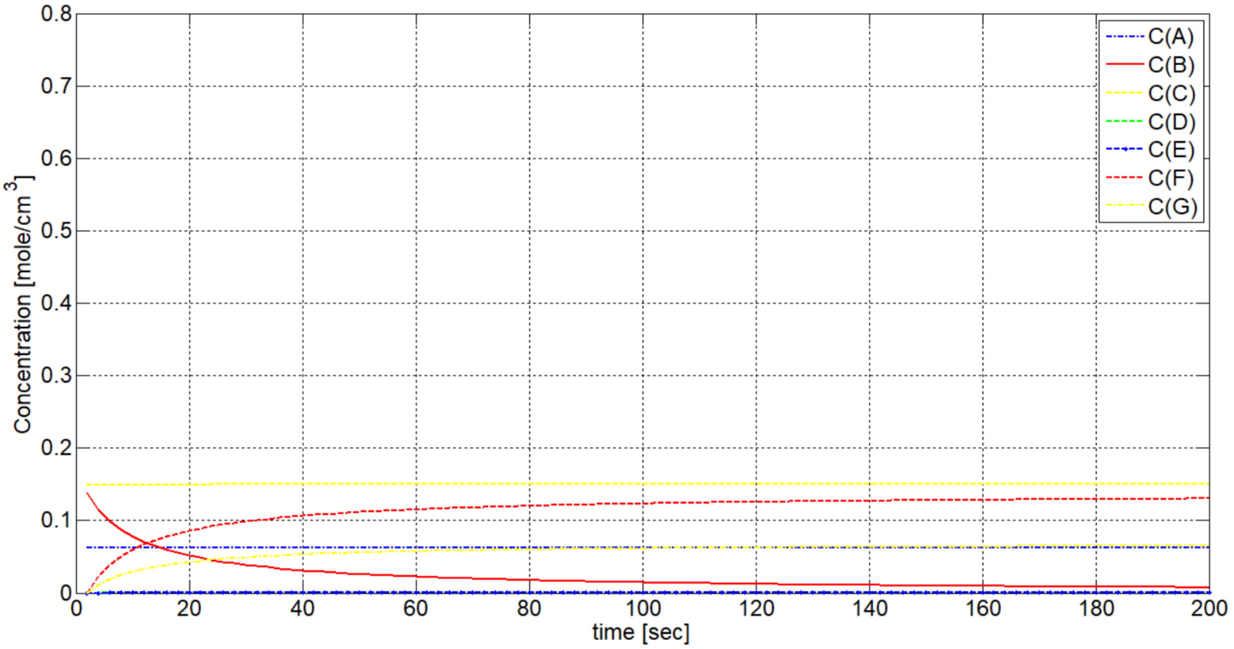
  C_D_diff(i) = abs(C_D(i) - C_D2(i));
  C_E_diff(i) = abs(C_E(i) - C_E2(i));
  C_F_diff(i) = abs(C_F(i) - C_F2(i));
  C_G_diff(i) = abs(C_G(i) - C_G2(i));
  fprintf('%.0f: %.7f - %.7f = %.7f\n', i, C_A(i), C_A2(i), abs(C_A(i) - C_A2(i)));
end
time = dt * (1:100);
fig = figure();
set(fig, 'color', 'white')
plot(time, C_A2, 'b-.', 'LineWidth', 2)
hold on
plot(time, C_B2, 'r', 'LineWidth', 2)
hold on
plot(time, C_C2, 'y--', 'LineWidth', 2)
hold on
plot(time, C_D2, 'g--', 'LineWidth', 2)
hold on
plot(time, C_E2, 'b-', 'LineWidth', 2)
hold on
plot(time, C_F2, 'r--', 'LineWidth', 2)
hold on
plot(time, C_G2, 'y-.', 'LineWidth', 2)
hold on
set(gca, 'FontSize', 18)
set(fig, 'color', 'white')
grid on
xlabel('time [sec]')
ylabel('Concentration [mole/cm^3]')
ylim([min(0.0) max(0.8)])
legend('C(A)','C(B)','C(C)', 'C(D)', 'C(E)', 'C(F)', 'C(G)');

fig = figure();
set(fig, 'color', 'white')
plot(time, C_A_diff, 'b-.', 'LineWidth', 2)
hold on
plot(time, C_B_diff, 'k--', 'LineWidth', 2)
hold on
plot(time, C_C_diff, 'y', 'LineWidth', 2)
hold on
plot(time, C_D_diff, 'g', 'LineWidth', 2)
hold on
plot(time, C_E_diff, 'b--', 'LineWidth', 2)
hold on
plot(time, C_F_diff, 'c-.', 'LineWidth', 2)

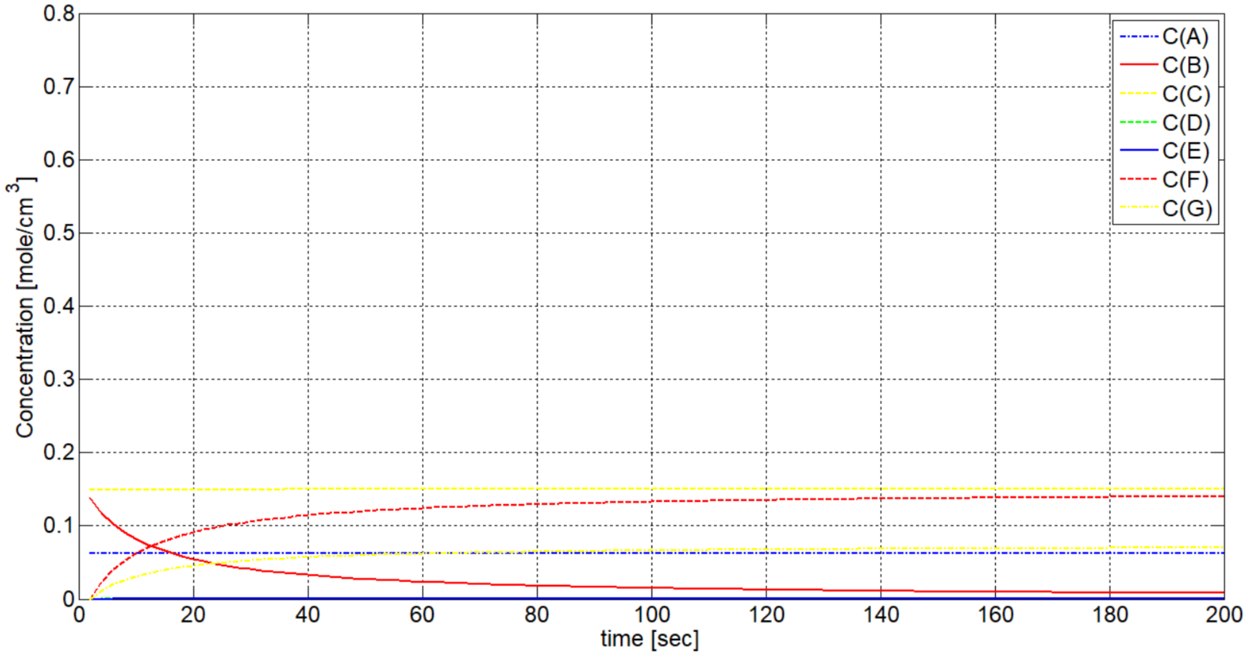
hold on
plot(time, C_G_diff, 'y--', 'LineWidth', 2)
hold on
set(gca, 'FontSize', 18)
set(fig, 'color', 'white')
ax = gca;
ax.YAxis.Exponent = 0;
%ylim([0 0.25])
grid on
xlabel('time [sec]')
ylabel('Concentration [mole/cm^3]')
ylim([min(0.0) max(0.8)])
legend('C(A)','C(B)','C(C)', 'C(D)','C(E)', 'C(F)', 'C(G)');
```

To run follow this link https://drive.google.com/file/d/1gESl5d9Sd-w8b35ziCmw9Fyn8lMFopuC/view?usp=sharing

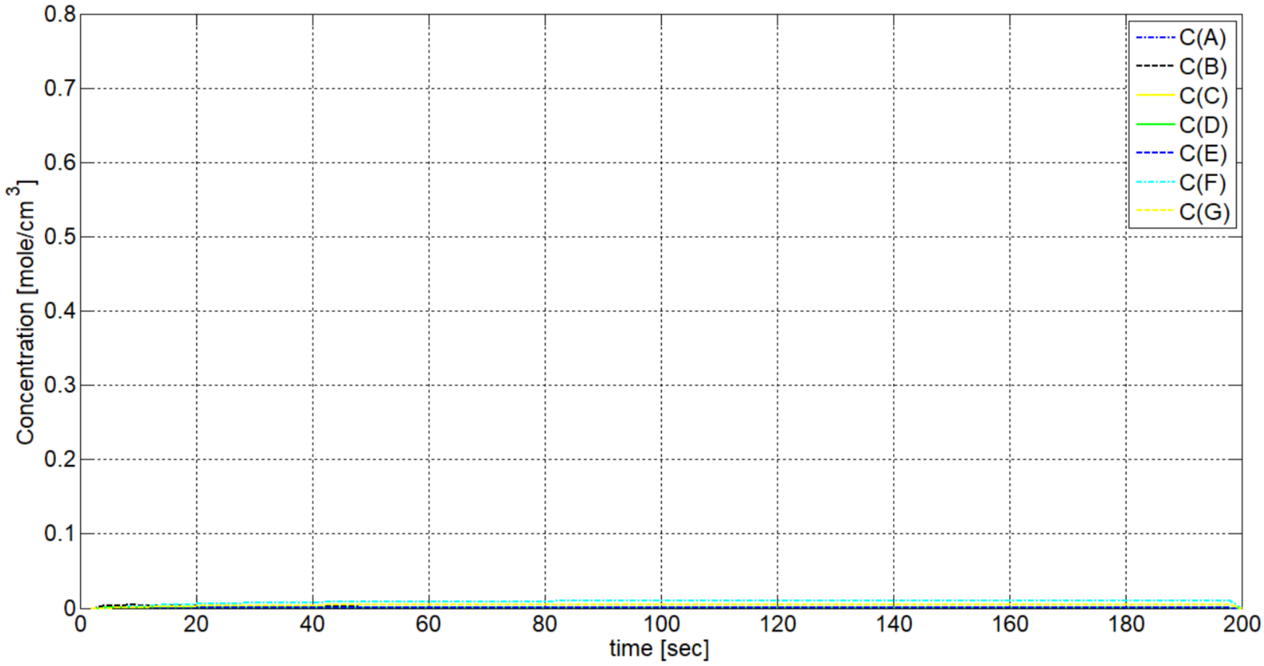
Results:
Euler numerical method:



Runge-Kutta numerical method:



Difference between two numerical methods:



Conclusion: We have created the mathematical model for the given chemical process and created the computer model with the implementation of Euler and Runge Kutta numerical methods in MATLAB. We can say that in the first and second figures computation was well done. In the last figure was shown the difference between two methods and as you can see the difference between them is too small. Also, we have found the masses of each matter of reagent from which we got product and found out that the addition of reagents` masses are equal with product masses. Moreover, we called the type of each chemical reaction and drawn the structural form of all matters.

4. *Practical task №2:* In one-dimensional space the concentration of matter A (blue line) is given (figure – B.1).

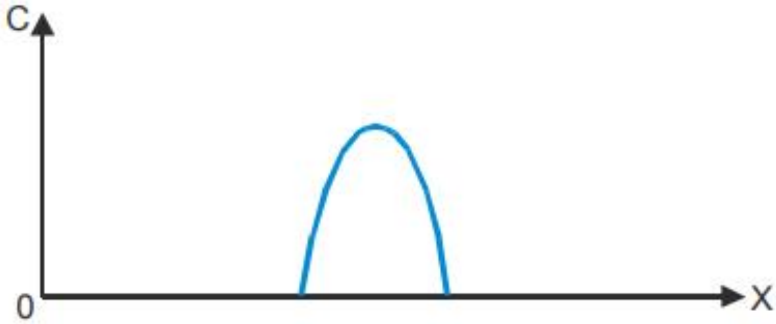


figure – B.1

With respect to time it is spreading along the axis X (diffusion). Since the matter A is dangerous and harmful gas, the helicopter is releasing the matter B over it starting from certain moment of time at point X_B (figure – B.2).

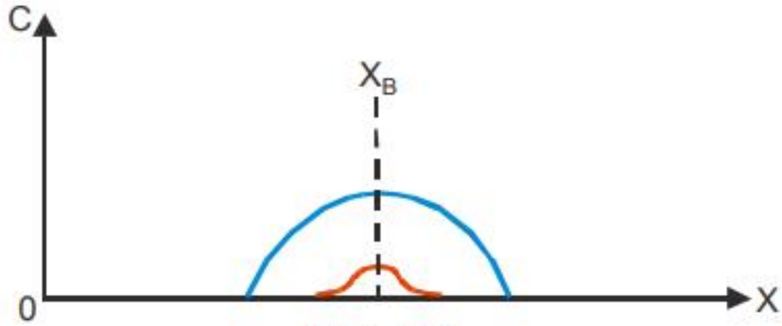


figure – B.2

During the interaction of matters A and B the following reaction occurs:

$$2A + B \rightarrow C + 3D$$

where C and D – concentration of gaseous matters, which are appearing due to the reaction (products of reaction). Matter C is known as heavy gas, so it won't move along the axis X, while matter D is extremely easy, so it will transfer with the force of winf from left to right. Diffusion coefficient of matter C and advection coefficient of matter D take as you wish.

Make mathematical and computer modeling of this process. Initial value of the concentration of matter A, time step, constant of the speed of reaction take as you want.

Solution:

$$\frac{\partial A}{\partial t} = -2kA^2B + a\frac{\partial^2 A}{\partial x^2}$$

$$\frac{\partial B}{\partial t} = -kA^2B - b_1\frac{\partial B}{\partial x} + b_2\frac{\partial^2 B}{\partial x^2}$$

$$\frac{\partial C}{\partial t} = kA^2B + c\frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial D}{\partial t} = 3kA^2B - d\frac{\partial D}{\partial x}$$

$$A_{new}(i) = A_{old}(i) + dt * (-2 * k * A_{old}^2(i) * B_{old}(i) + \frac{a}{dx * dx} * (A_{old}(i+1) - 2 * A_{old}(i) + A_{old}(i-1)));$$

$$B_{new}(i) = B_{old}(i) + dt * (-k * A_{old}^2(i) * B_{old}(i) - \frac{b1}{dx} * \left(B_{old}(i) - B_{old}(i-1)\right) + \frac{b2}{dx * dx} * (B_{old}(i+1) - 2 * B_{old}(i) + B_{old}(i-1)));$$

$$C_{new}(i) = C_{old}(i) + dt * (k * A_{old}^2(i) * B_{old}(i) + \frac{c}{dx * dx} * (C_{old}(i+1) - 2 * C_{old}(i) + C_{old}(i-1)));$$

$$D_{new}(i) = D_{old}(i) + dt * (3 * k * A_{old}^2(i) * B_{old}(i) - \frac{d}{dx} * (D_{old}(i) - D_{old}(i-1)));$$

Code:

```
clear
figure('units','normalized','outerposition',[0 0 1 1])

x_min = 0;
x_max = 15;

N = x_max * 10;

dx = (x_max - x_min)/N; % 0.1
x = x_min : dx : x_max;

t = 0;
t_max = 4;
dt = dx * dx;
n_steps = t_max/dt;


a = 5 * dx * dx;
b1 = 0.5;
b2 = 4 * dx * dx;
c = 3 * dx * dx;
d = 1;

k = 0.5;

for i = 1 : N+1
    A0(i) = 0;
    B0(i) = 0;
    C0(i) = 0;
```

```
    D0(i) = 0;
end

for i = 1: N+1
    if dx * i <= 6.086 || dx * i >= 8.914
        A0(i) = 0 * dx * i;
    else
        A0(i) = sqrt(20-(dx * i-7.5)^2/0.1);
    end
end


A_old = A0;
A_new = A0;
B_old = B0;
B_new = B0;
C_old = C0;
C_new = C0;
D_old = D0;
D_new = D0;


for i = 1 : n_steps
    A_old(1)=A_old(2);
    A_old(N+1)=A_old(N);
    B_old(1)=B_old(2);
    B_old(N+1)=B_old(N);
    C_old(1)=C_old(2);
    C_old(N+1)=C_old(N);
    D_old(1)=D_old(2);
    D_old(N+1)=D_old(N);

    for i=2: N
        A_new(i) = A_old(i) + dt * (-2 * k * A_old(i)^2 * B_old(i)                              + a  / (dx
* dx) * (A_old(i+1) - 2 * A_old(i) + A_old(i-1)) );

        B_new(i) = B_old(i) + dt * (    -k * A_old(i)^2 * B_old(i) - b1 /  dx * (B_old(i) - B_old(i-
1)) + b2 / (dx * dx) * (B_old(i+1) - 2 * B_old(i) + B_old(i-1)) );

        C_new(i) = C_old(i) + dt * (     k * A_old(i)^2 * B_old(i)                              + c  / (dx *
dx) * (C_old(i+1) - 2 * C_old(i) + C_old(i-1)) );

        D_new(i) = D_old(i) + dt * ( 3 * k * A_old(i)^2 * B_old(i) - d  /  dx * (D_old(i) - D_old(i-
1))                                              );
    end

    if t >= 0.5 && t <= 1.0
        B_new = (t-0.5)*4*exp(-3*(x - 7.5).^2);
    end

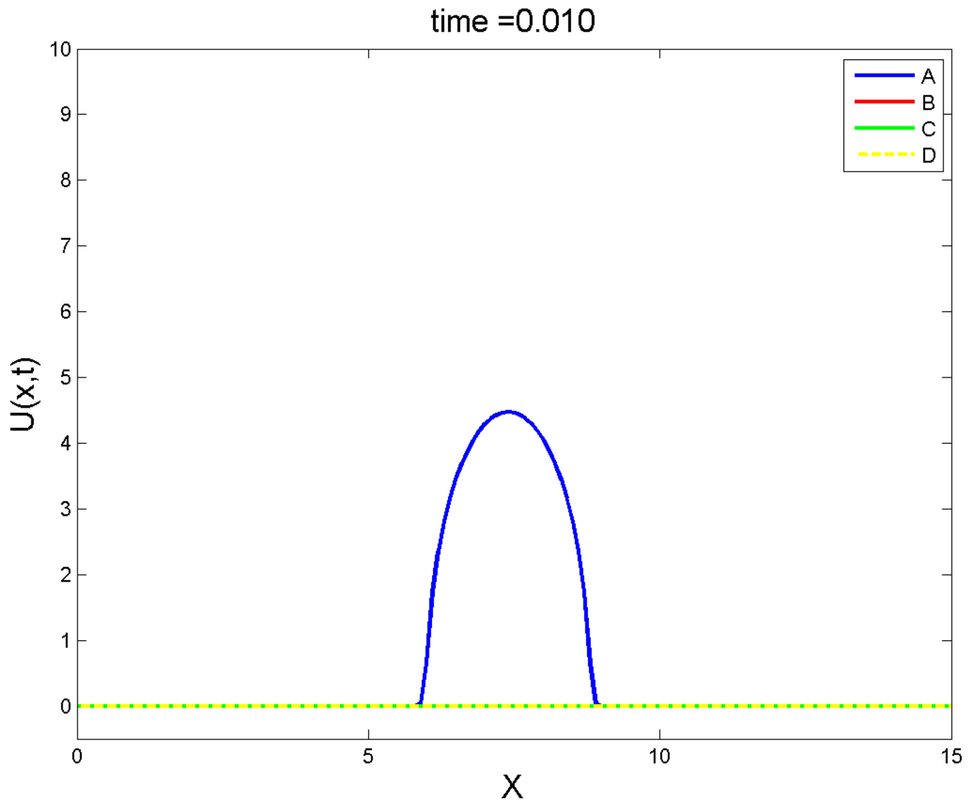
    t=t+dt;
    A_old=A_new;
```

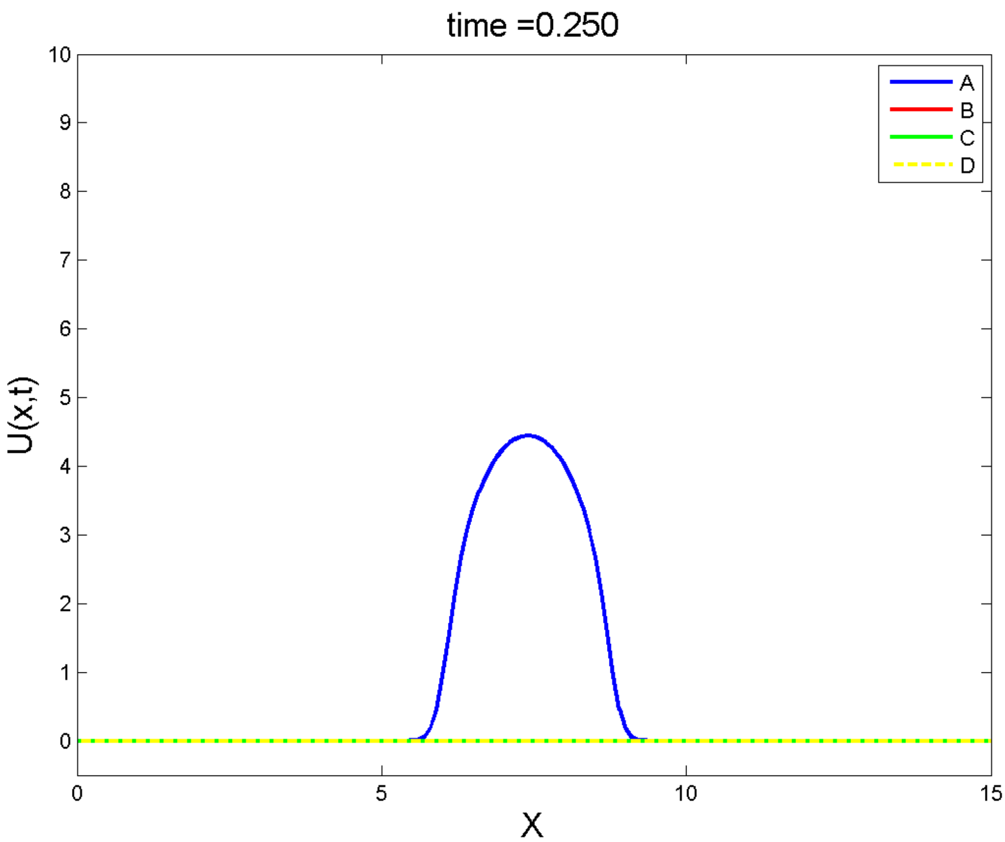
```
    B_old=B_new;
    C_old=C_new;
    D_old=D_new;

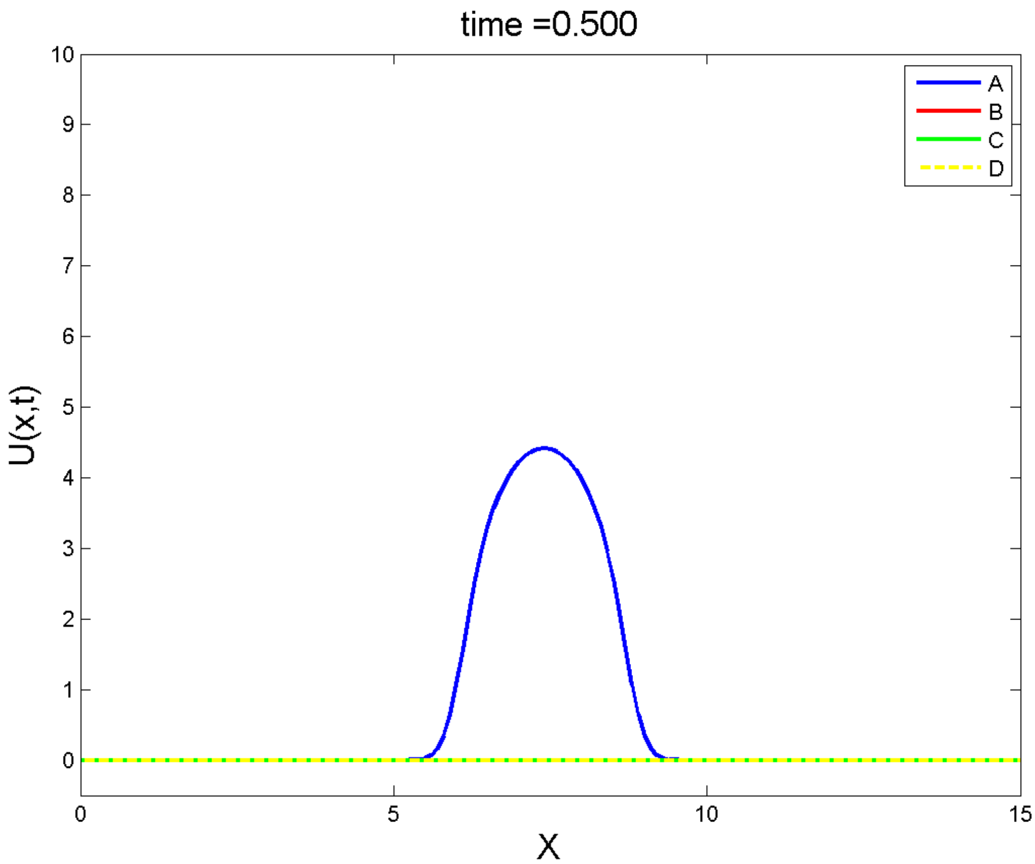
    plot(x,A_old,'b-','LineWidth',3);
    hold on
    plot(x,B_old,'r-','LineWidth',3);
    hold on
    plot(x,C_old,'g-','LineWidth',3);
    hold on
    plot(x,D_old,'y--','LineWidth',3);
    hold off
    axis([x_min x_max -0.5 10])
    xlabel('X','FontSize',16)
    ylabel('U(x,t)','FontSize',16)
    title(sprintf('time =%1.3f',t),'FontSize',16)
    legend('A','B','C', 'D');

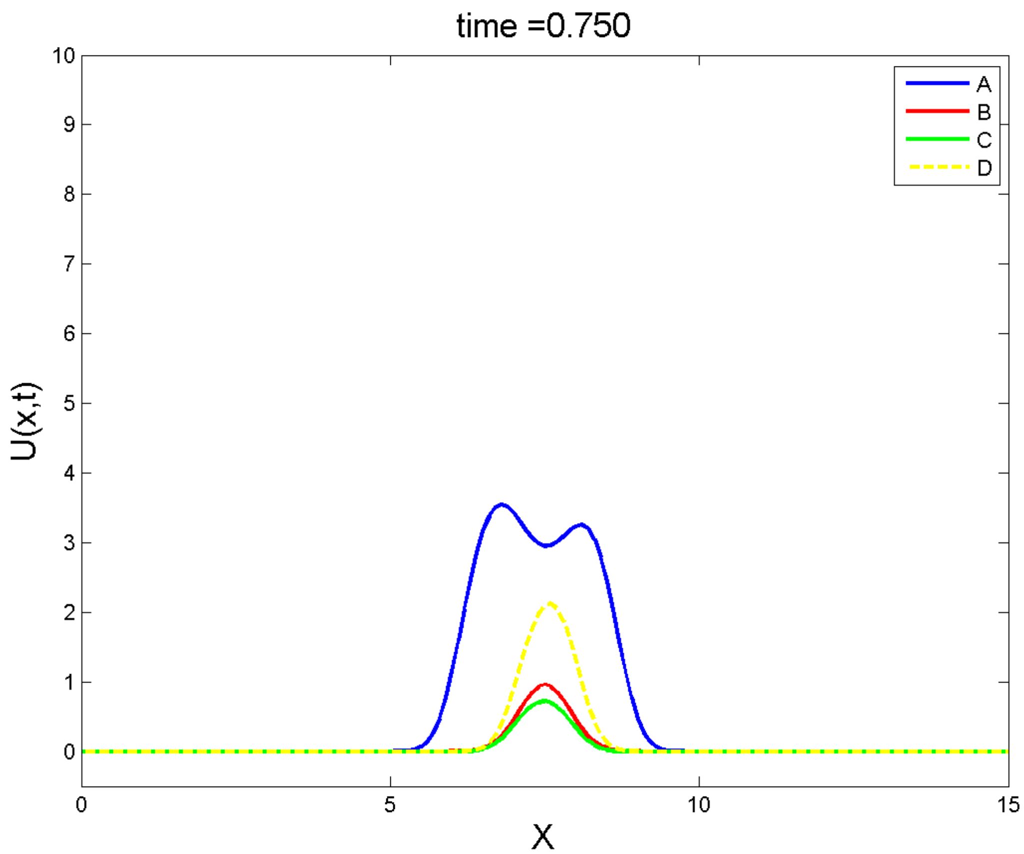
    pause(dt);
end
```

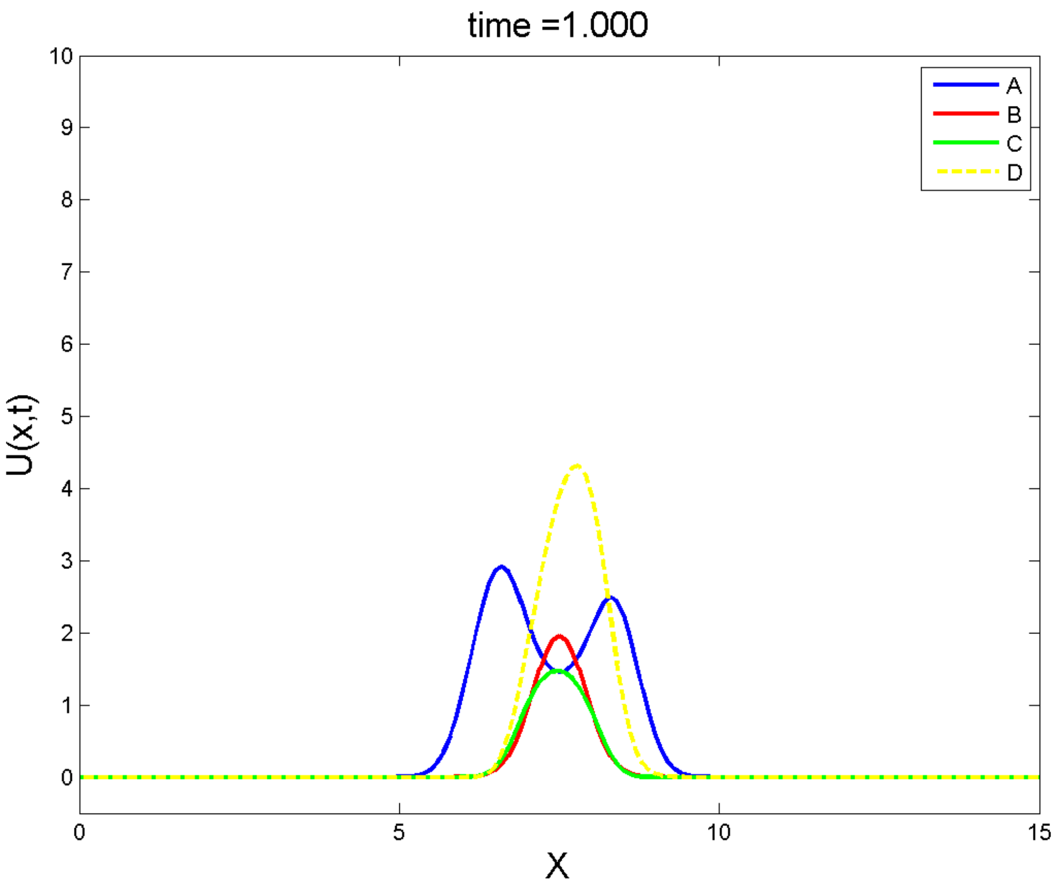
Results:

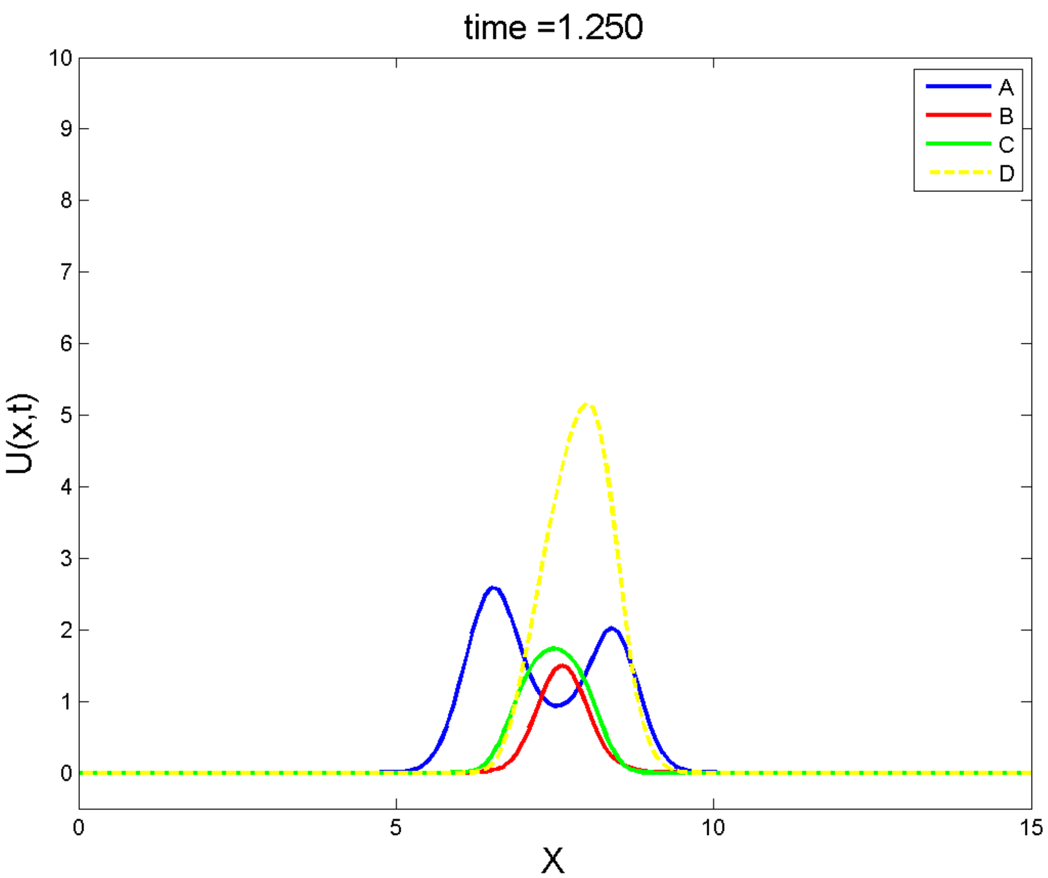

time =0.010
U(x,t)
X
A
B
C
D
0
1
2
3
4
5
6
7
8
9
10
0
5
10
15

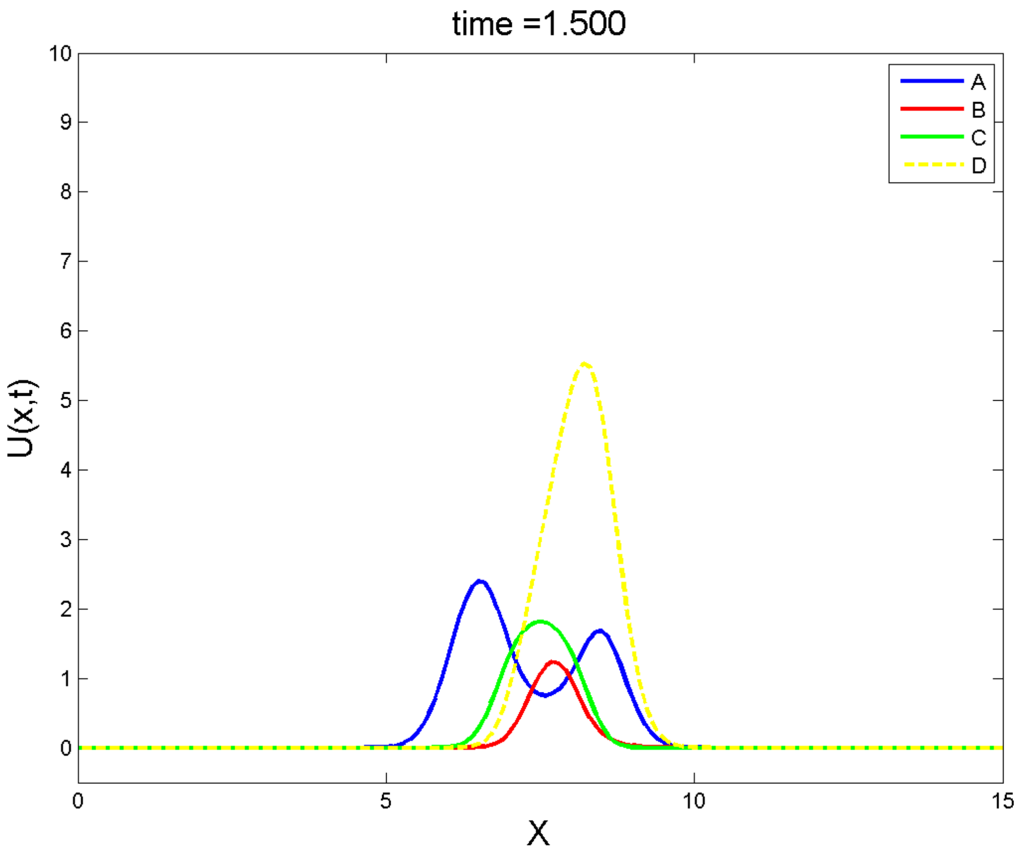

time =0.250
U(x,t)
X
A
B
C
D
0
1
2
3
4
5
6
7
8
9
10
0
5
10
15

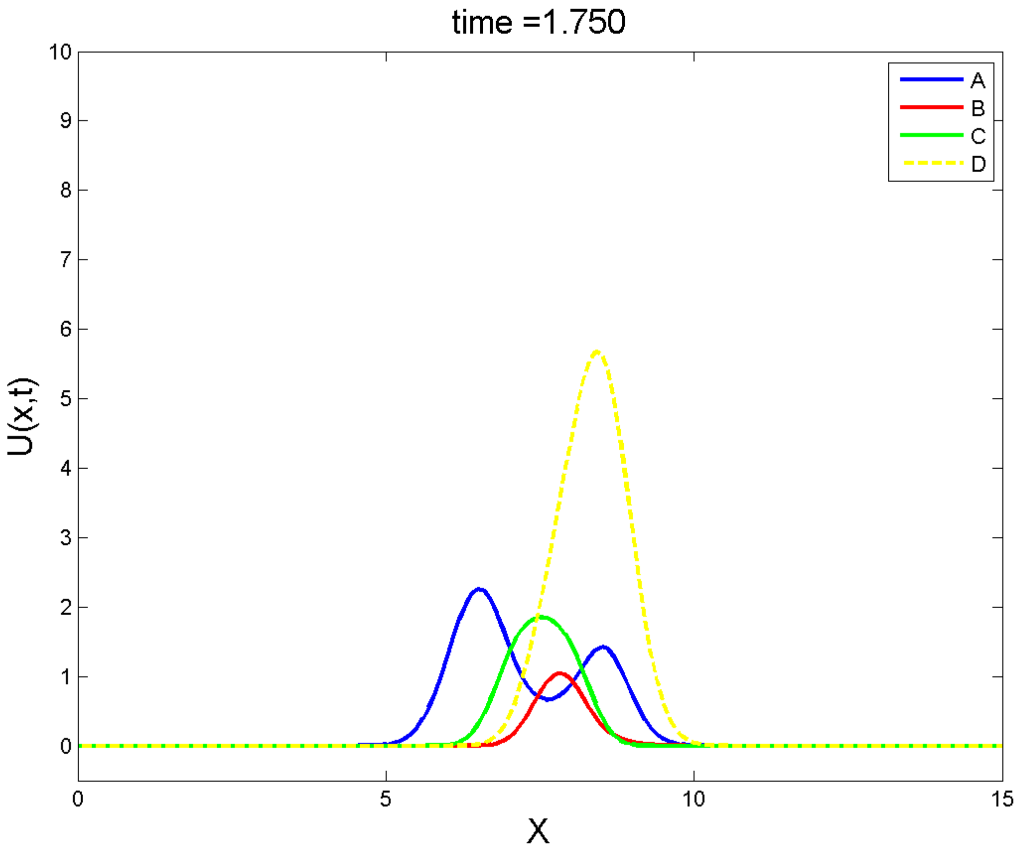

time =0.500
U(x,t)
X
A
B
C
D
0
5
10
15
0
1
2
3
4
5
6
7
8
9
10

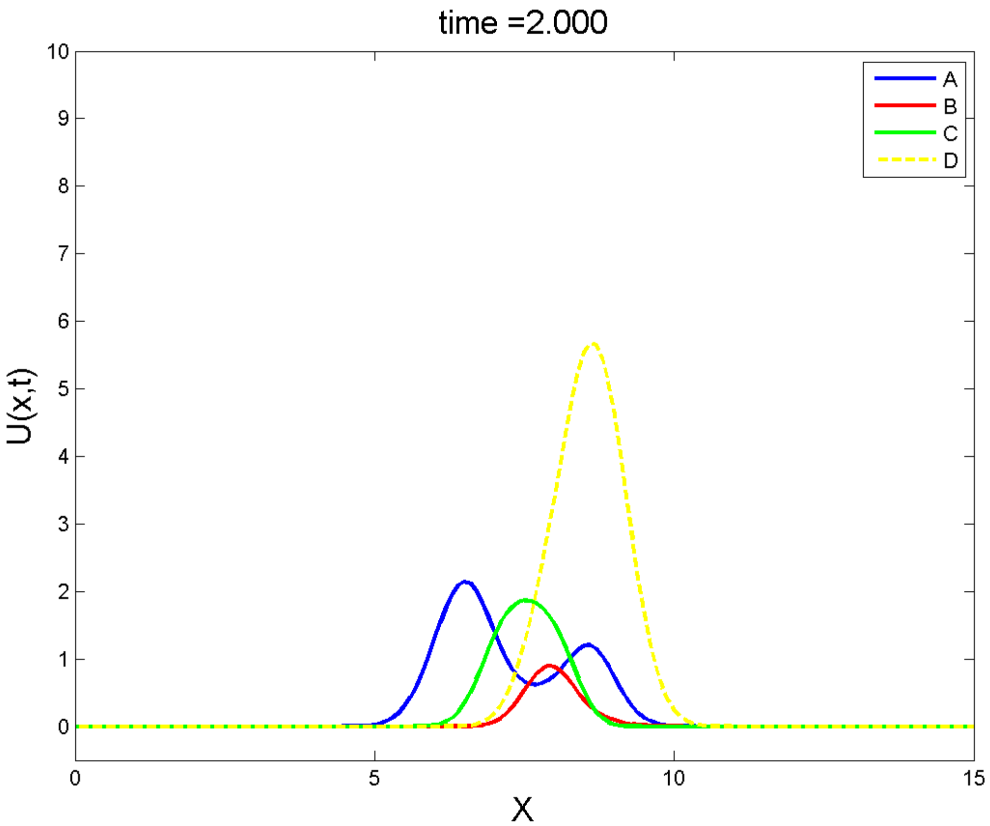

time =0.750
U(x,t)
X
A
B
C
D
0
5
10
15
0
1
2
3
4
5
6
7
8
9
10

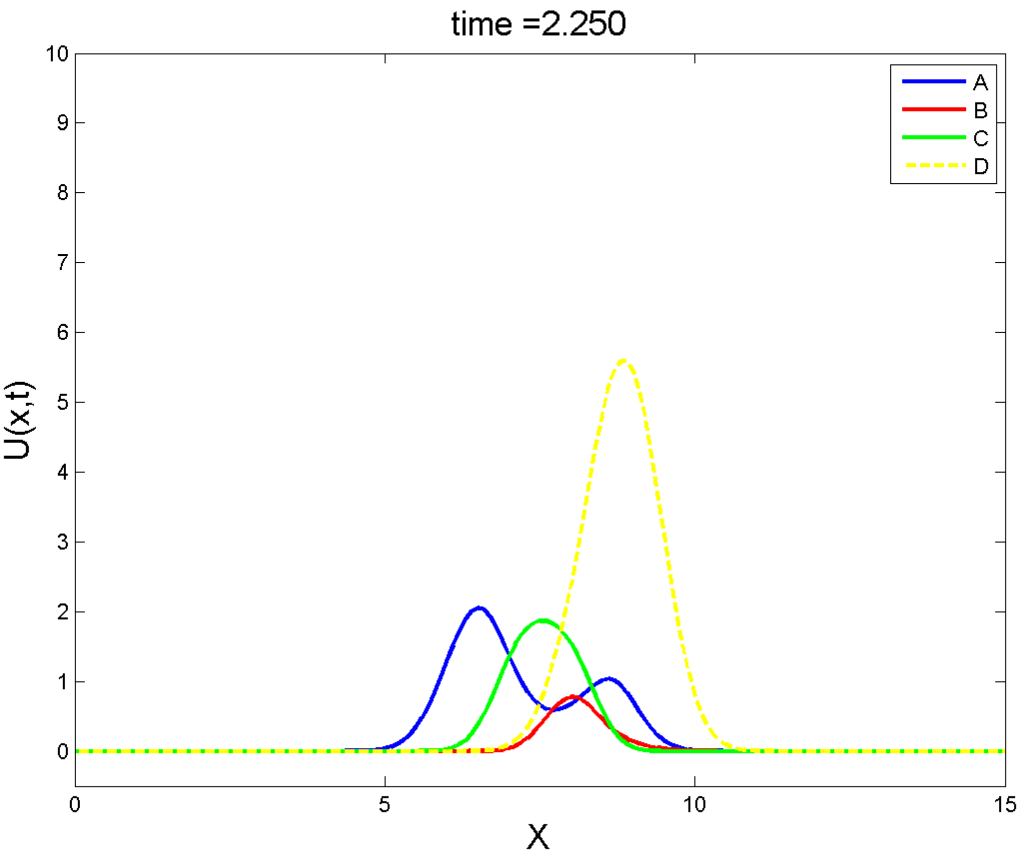

time =1.000
U(x,t)
X
A
B
C
D
0
5
10
15
0
1
2
3
4
5
6
7
8
9
10

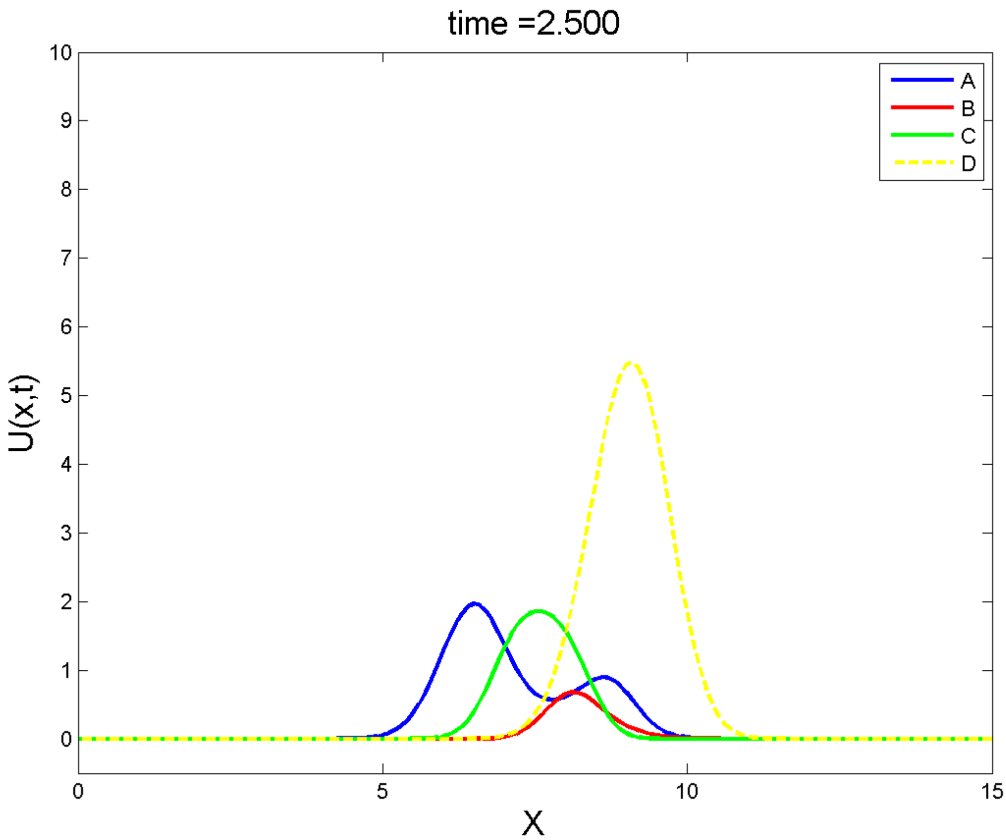

time =1.250
U(x,t)
X
A
B
C
D
0
5
10
15
0
1
2
3
4
5
6
7
8
9
10

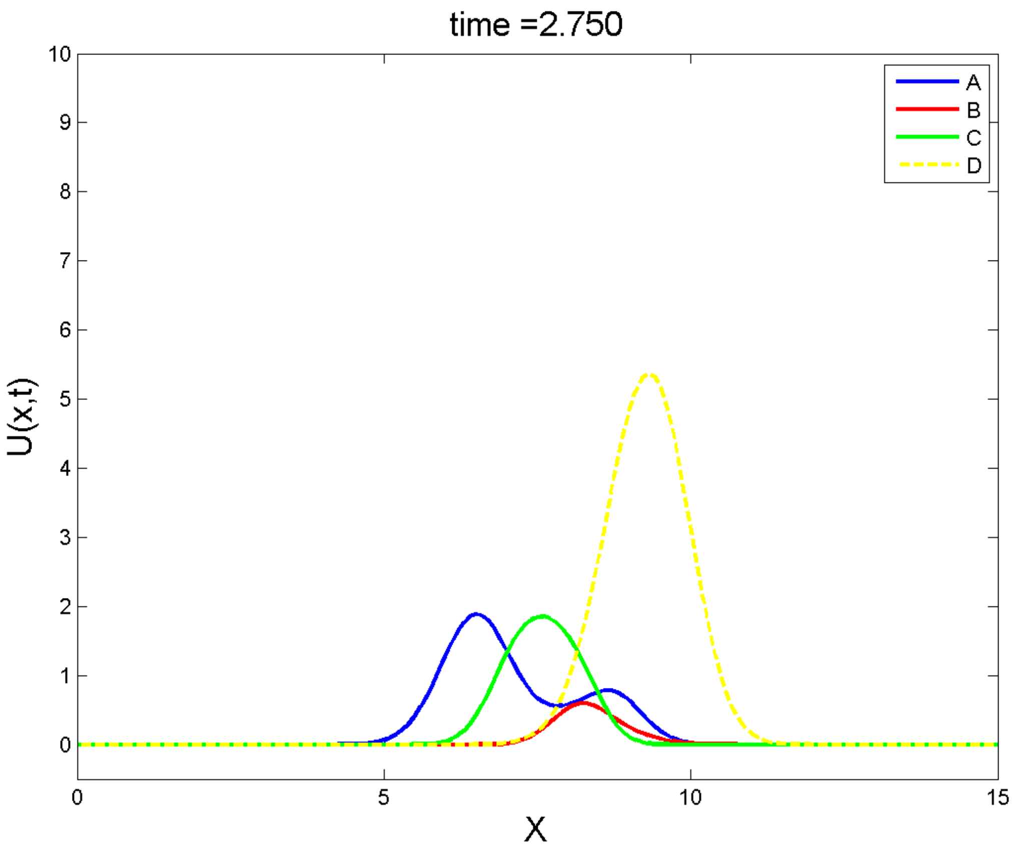

time =1.500
U(x,t)
X
A
B
C
D
0
5
10
15

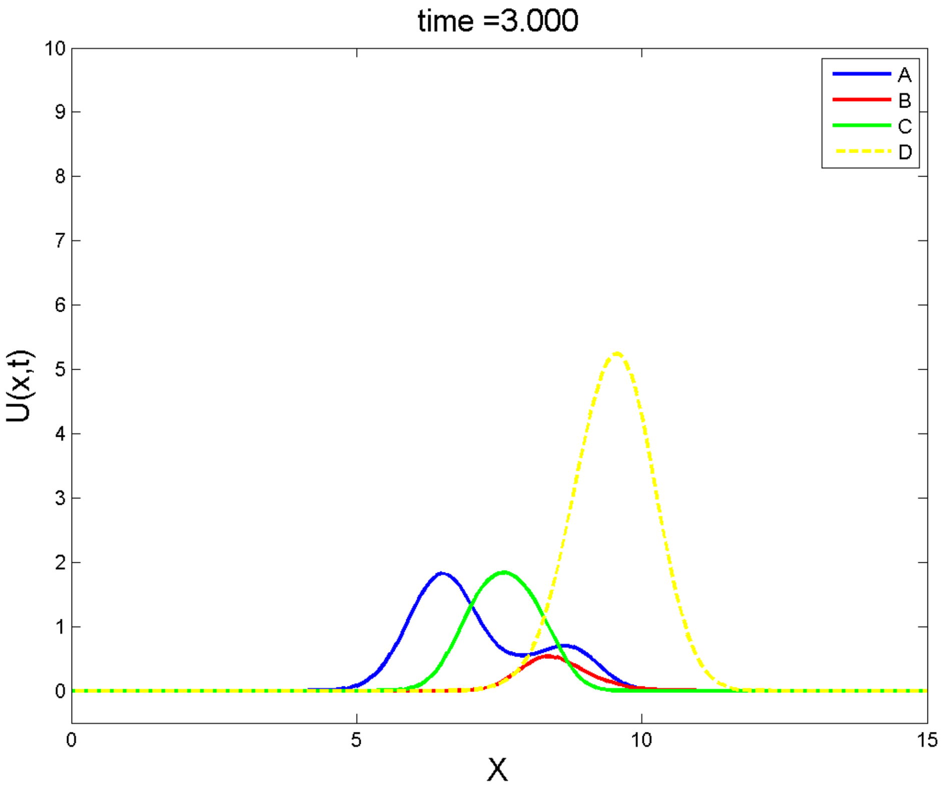

time =1.750
U(x,t)
X
A
B
C
D
0
5
10
15


time =2.000
U(x,t)
X
A
B
C
D

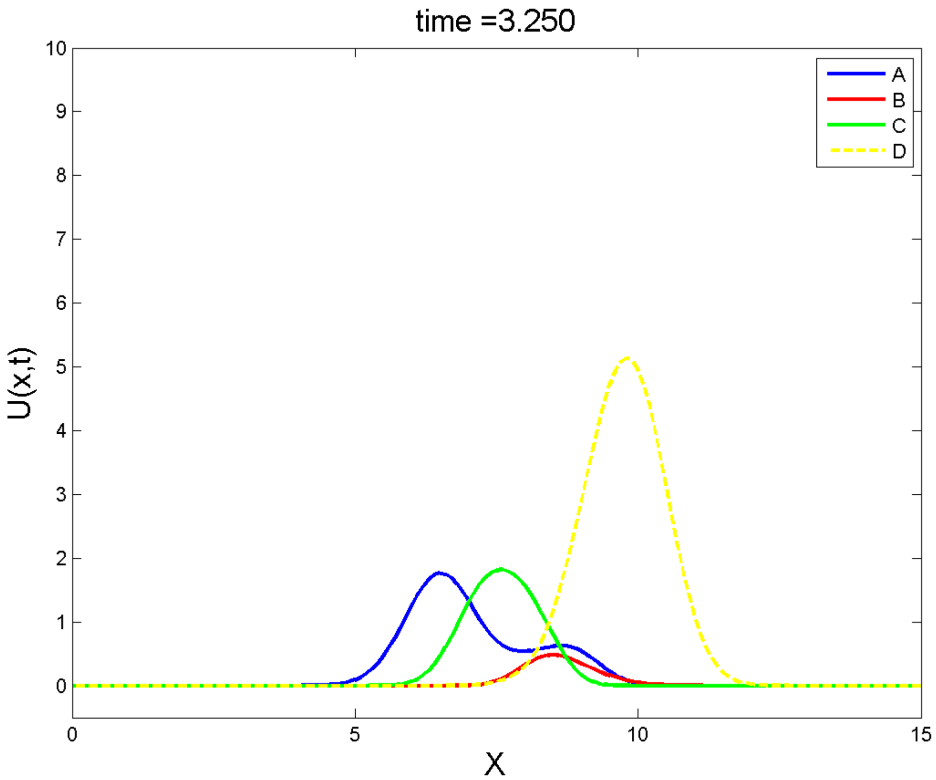

time =2.250
U(x,t)
X
A
B
C
D


time =2.500
U(x,t)
X
A
B
C
D
0
1
2
3
4
5
6
7
8
9
10
0
5
10
15

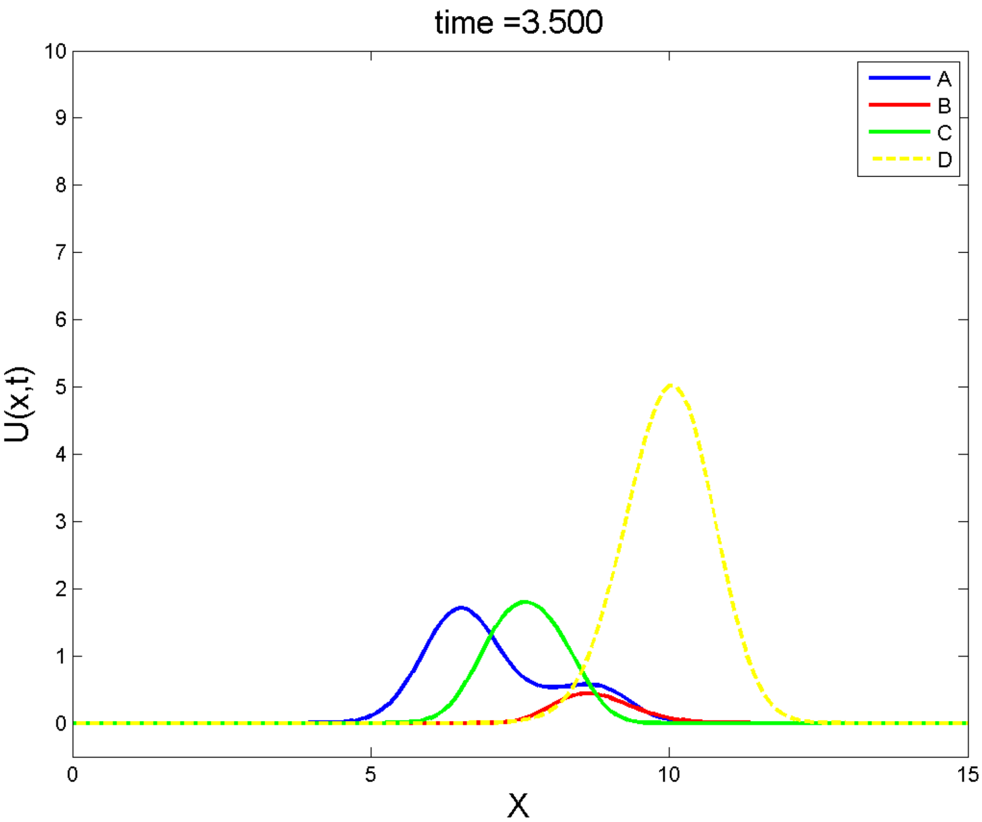

time =2.750
U(x,t)
X
A
B
C
D
0
1
2
3
4
5
6
7
8
9
10
0
5
10
15

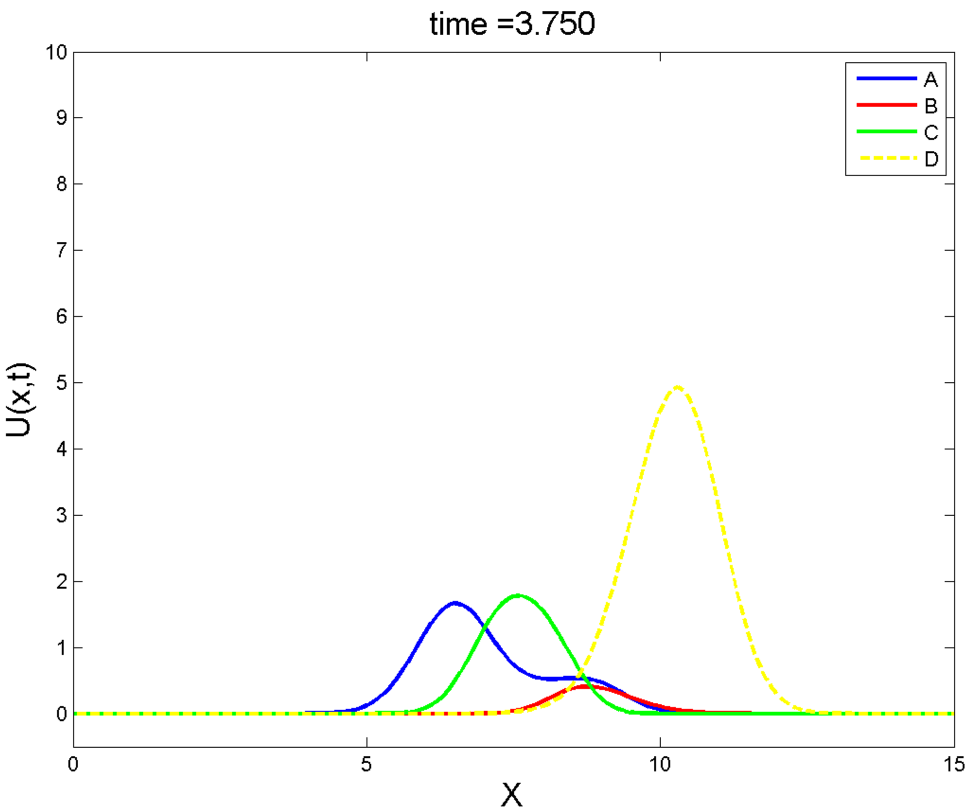


time =3.000
A
B
C
D
U(x,t)
X



time =3.250
A
B
C
D
U(x,t)
X


time =3.500
U(x,t)
X
A
B
C
D
0
5
10
15
0
1
2
3
4
5
6
7
8
9
10


time =3.750
U(x,t)
X
A
B
C
D
0
5
10
15
0
1
2
3
4
5
6
7
8
9
10

Conclusion:

To sum up, we have considered two matters` reaction in one-dimensional space. Our 1st matter A is very dangerous gas, and to destroy it, after 0.5 sec we added new matter B. For A was used the diffusion, and with the respect to time it was spreading along the X -axis. For B we used both diffusion and convection. In the result of their reaction we get two new products: C and D. Here, C is known as heavy gas and it won`t move, because of this we used the diffusion. Vice versa D is very light, and it will transfer easily with the force of wind, so we used the convection for it. As shown in results, you can see how reagents react with each other, and consequently we receive two products.

5. *Practical task №3*: Make mathematical and computer modeling of the same process as in practical task №2, but for two-dimensional space. The initial condition of the concentration of matter *A* take according to the figure – B.3:

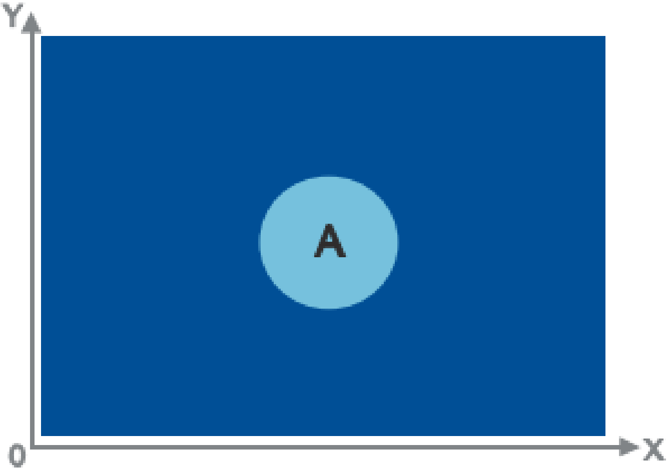


figure – B.3

Starting from the certain moment of time the helicopter is releasing the matter *B* at point X_B for counteraction to matter *A* (figure – B.4).

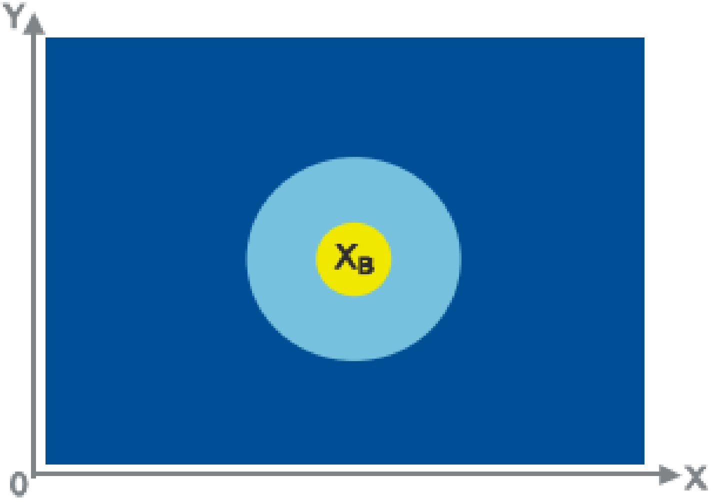


figure – B.4

Parameters of computation (time step, constant of the speed of reaction and others) take as you want.

Solution:

$$\frac{\partial A}{\partial t} = -2kA^2B + a(\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2})$$

$$\frac{\partial B}{\partial t} = -kA^2B - b_1(\frac{\partial B}{\partial x} + \frac{\partial B}{\partial y}) + b_2(\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2})$$

$$\frac{\partial C}{\partial t} = kA^2B + c(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2})$$

$$\frac{\partial D}{\partial t} = 3kA^2B - d(\frac{\partial D}{\partial x} + \frac{\partial D}{\partial y})$$

$$A_{new}(i,j) = A_{old}(i,j) + dt * (-2 * k * A_{old}^2(i,j) * B_{old}(i,j) + \frac{a_1}{dx * dx} * \left(A_{old}(i+1,j) - 2 * A_{old}(i,j) + A_{old}(i-1,j)\right) + \frac{a_2}{dy * dy} * (A_{old}(i,j+1) - 2 * A_{old}(i,j) + A_{old}(i,j-1)));$$

$$B\_new(i,j) = B_{old}(i,j) + dt * (-k * A_{old}^2(i,j) * B_{old}(i,j) - \frac{b_1}{dx} * \left(B_{old}(i,j) - B_{old}(i-1,j)\right) - \frac{b_2}{dx} * \left(B_{old}(i,j) - B_{old}(i,j-1)\right) + \frac{b_3}{dx * dx} * \left(B_{old}(i+1,j) - 2 * B_{old}(i,j) + B_{old}(i-1,j)\right) + \frac{b_4}{dy * dy} * (B_{old}(i,j+1) - 2 * B_{old}(i,j) + B_{old}(i,j-1)));$$

$$C\_new(i,j) = C_{old}(i,j) + dt * (k * A_{old}^2(i,j) * B_{old}(i,j) + \frac{c_1}{dx * dx} * \left(C_{old}(i+1,j) - 2 * C_{old}(i,j) + C_{old}(i-1,j)\right) + \frac{c_2}{dy * dy} * (C_{old}(i,j+1) - 2 * C_{old}(i,j) + C_{old}(i,j-1)));$$

$$D\_new(i,j) = D_{old}(i,j) + dt * (3 * k * A_{old}^2(i,j) * B_{old}(i,j) - \frac{d_1}{dx} * \left(D_{old}(i,j) - D_{old}(i-1,j)\right) - \frac{d_2}{dx} * (D_{old}(i,j) - D_{old}(i,j-1)));$$

Code:

```
    clc;
clear;
x_min = 0;
x_max = 15;

N = x_max * 10;
M = x_max * 10;

dx = (x_max - x_min)/N;
dy = (x_max - x_min)/N;

figure('units','normalized','outerposition',[0 0 1 1]);
```

```
x = linspace(0,x_max,N);
y = linspace(0,x_max,M);
[X,Y] = meshgrid(x,y);
T_0 = 0;

A_old = ones(N,M)*T_0;
A_new = ones(N,M)*T_0;
B_old = ones(N,M)*T_0;
B_new = ones(N,M)*T_0;
C_old = ones(N,M)*T_0;
C_new = ones(N,M)*T_0;
D_old = ones(N,M)*T_0;
D_new = ones(N,M)*T_0;

for i = 1:N
    for j = 1:M
        if sqrt((7.5 - i * dx)^2 + (7.5 - j * dy)^2) <= 1
            A_old(i,j) = 7;
        end
    end
end



t = 0; t_end = 24;
dt = 2 * dx * dy;

a_1 = 5 * dx * dx;
a_2 = 5 * dx * dx;
b_1 = 0.5;
b_2 = 0.5;
b_3 = 4 * dx * dx;
b_4 = 4 * dx * dx;
c_1 = 3 * dx * dx;
c_2 = 3 * dx * dx;
d_1 = 1;
d_2 = 1;

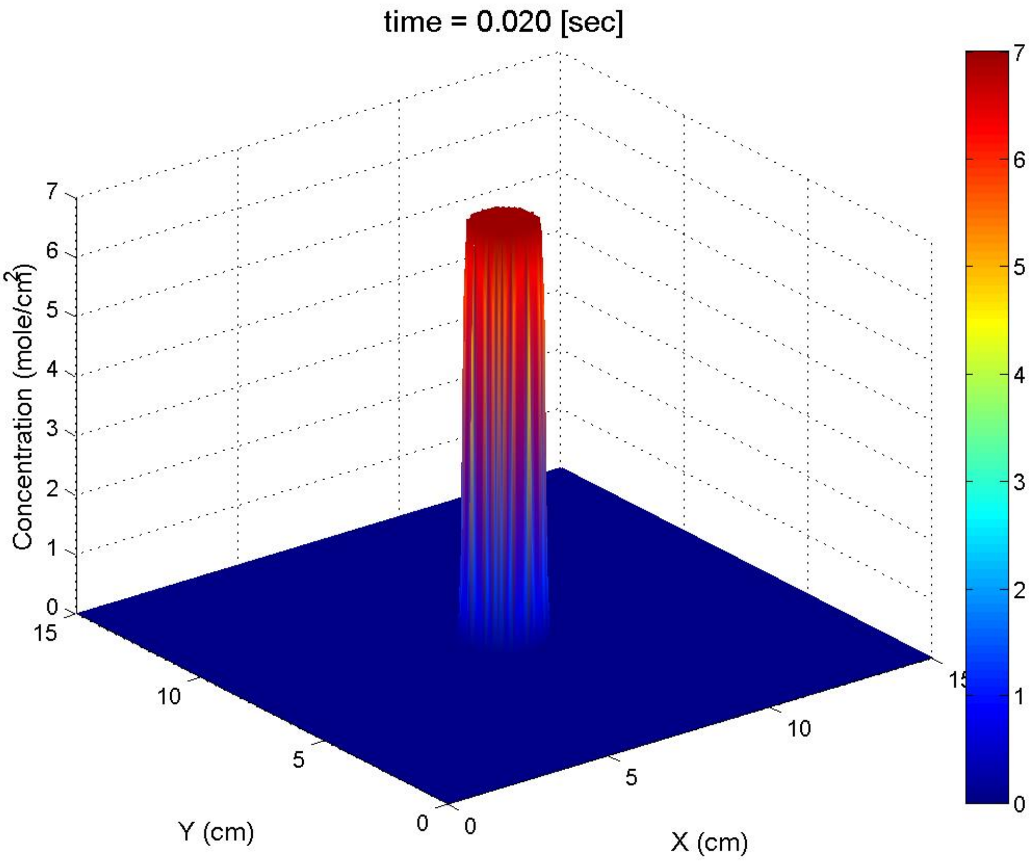
k = 0.1;

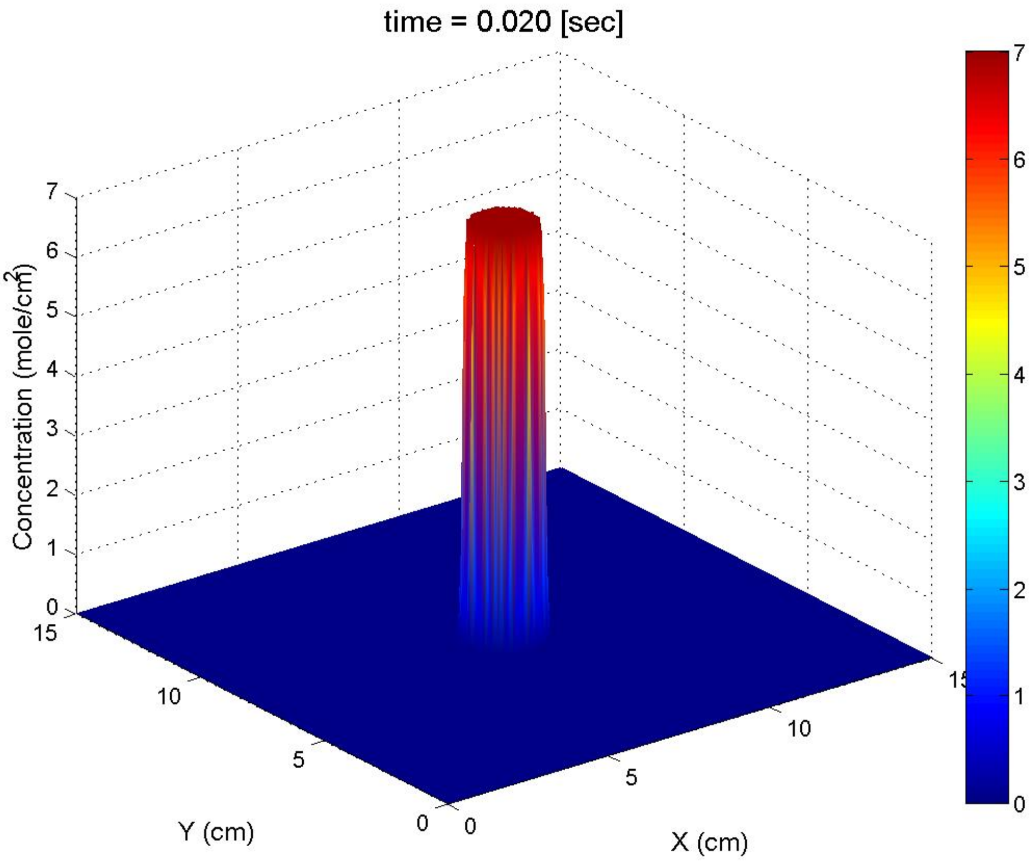
while t < t_end
    t = t + dt;
    for i = 2:N-1
        for j = 2:M-1
            A_new(i,j) = A_old(i,j) + dt * (-2 * k * A_old(i,j)^2 * B_old(i,j)
+ a_1 / (dx * dx) * (A_old(i+1,j) - 2 * A_old(i,j) + A_old(i-1,j)) + a_2 / (dy * dy) * (A_old(i,j+1)
- 2 * A_old(i,j) + A_old(i,j-1)) );
            B_new(i,j) = B_old(i,j) + dt * (    -k * A_old(i,j)^2 * B_old(i,j) - b_1 / dx * (B_old(i,j) -
B_old(i-1,j)) - b_2 / dx * (B_old(i,j) - B_old(i,j-1)) + b_3 / (dx * dx) * (B_old(i+1,j) - 2 *
B_old(i,j) + B_old(i-1,j)) + b_4 / (dy * dy) * (B_old(i,j+1) - 2 * B_old(i,j) + B_old(i,j-1)) );
```

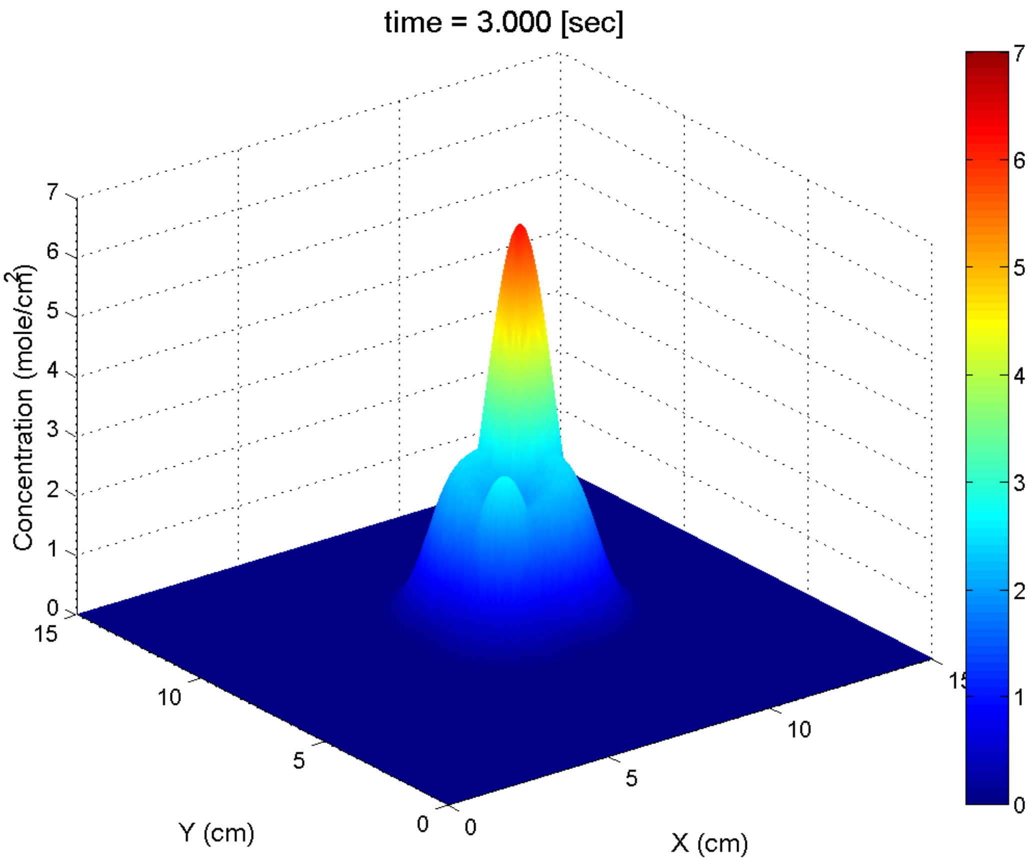
```
            C_new(i,j) = C_old(i,j) + dt * (     k * A_old(i,j)^2 * B_old(i,j)
+ c_1 / (dx * dx) * (C_old(i+1,j) - 2 * C_old(i,j) + C_old(i-1,j)) + c_2 / (dy * dy) * (C_old(i,j+1)
- 2 * C_old(i,j) + C_old(i,j-1)) );
            D_new(i,j) = D_old(i,j) + dt * ( 3 * k * A_old(i,j)^2 * B_old(i,j) - d_1 / dx * (D_old(i,j) -
D_old(i-1,j)) - d_2 / dx * (D_old(i,j) - D_old(i,j-1))
);
        end
    end
    if t >= 0.5 && t <= 1.0
        for i = 1:N
            for j = 1:M
                if sqrt((7.5/2 - i * dx/2)^2 + (7.5/2 - j * dy/2)^2) <= 1
                    B_new(i,j) = (t-0.5) * 3 * 2;
                end
            end
        end
    end
    A_old = A_new;
    B_old = B_new;
    C_old = C_new;
    D_old = D_new;

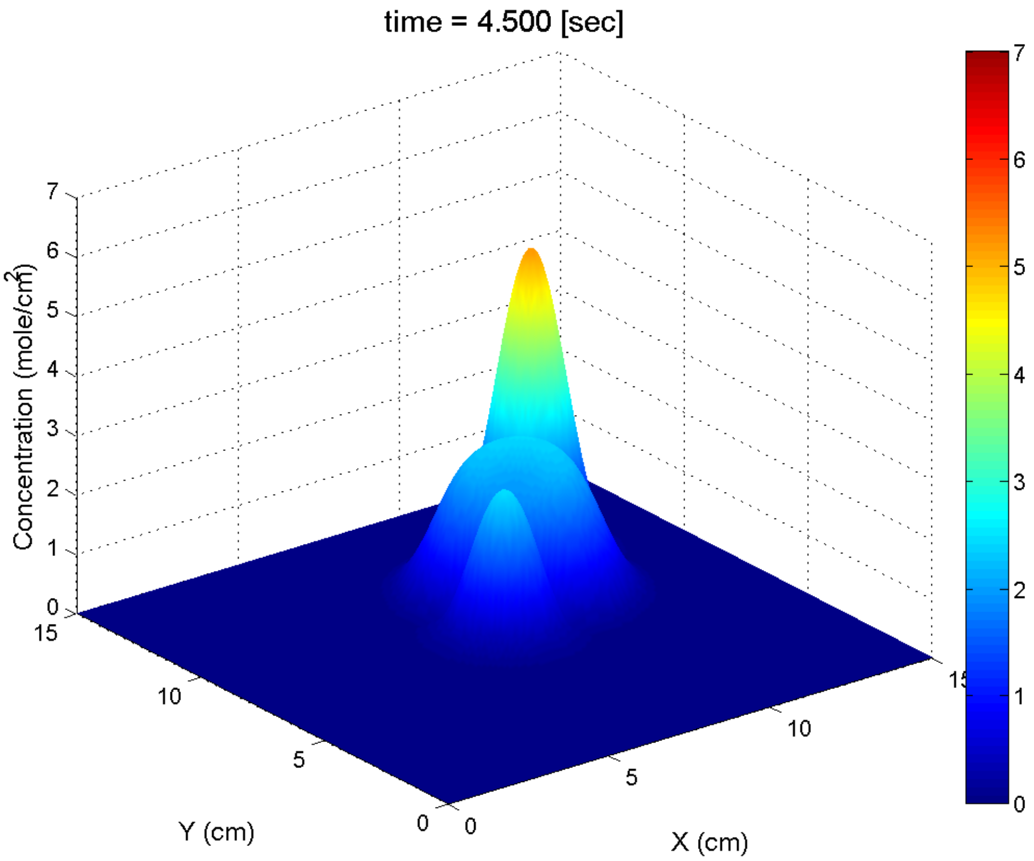
    surf(X,Y,A_old);
    shading interp;
    hold on;
    surf(X,Y,B_old);
    shading interp;
    hold on;
    surf(X,Y,C_old);
    shading interp;
    hold on;
    surf(X,Y,D_old);
    shading interp;
    hold off;
    %view(2);
    colormap(jet(90)), colorbar
    caxis([0 7])
    title({sprintf('\n time = %1.3f [sec]',t)},'FontSize',14)
    zlim([0 7])
    xlabel('X (cm)','FontSize',12);
    ylabel('Y (cm)','FontSize',12);
    zlabel('Concentration (mole/cm^{2})','FontSize',12);
    axis([0 x_max 0 x_max 0 7]);
    drawnow;
end
```

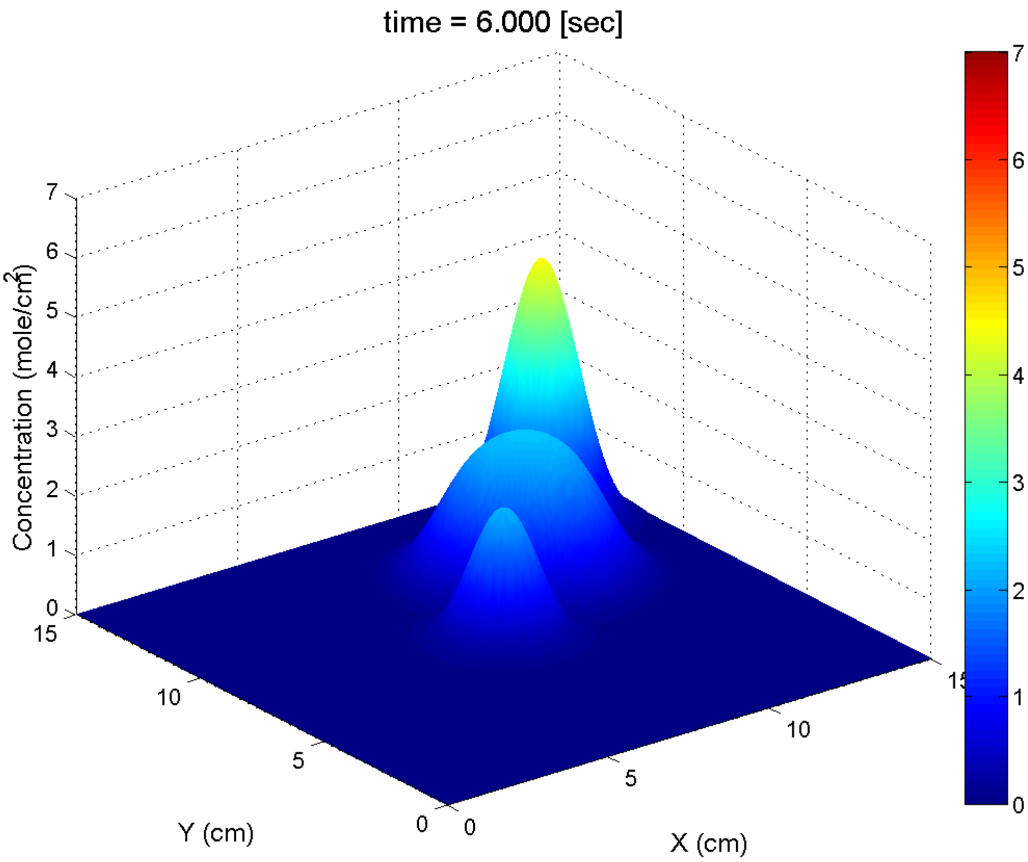
Results:

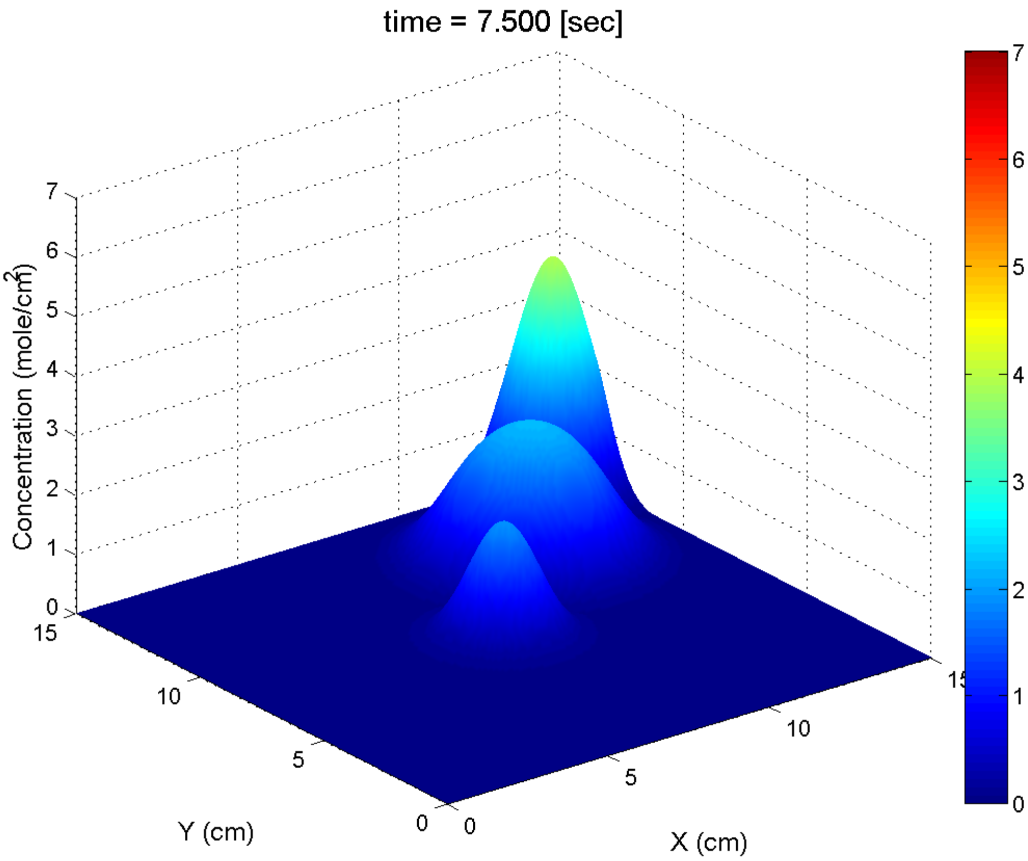

time = 0.020 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0

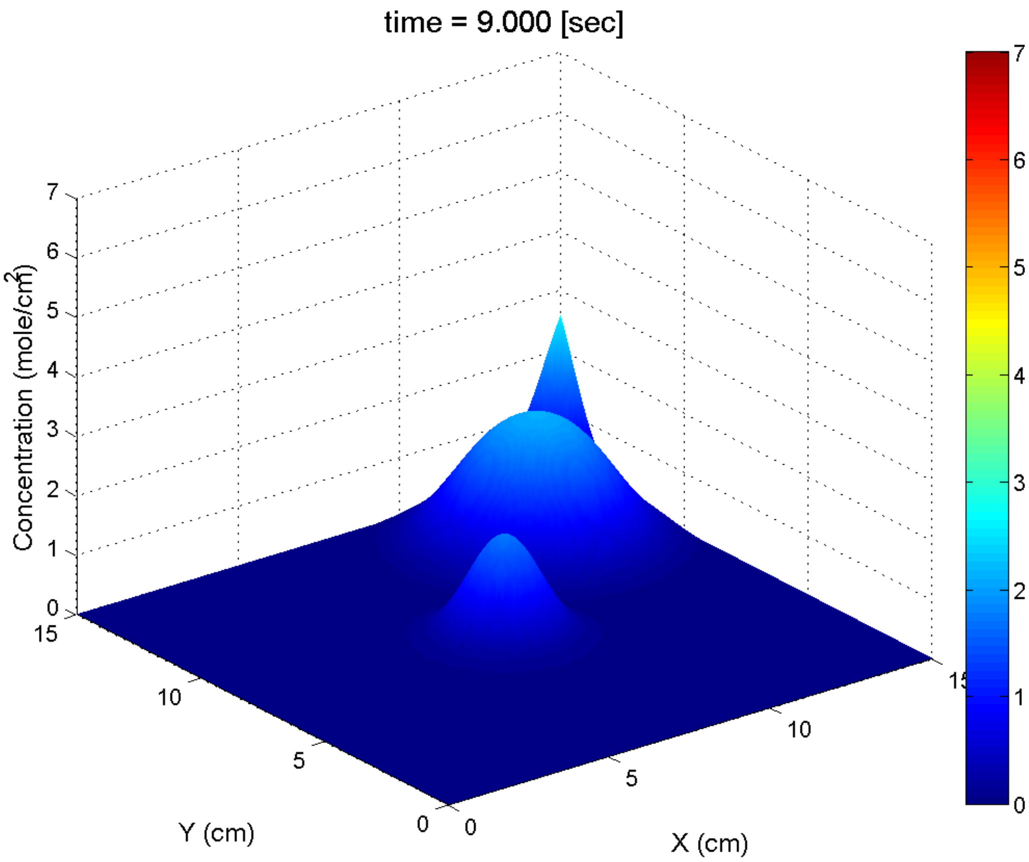

time = 0.020 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0

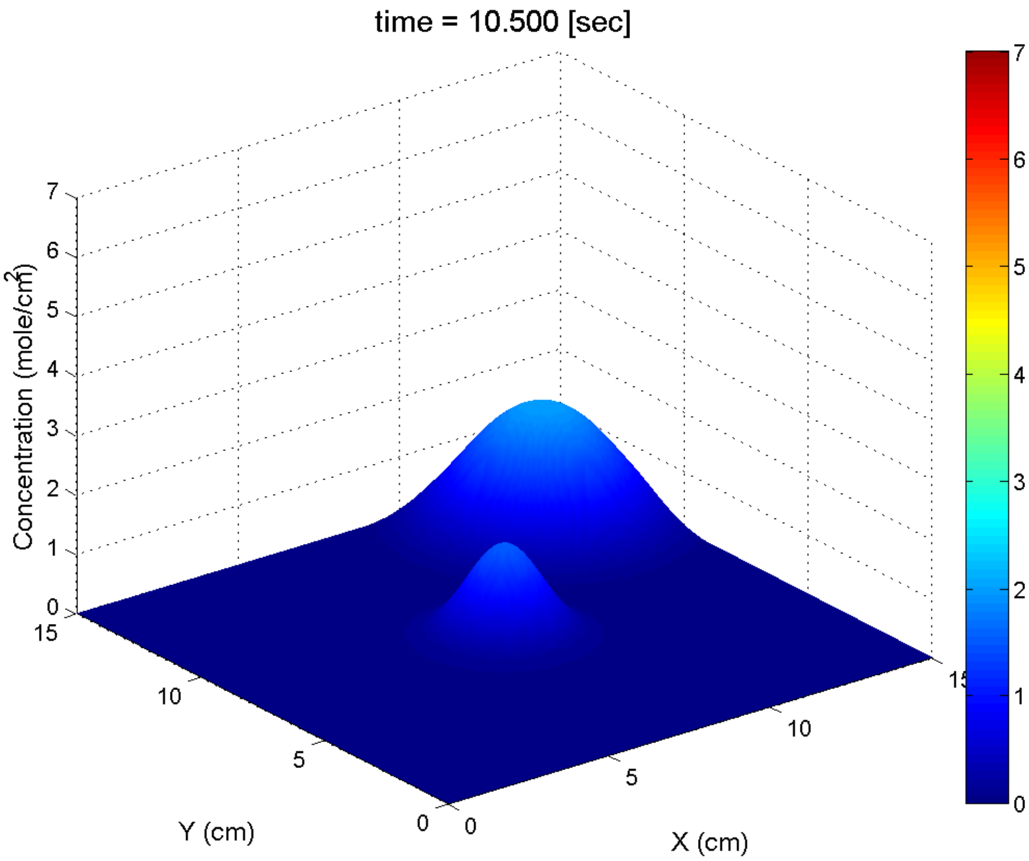

time = 3.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0

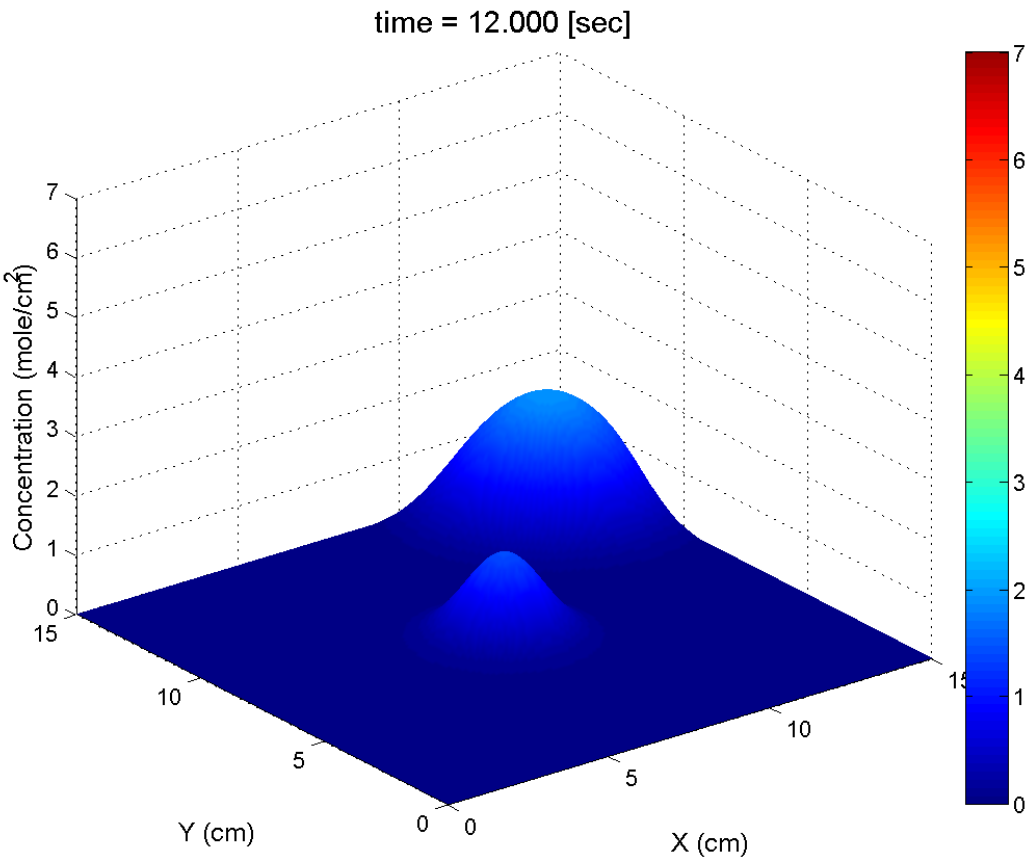

time = 4.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0

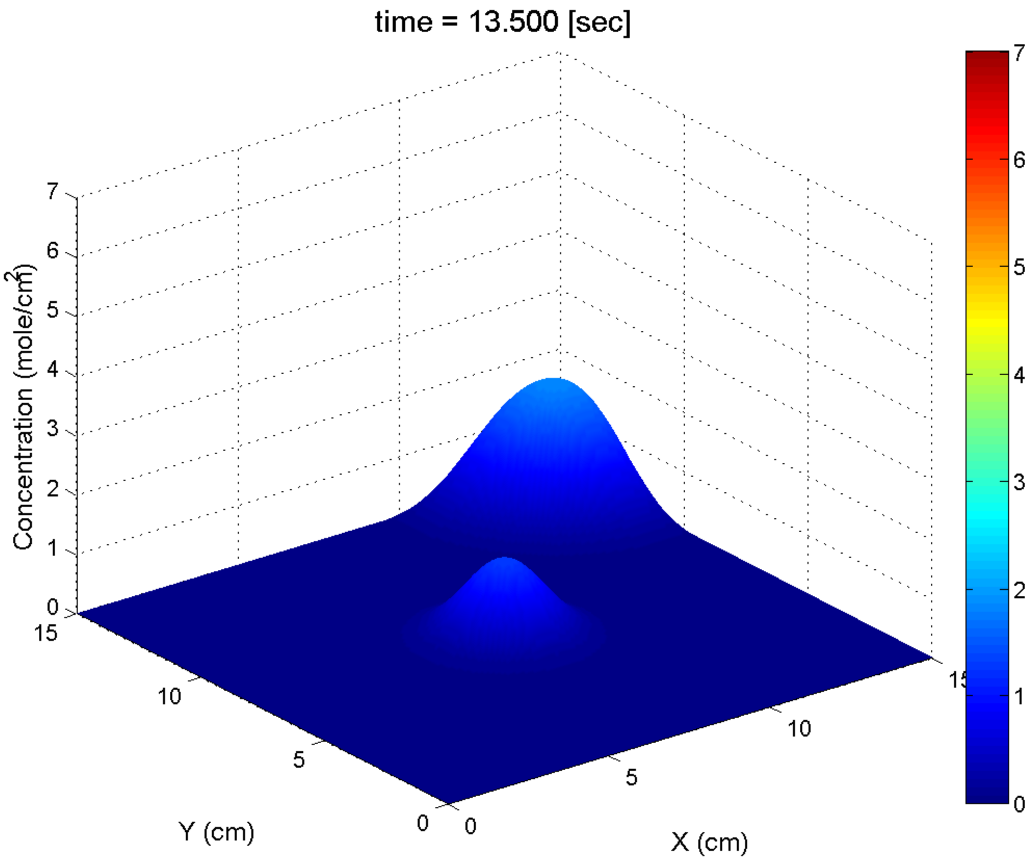

time = 6.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10
15

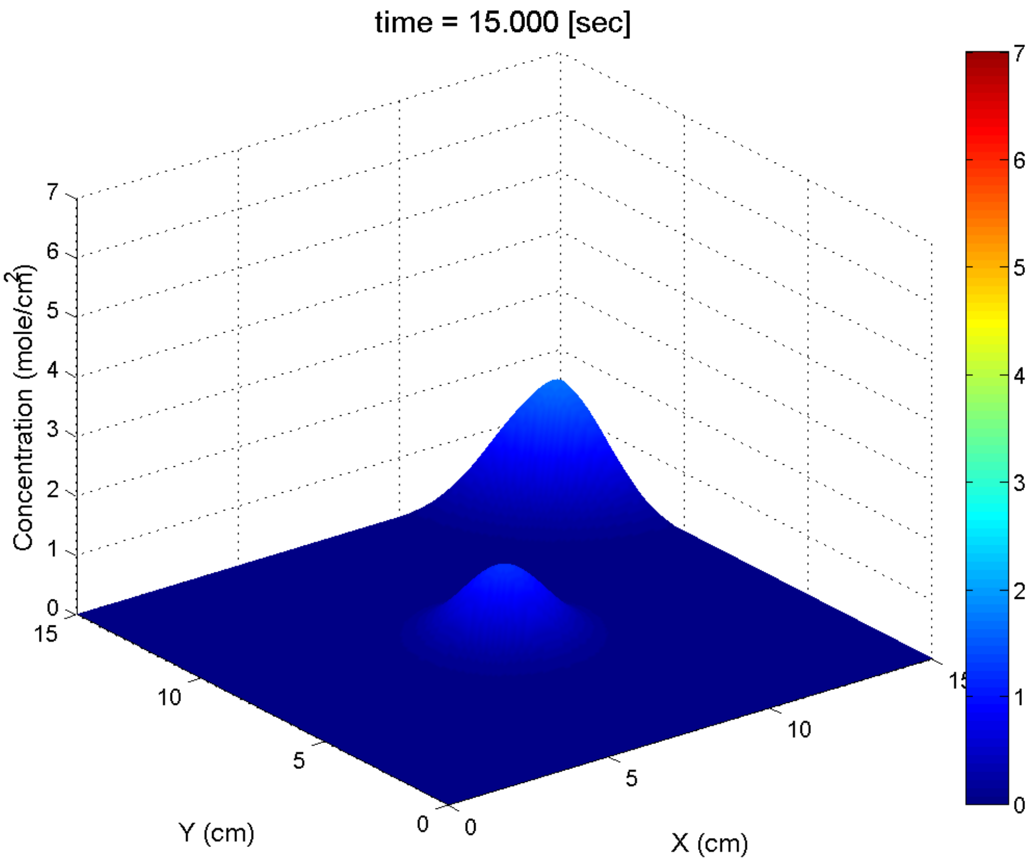

time = 7.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10
15

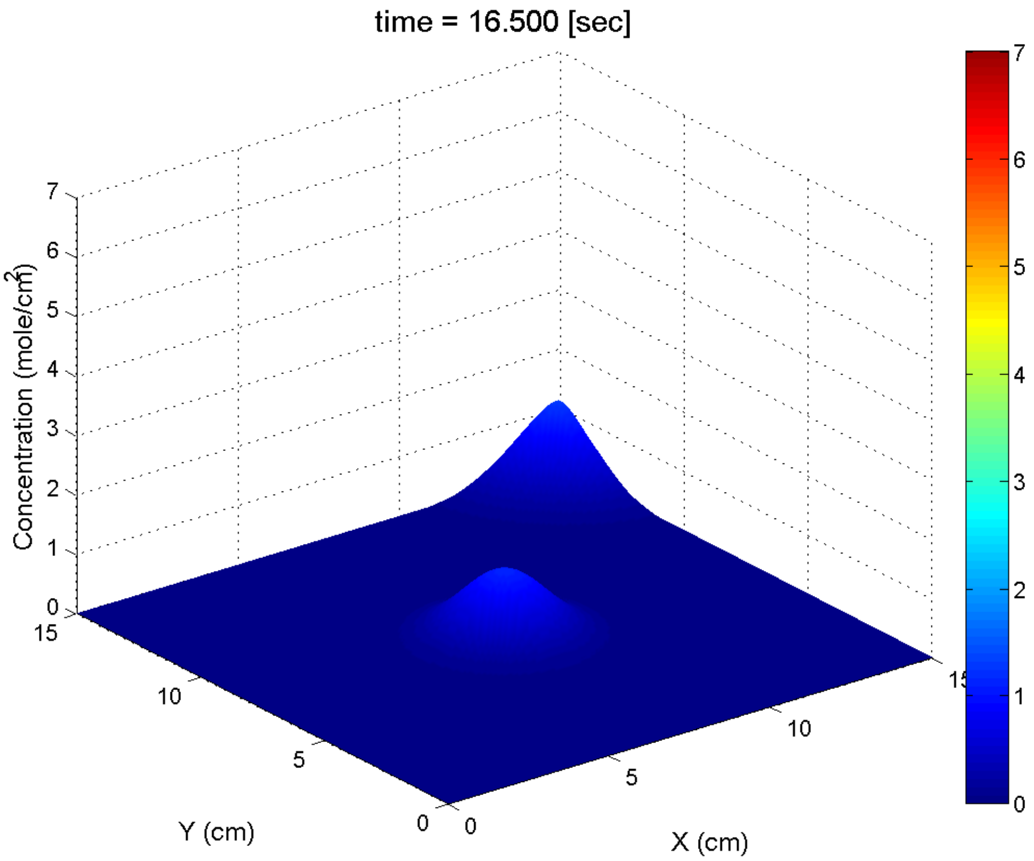

time = 9.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0

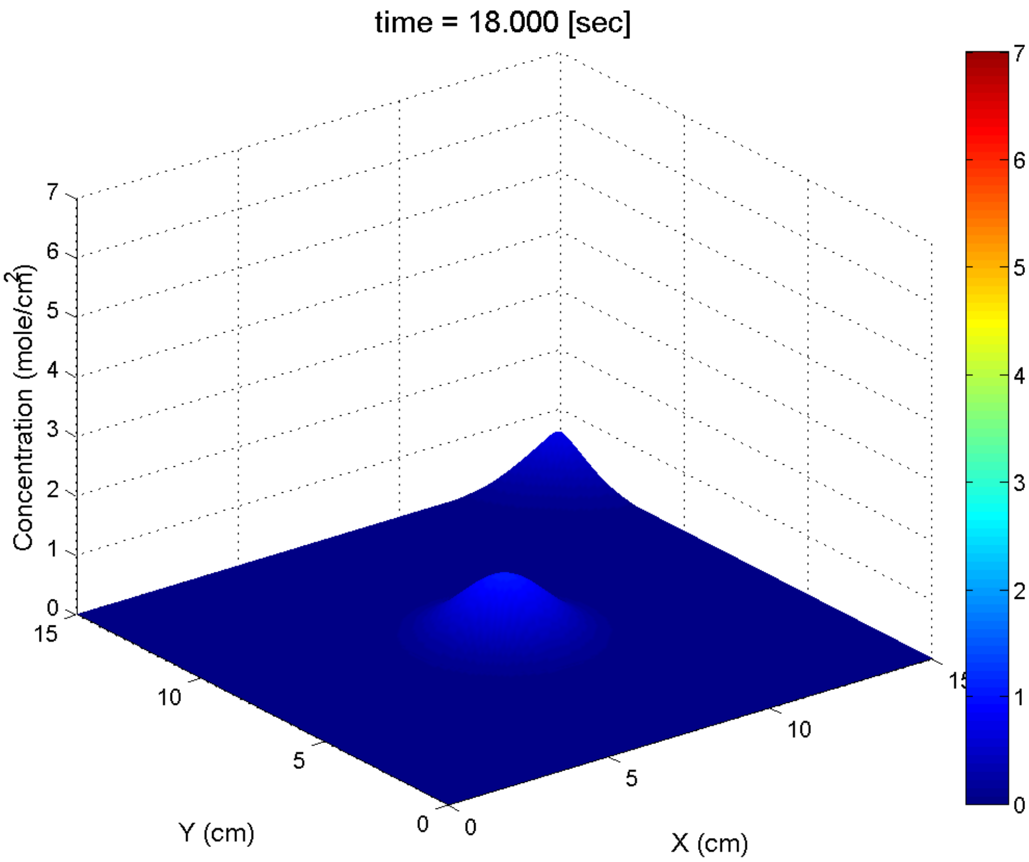

time = 10.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0

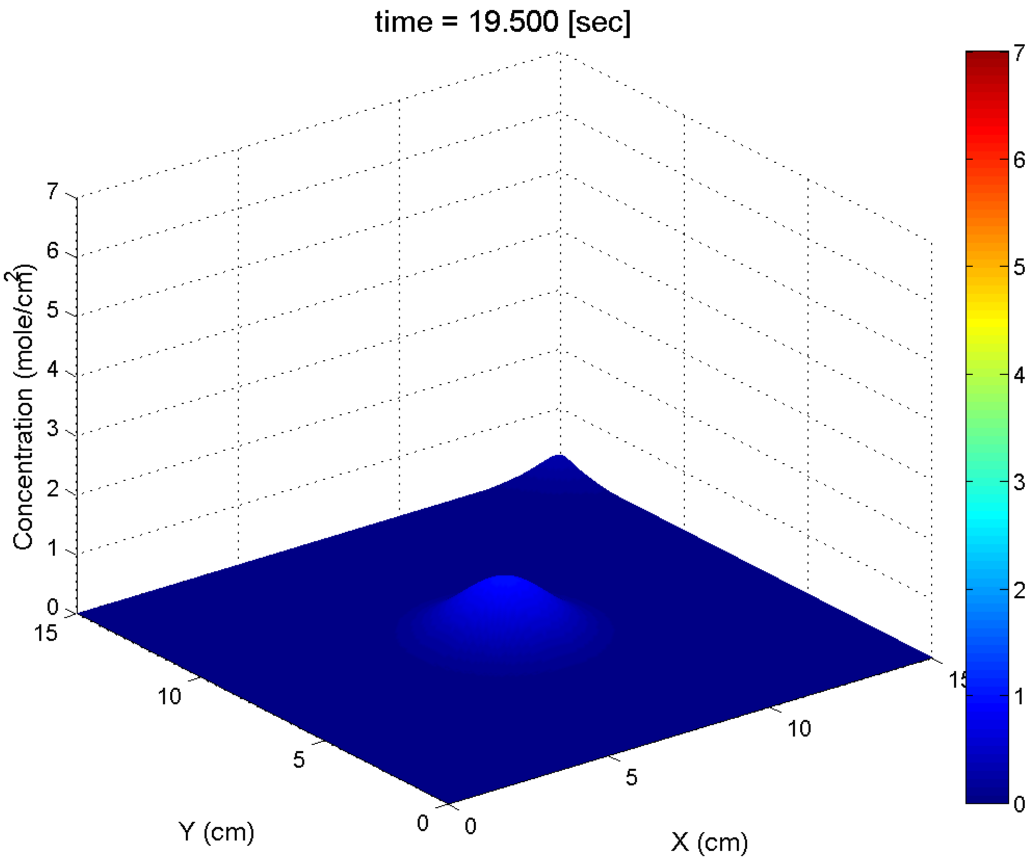

time = 12.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15
0
5
10
15

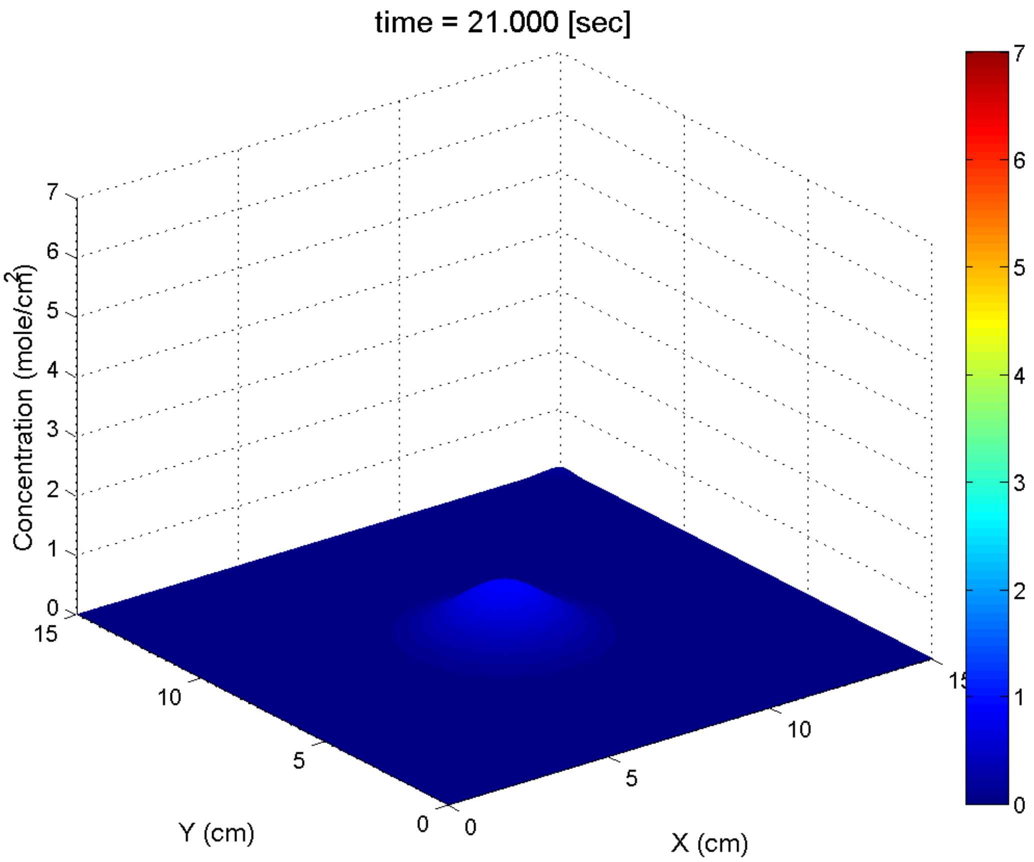

time = 13.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15
0
5
10
15

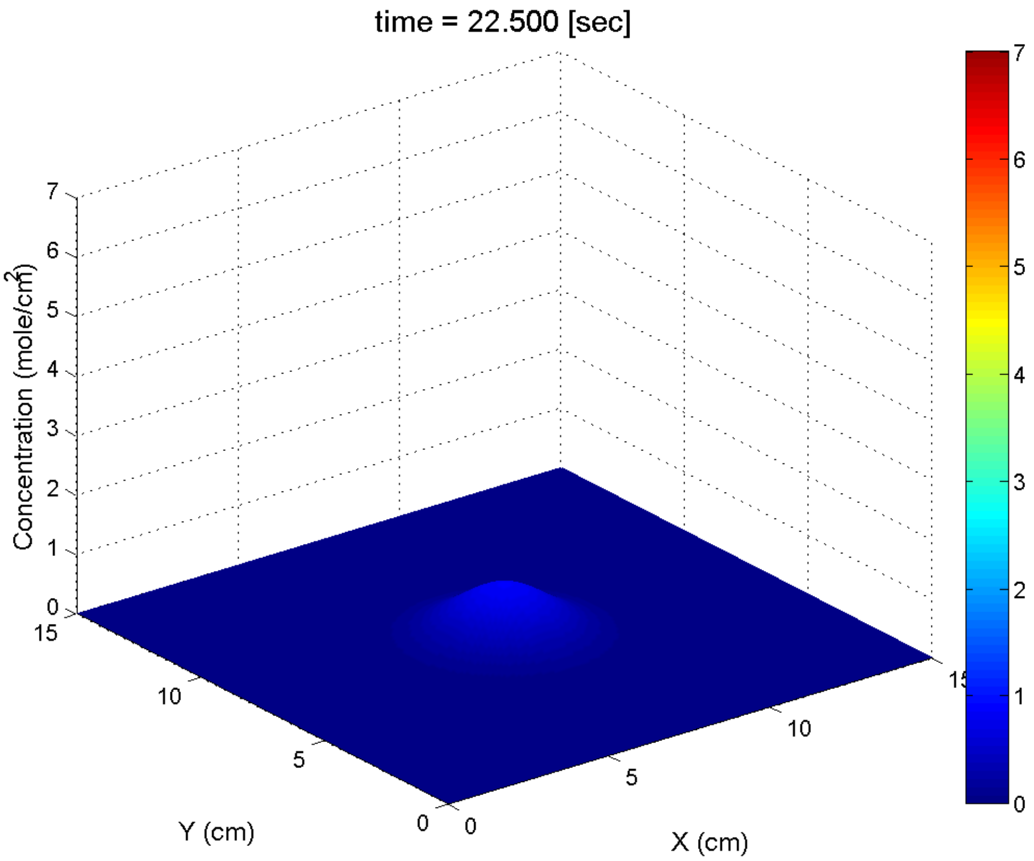

time = 15.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7

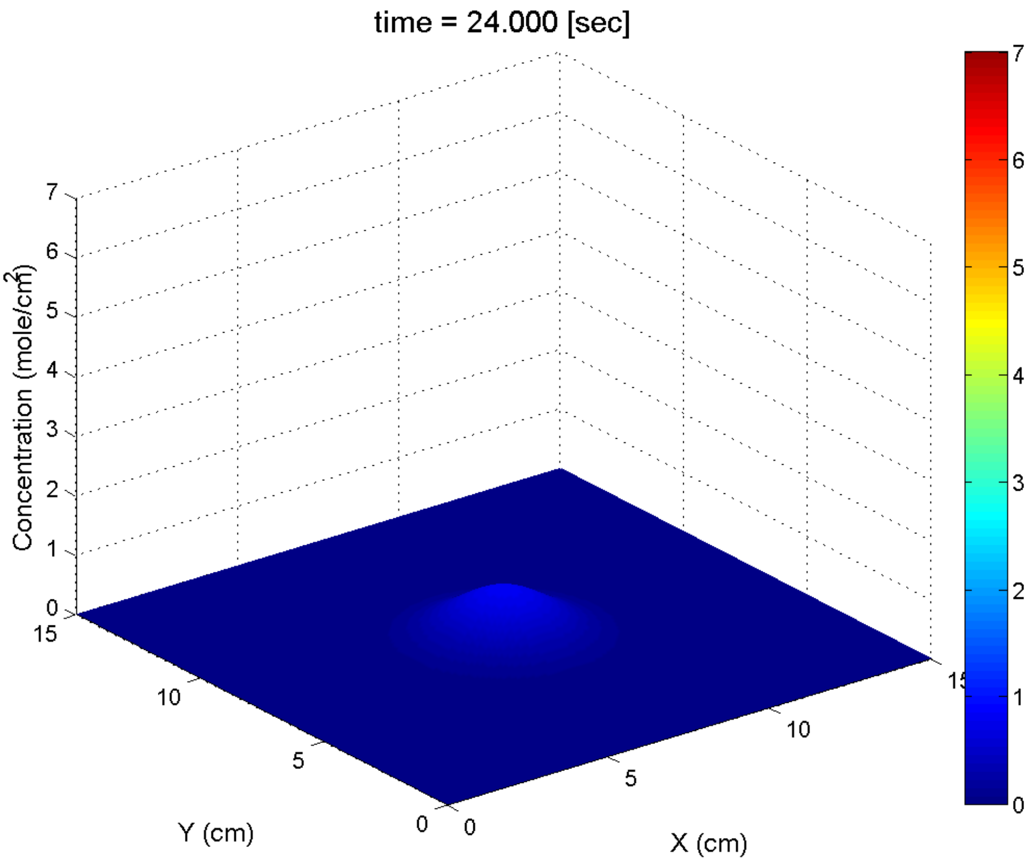

time = 16.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7


time = 18.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0


time = 19.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0


time = 21.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15

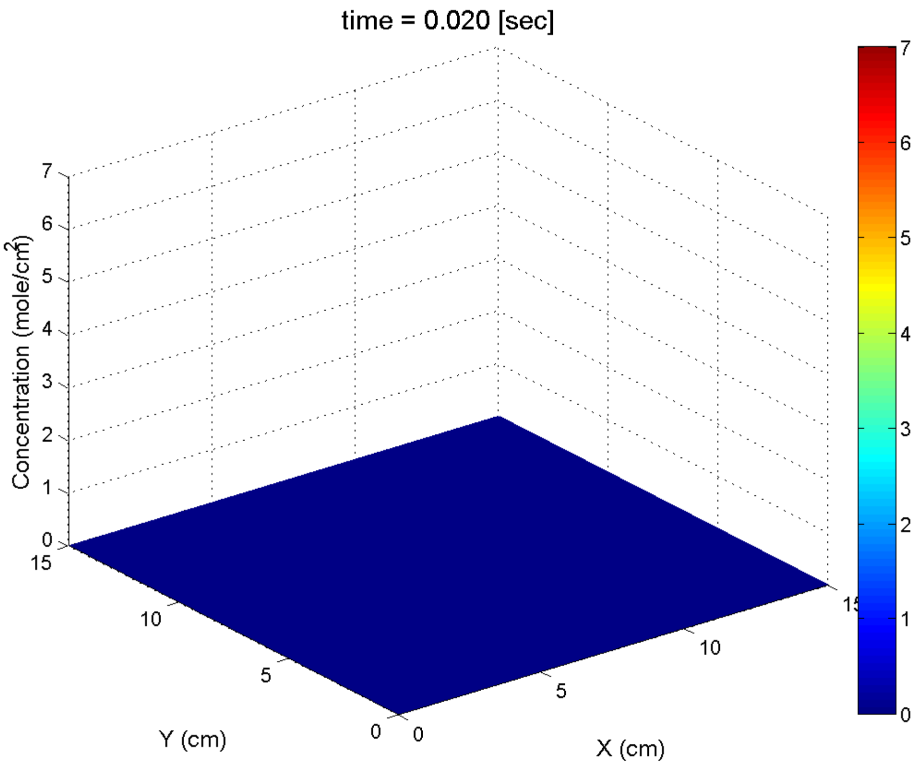

time = 22.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15

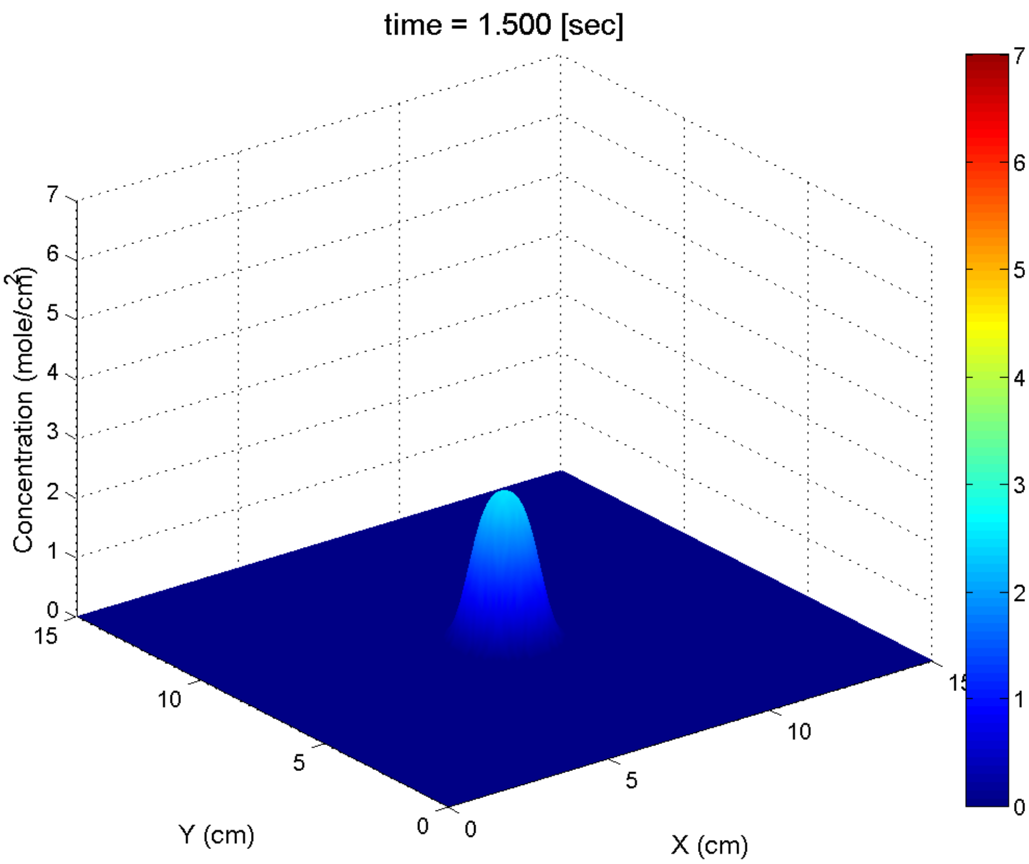


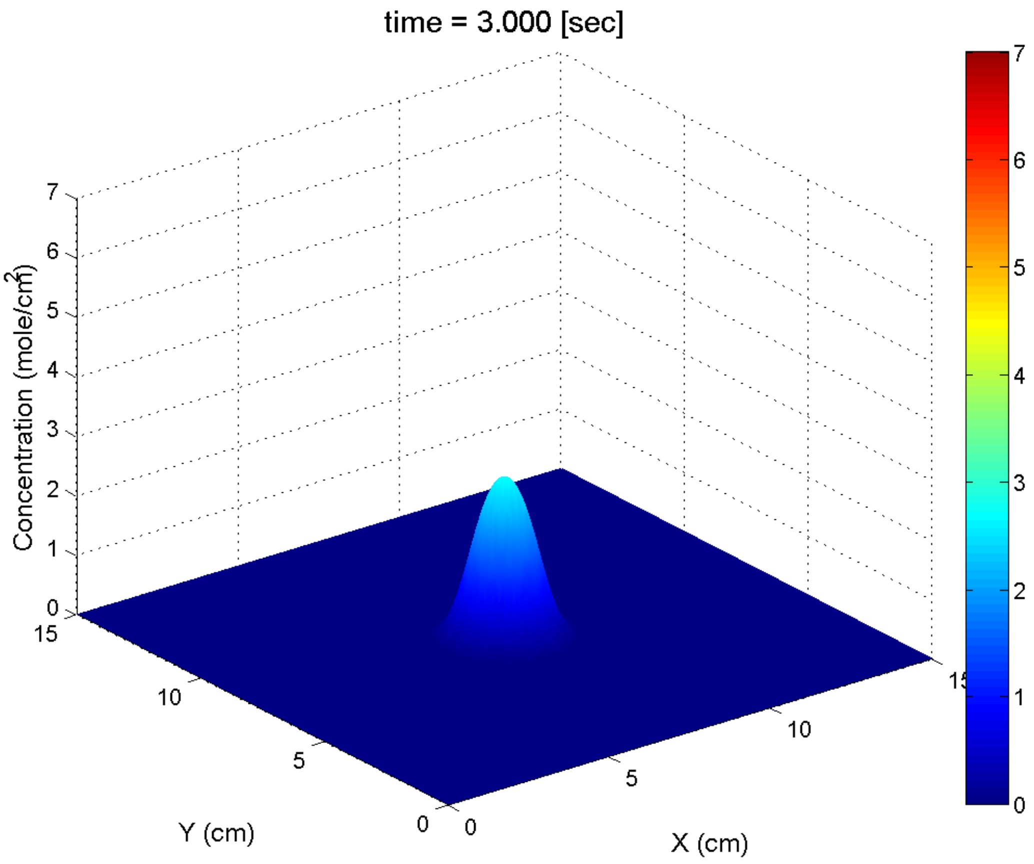
Conclusion:

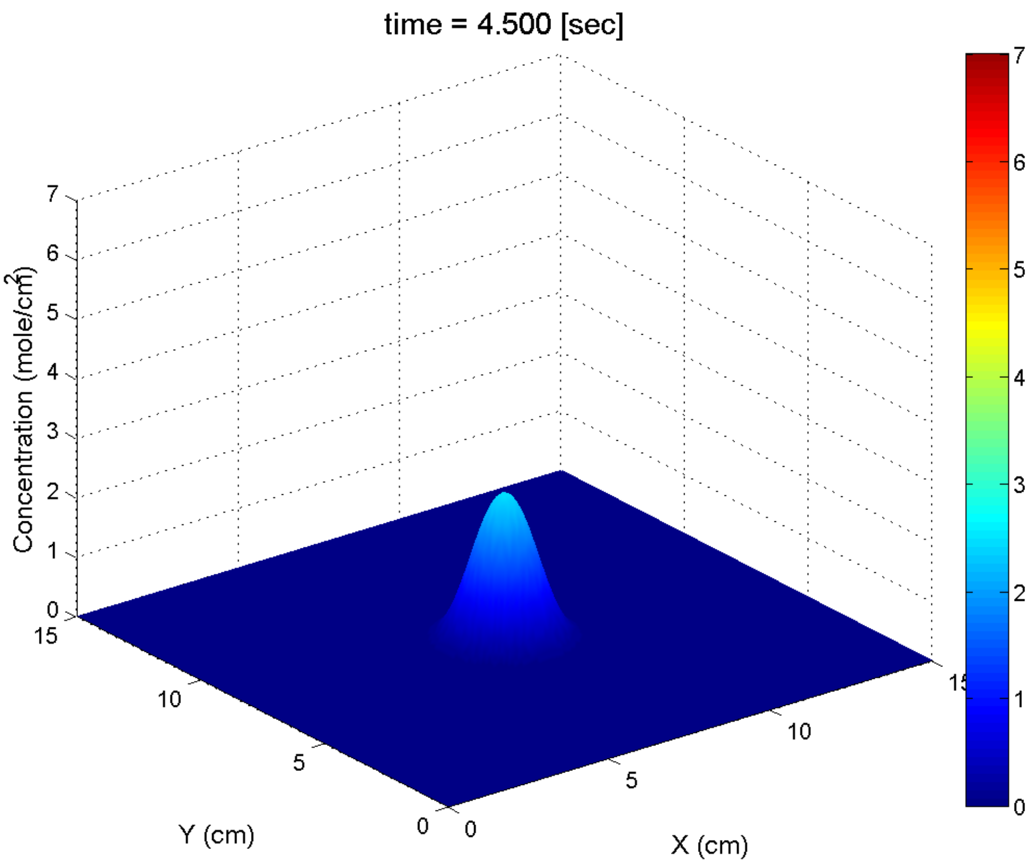
So, to sum up, we have considered previous two matters` reaction in two-dimensional space. Here we got same results but in two-dimensional space. Next, we will show the results of every product of the reaction. Because while all 4 matters on the same plane it will be hard to understand what is what. So, we need to animate each product to make understandable.

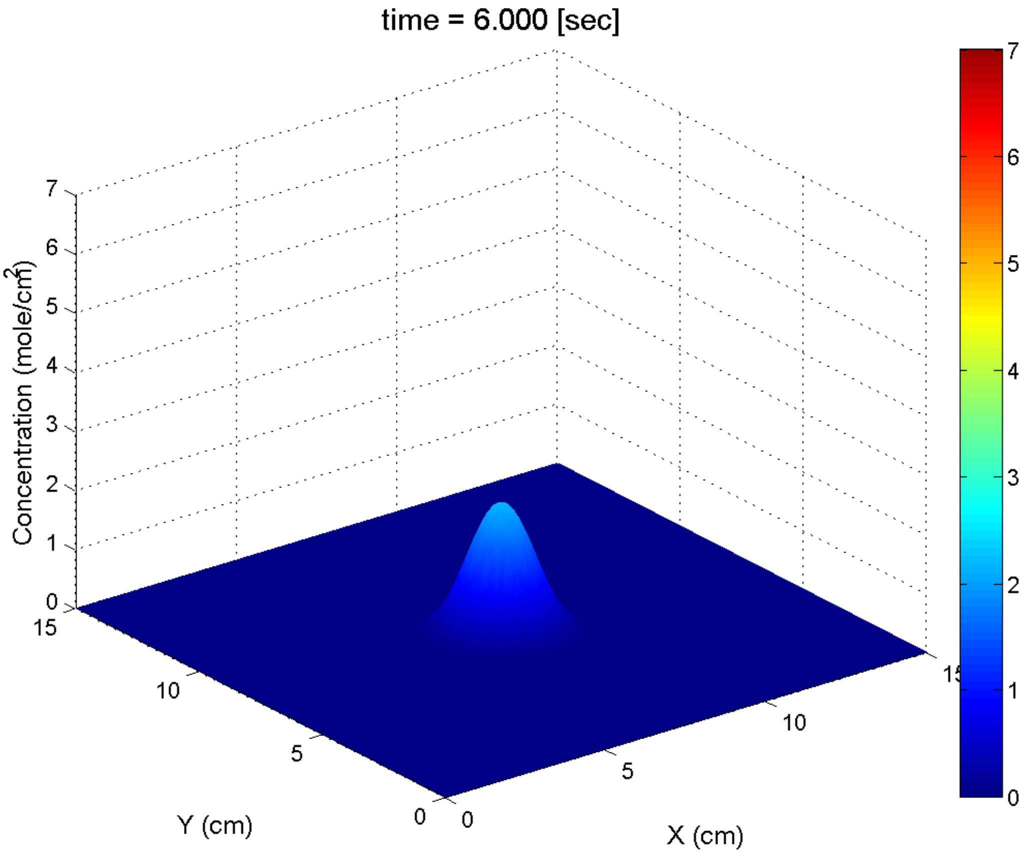
Product C:

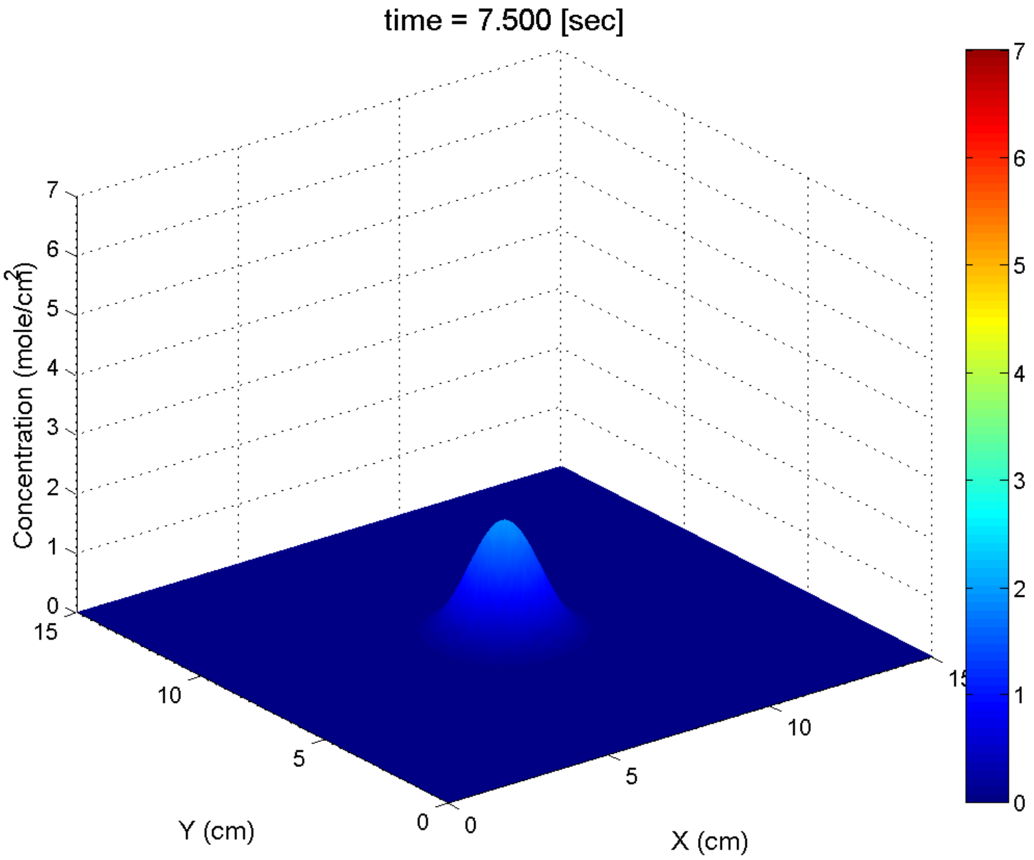

time = 0.020 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15

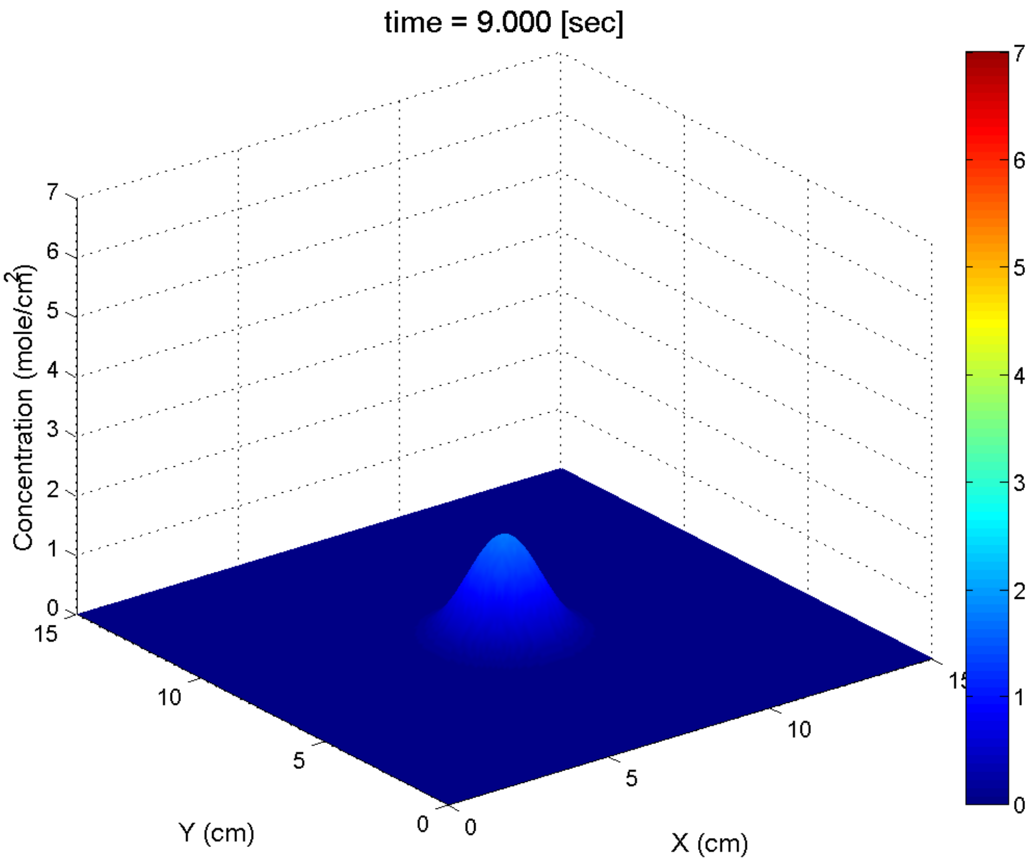

time = 1.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15

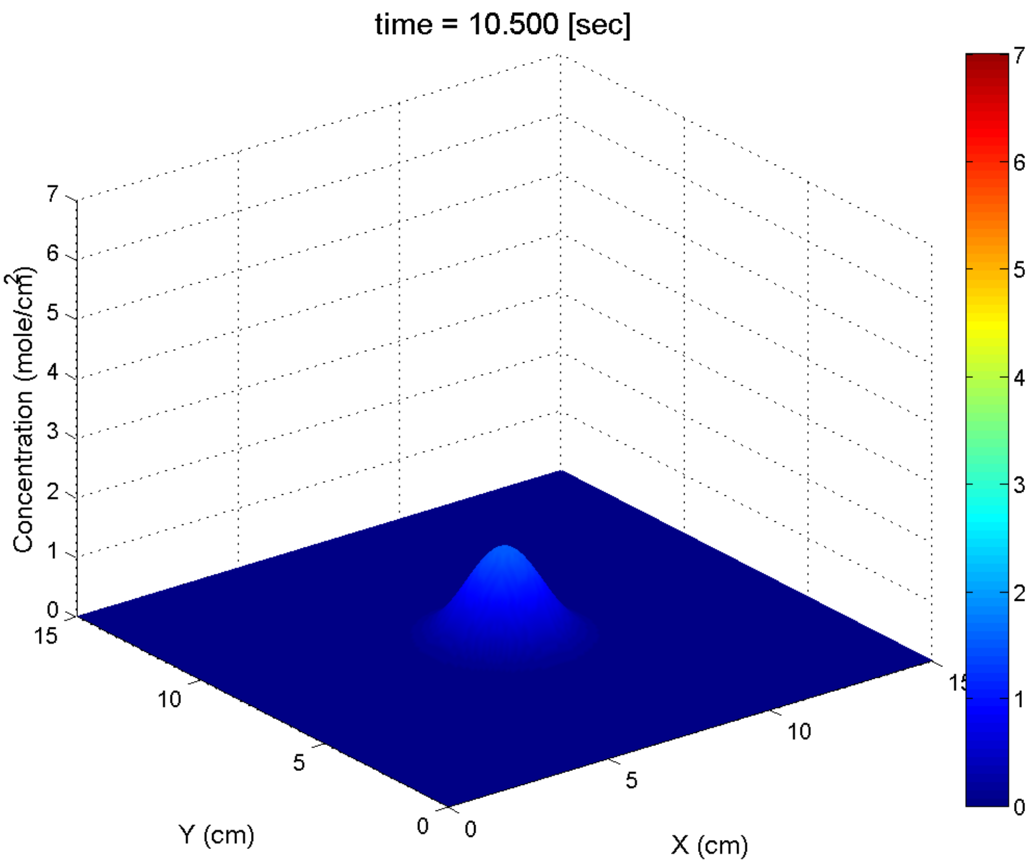

time = 3.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

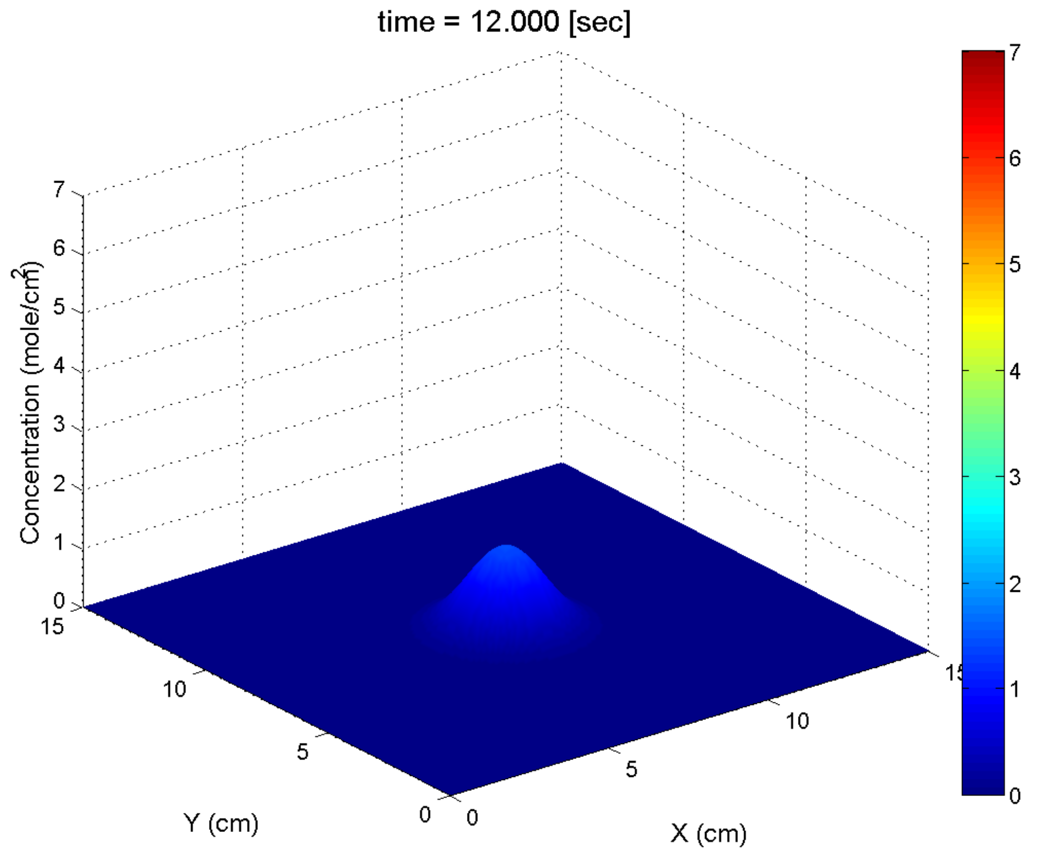

time = 4.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

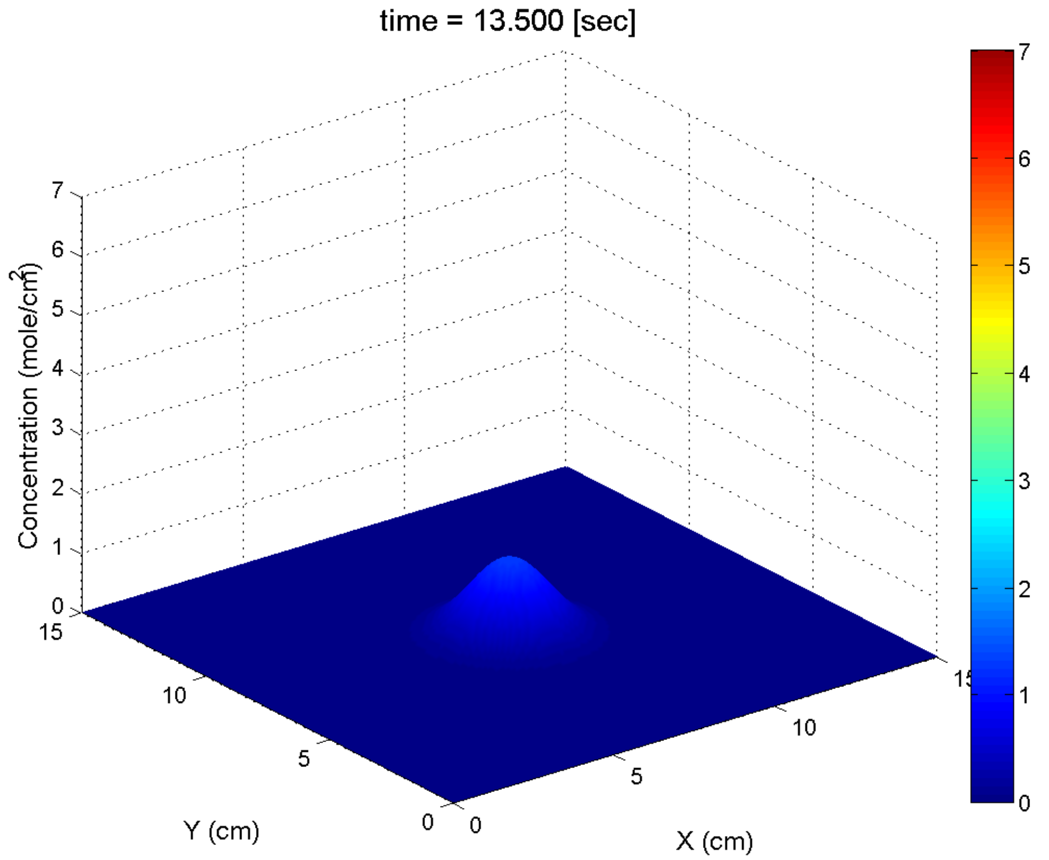

time = 6.000 [sec]
Concentration (mole/cm^2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10
15

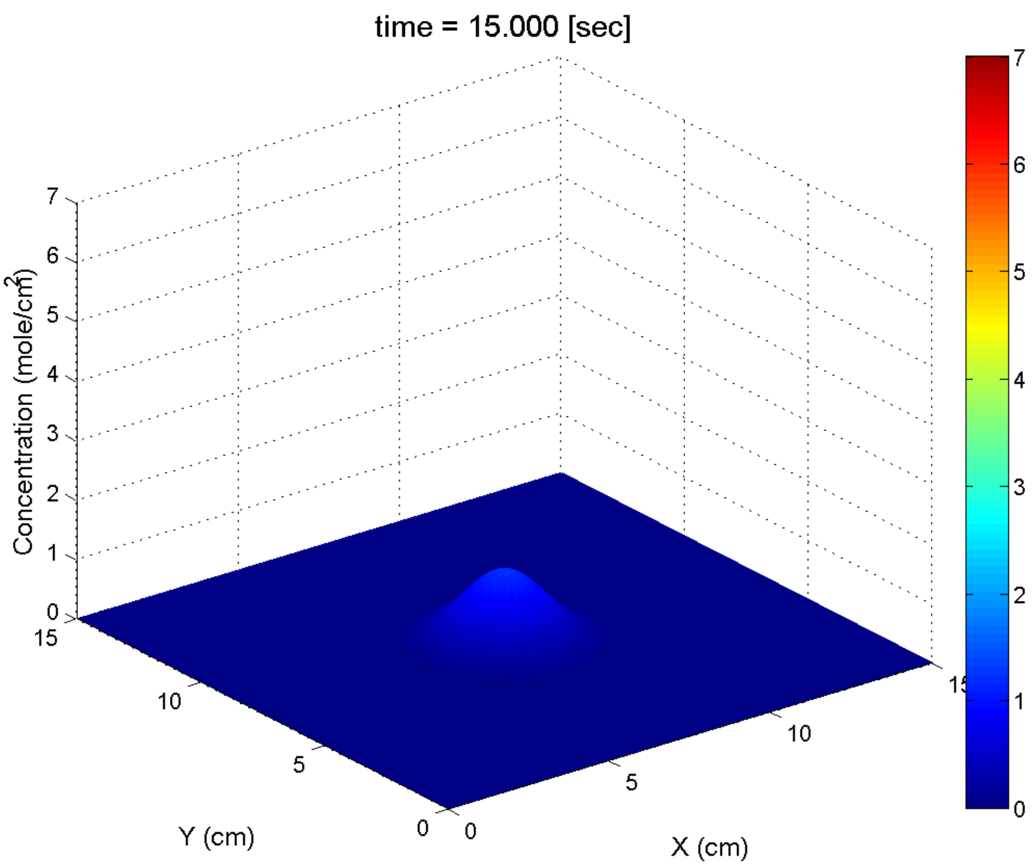

time = 7.500 [sec]
Concentration (mole/cm^2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10
15

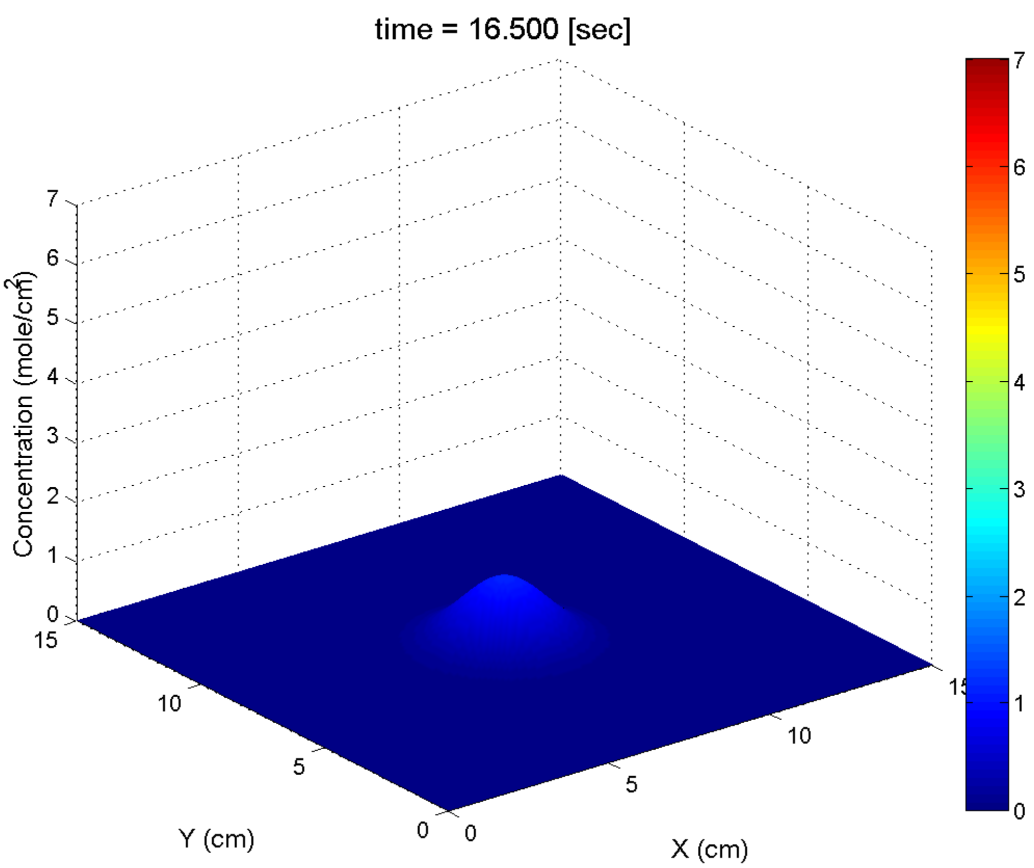

time = 9.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10

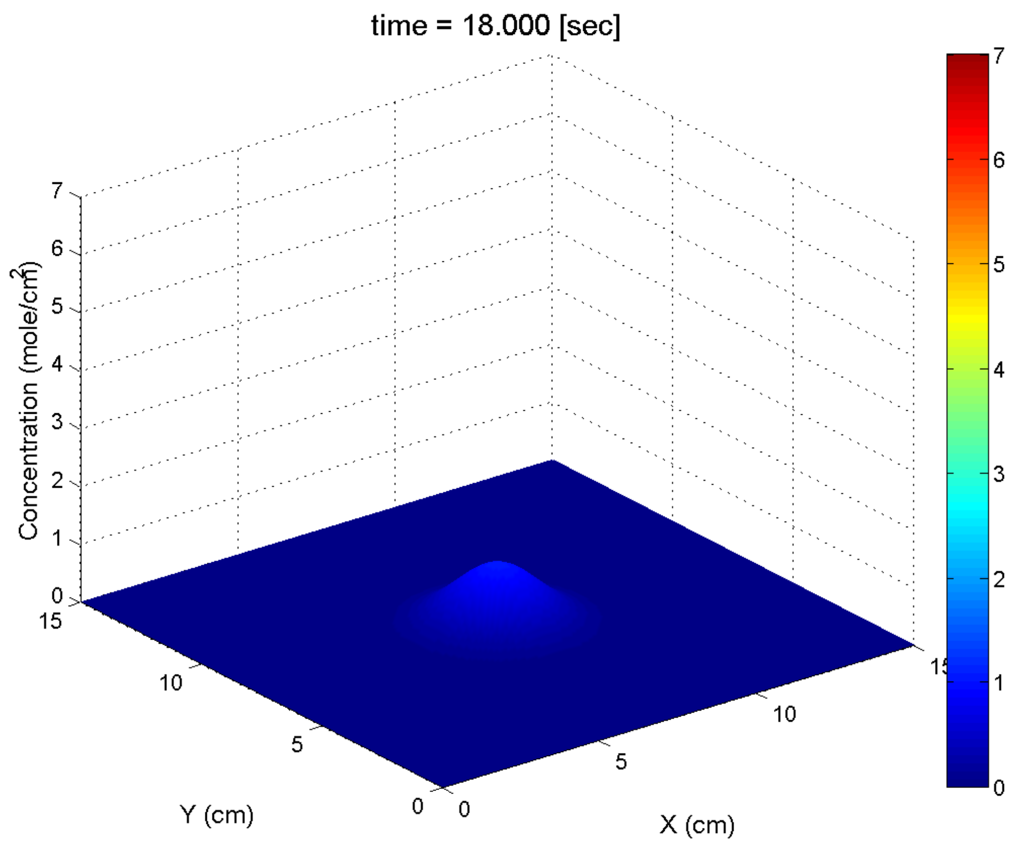

time = 10.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10

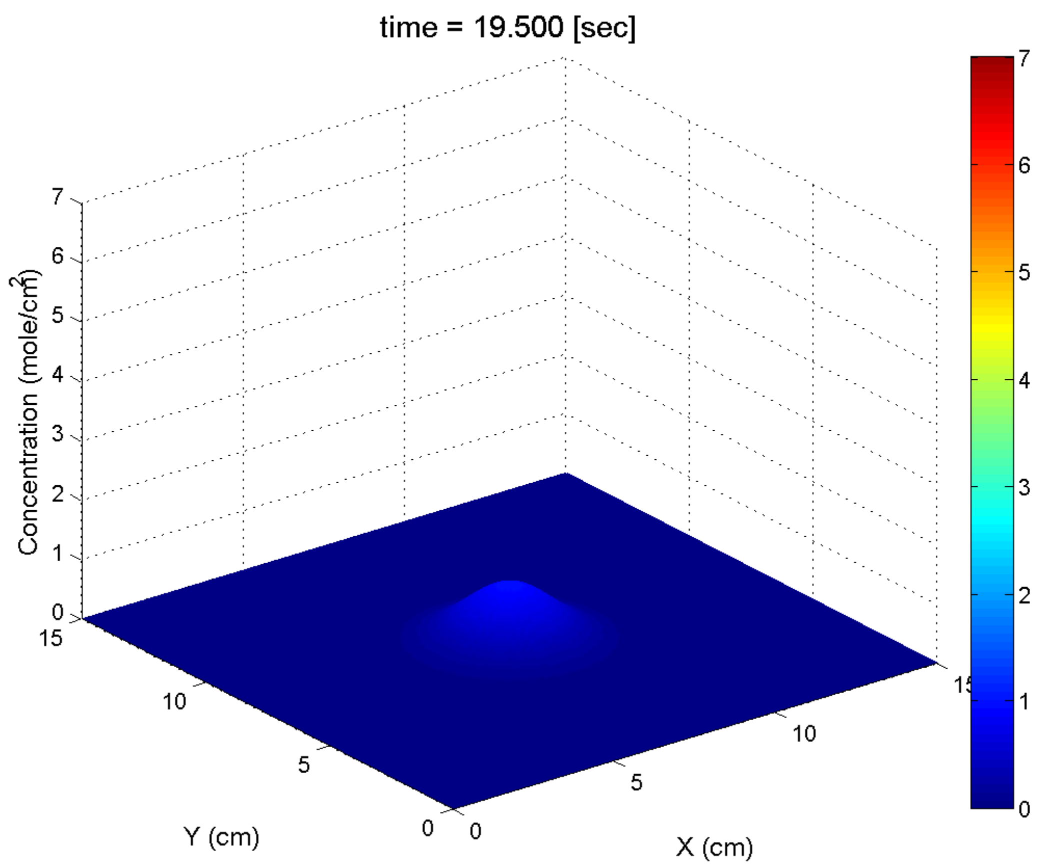

time = 12.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

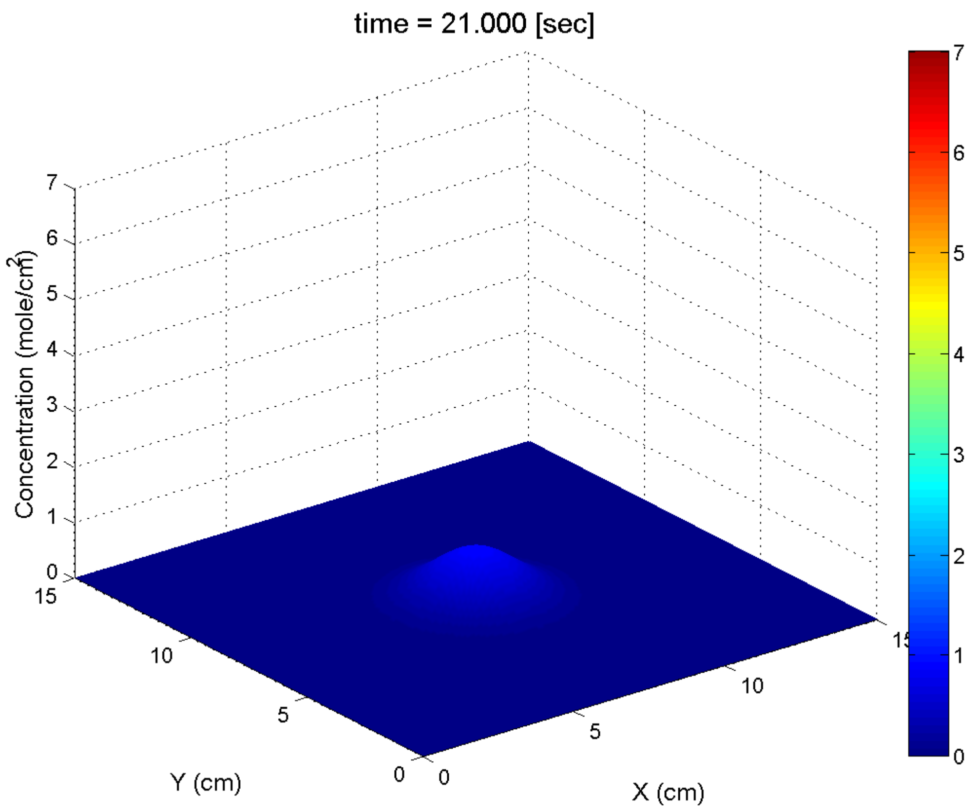

time = 13.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

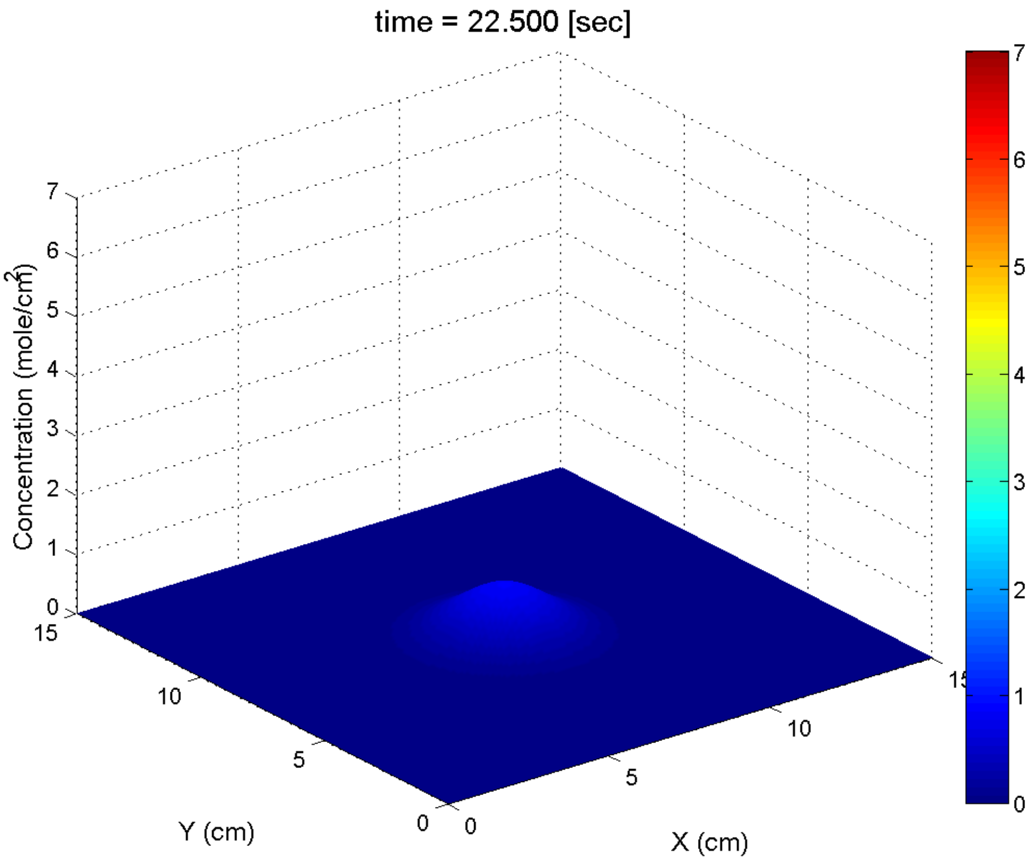

time = 15.000 [sec]
Concentration (mole/cm²)
Y (cm)
X (cm)

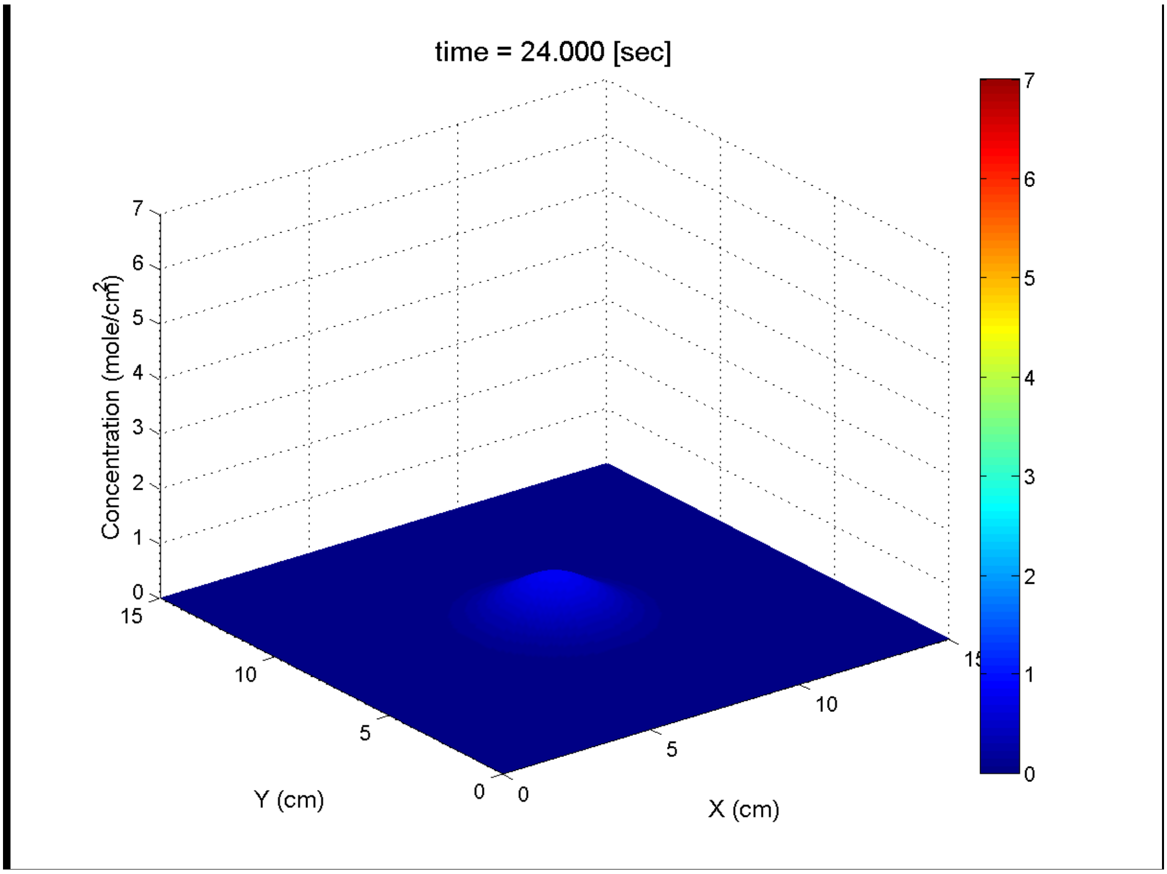

time = 16.500 [sec]
Concentration (mole/cm²)
Y (cm)
X (cm)


time = 18.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

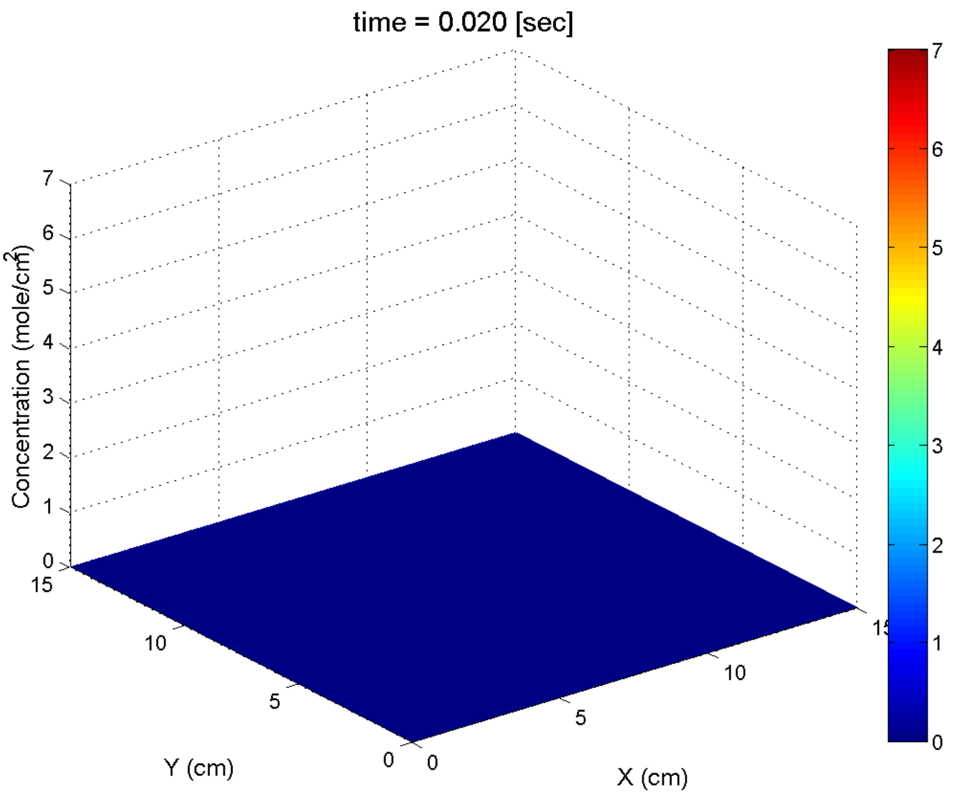

time = 19.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

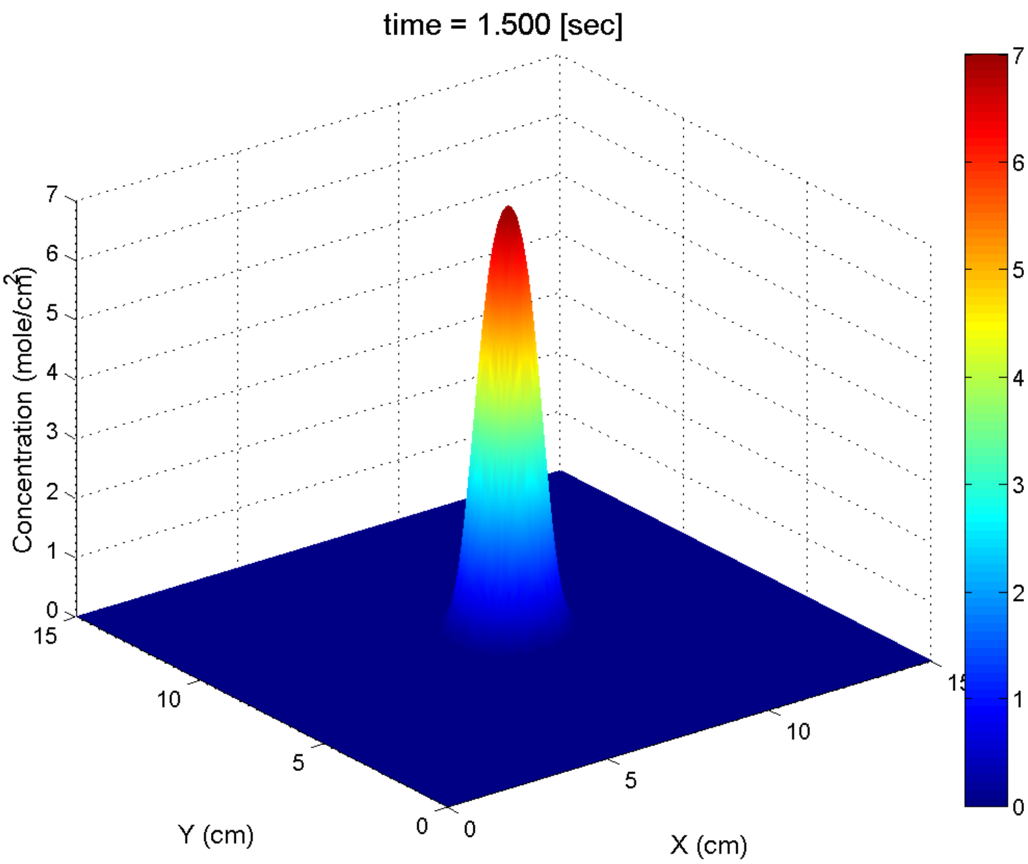

time = 21.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

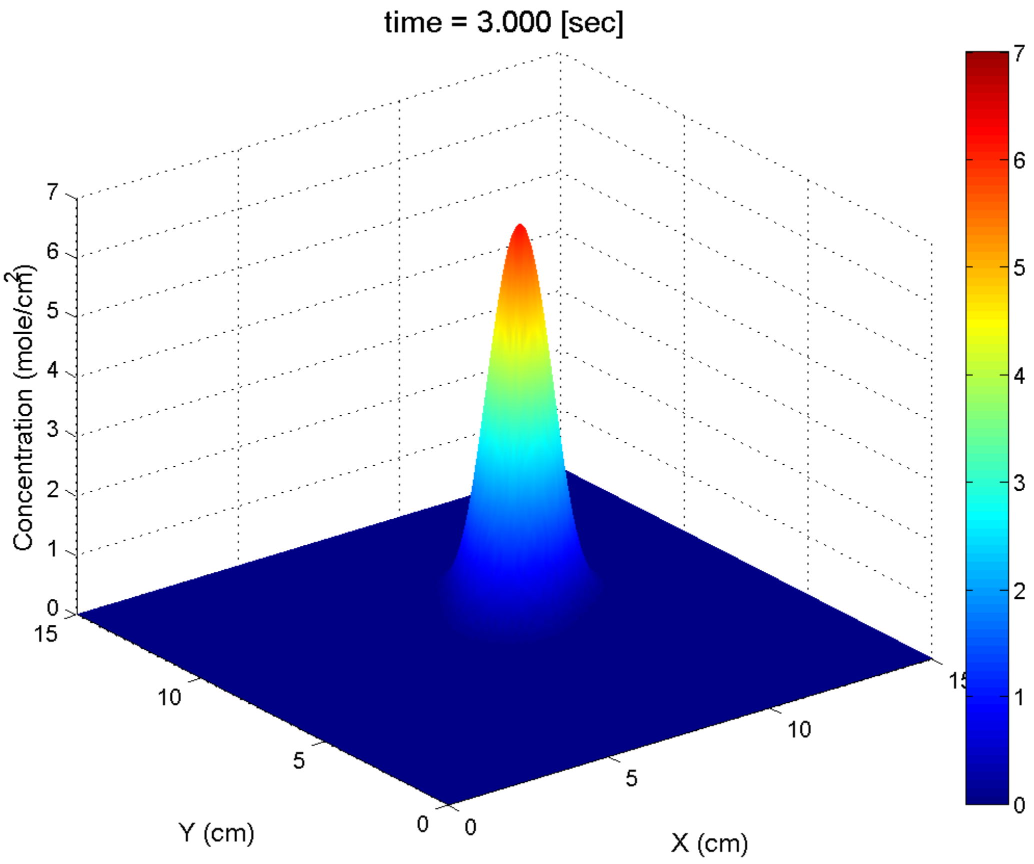

time = 22.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)


time = 24.000 [sec]
Concentration (mole/cm^2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
0
5
10
15

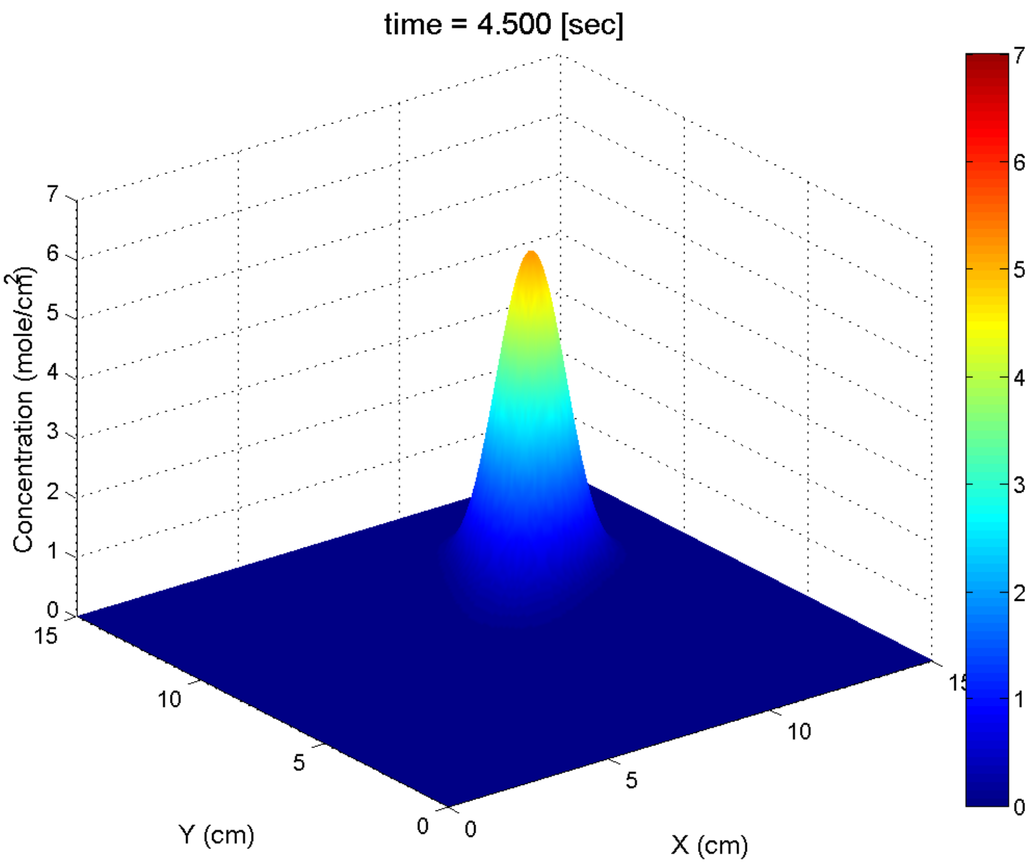
Product D:


time = 0.020 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

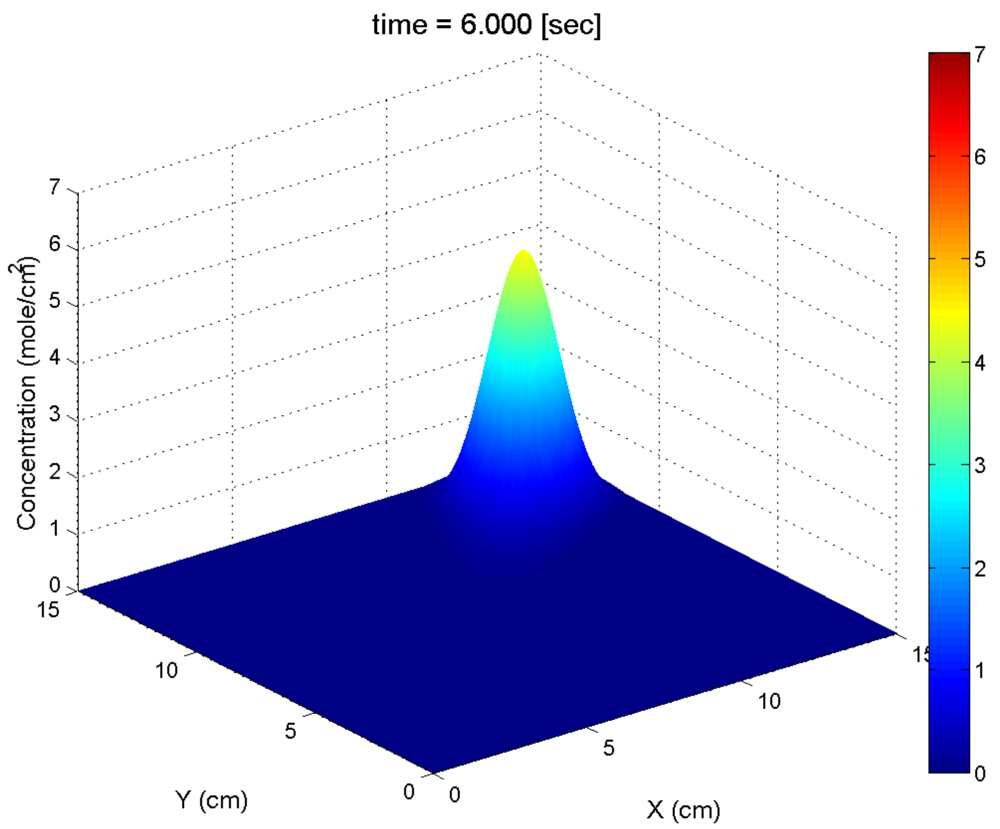

time = 1.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

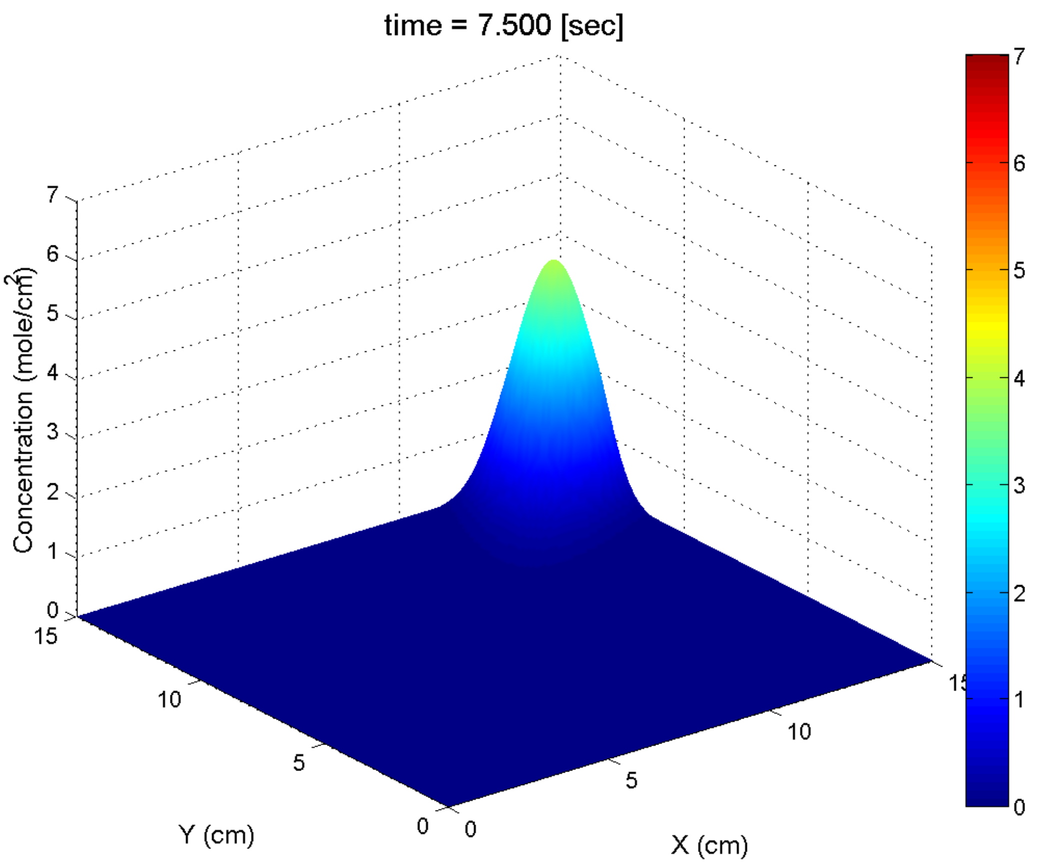


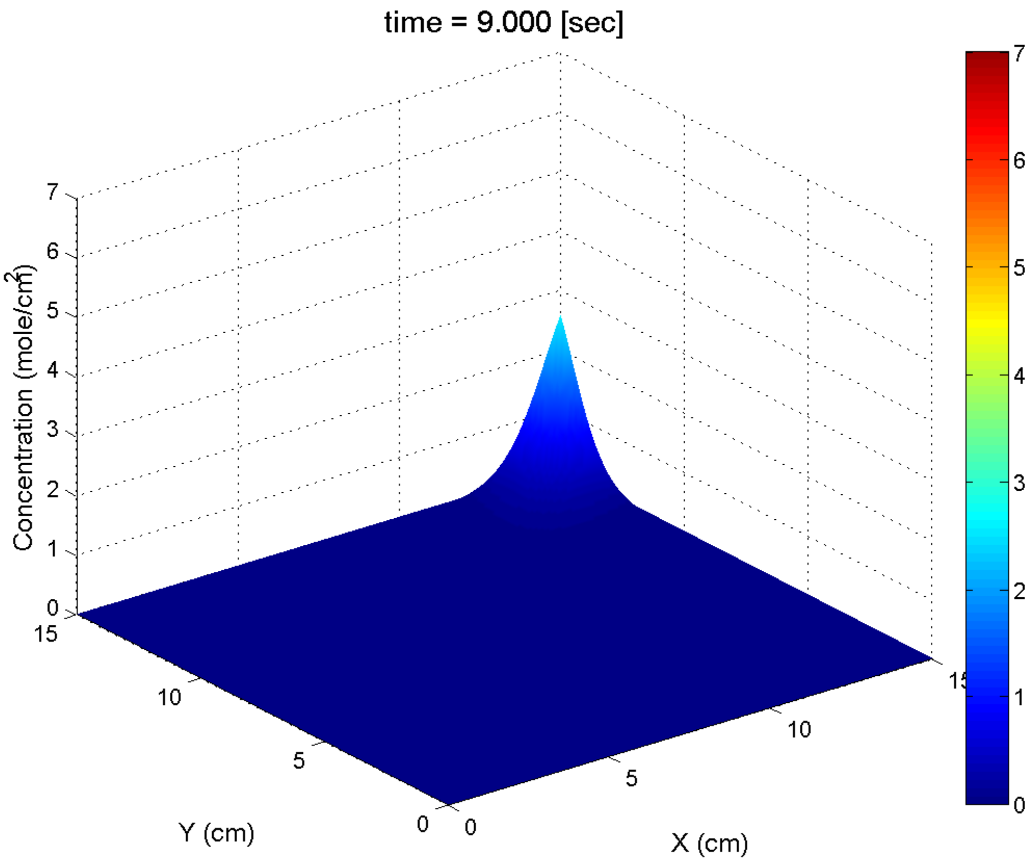
time = 3.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)



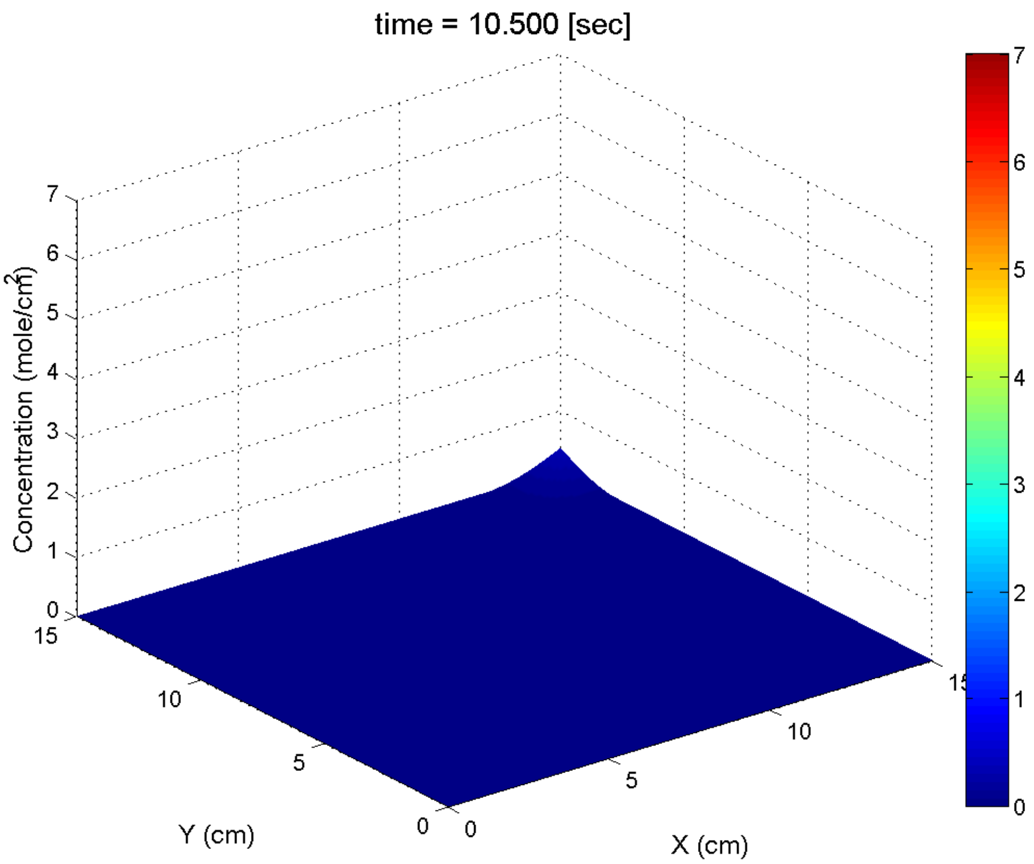
time = 4.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)


time = 6.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

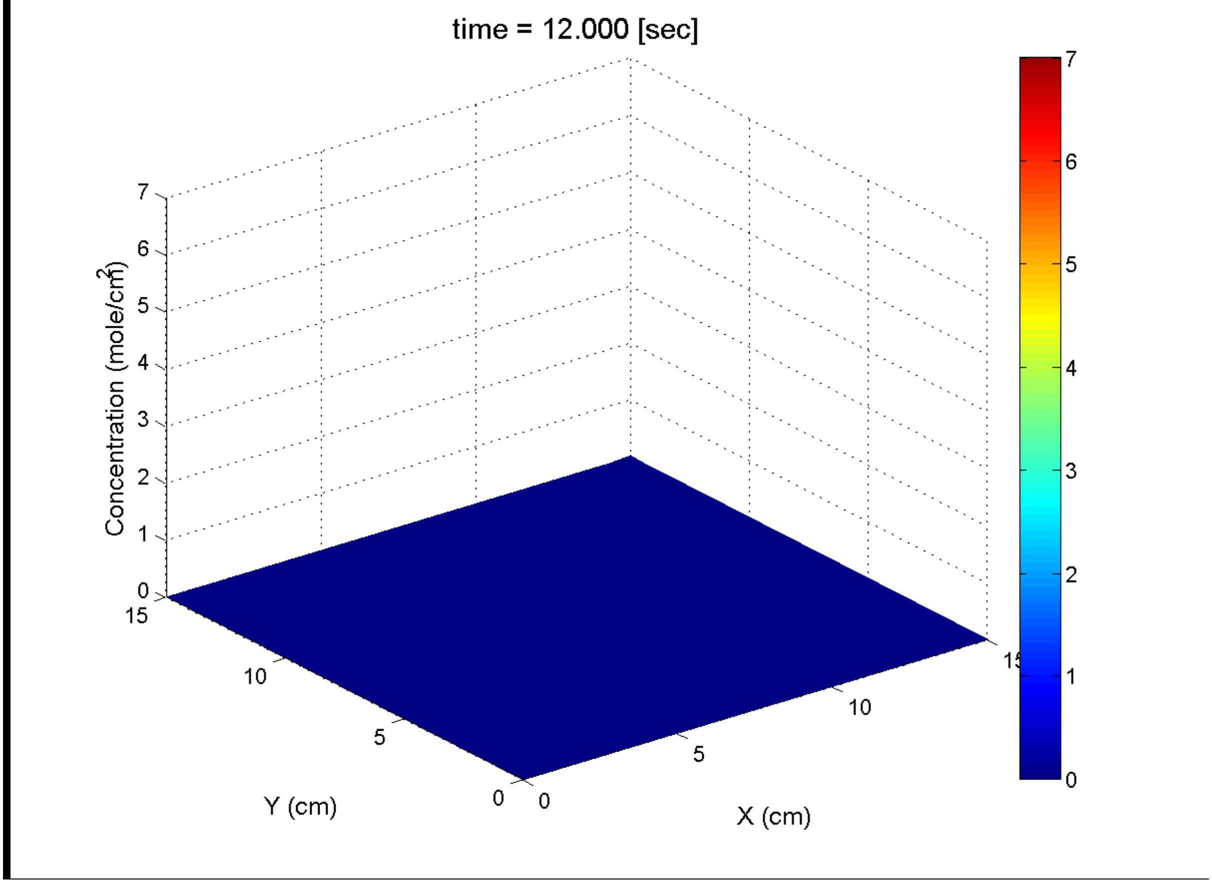

time = 7.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

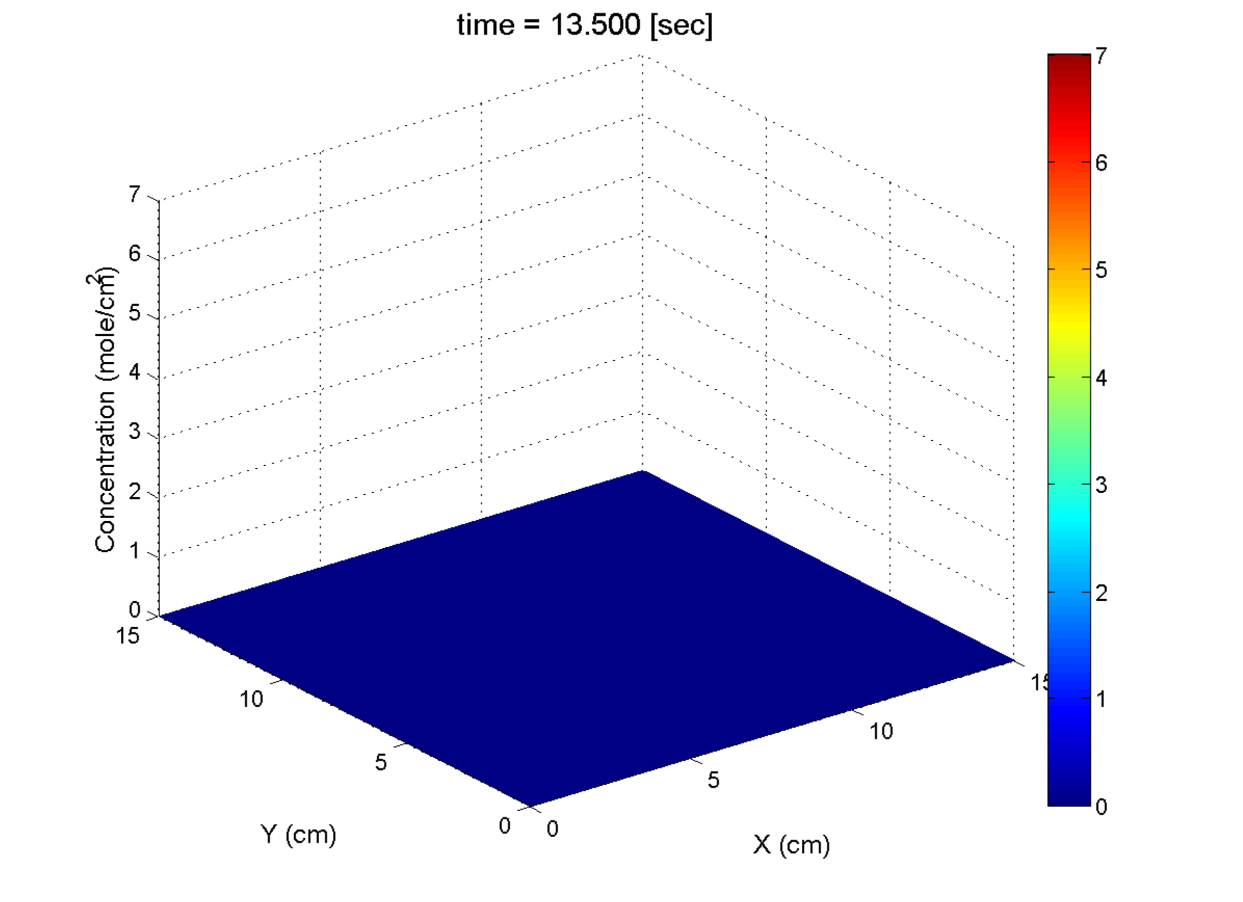


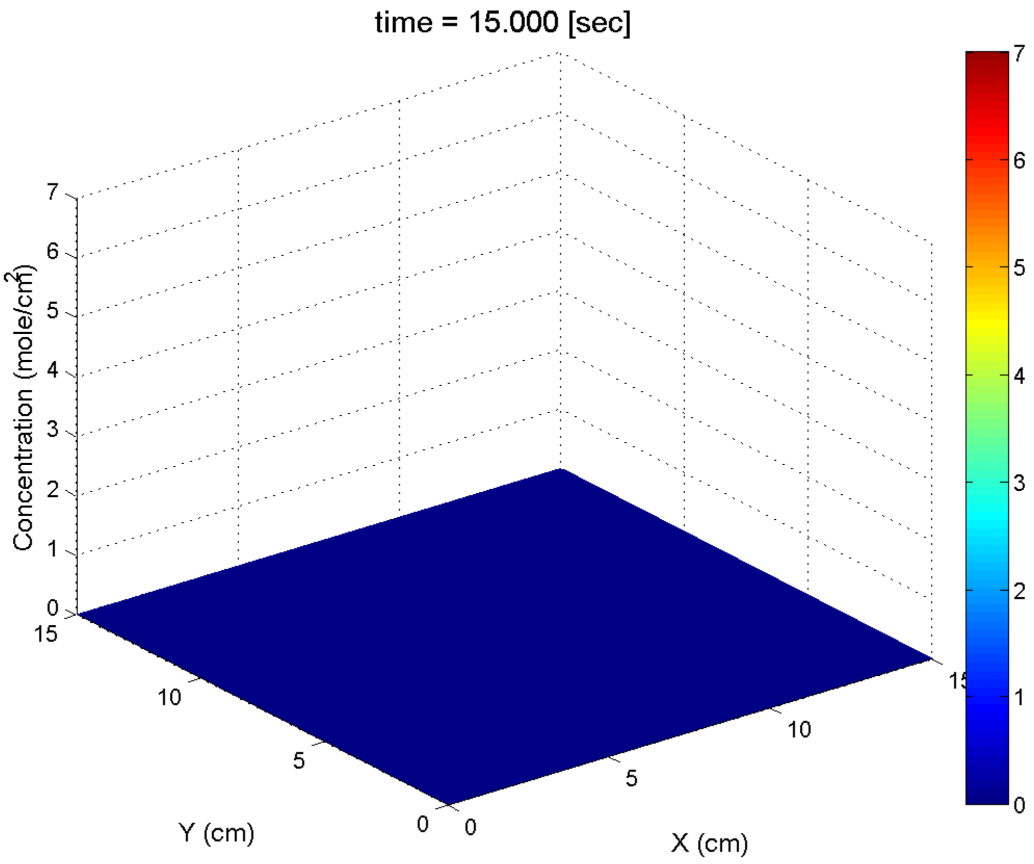
time = 9.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

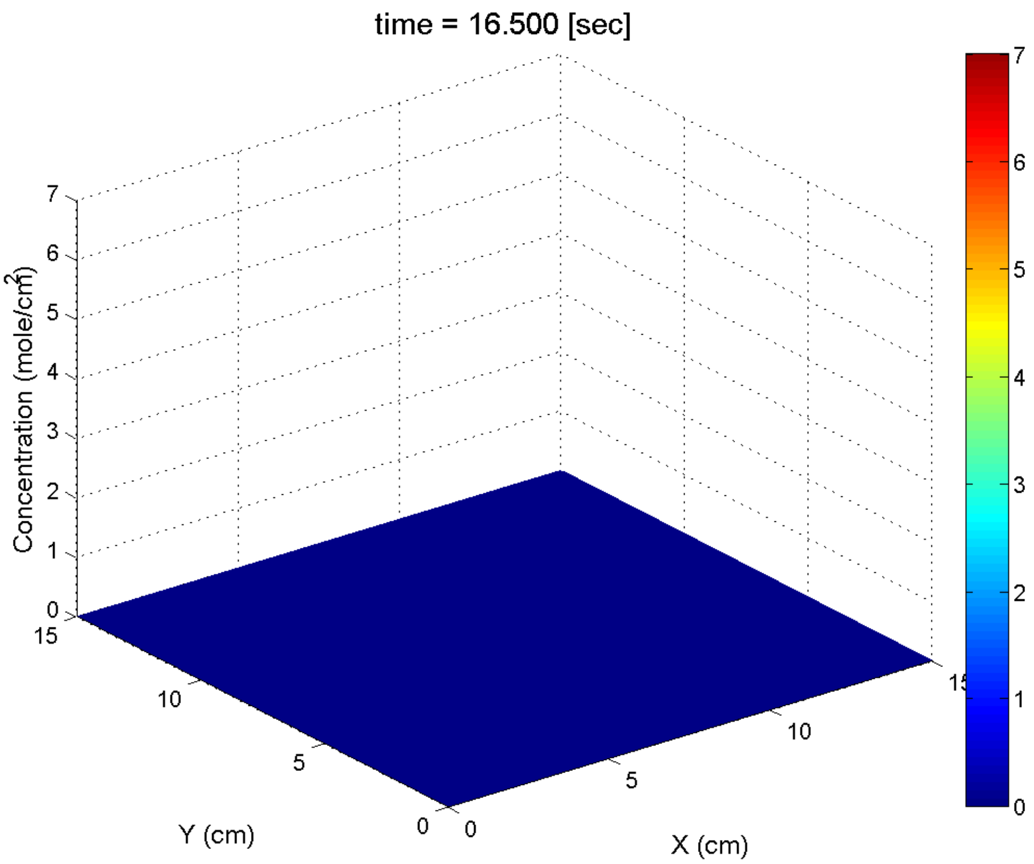


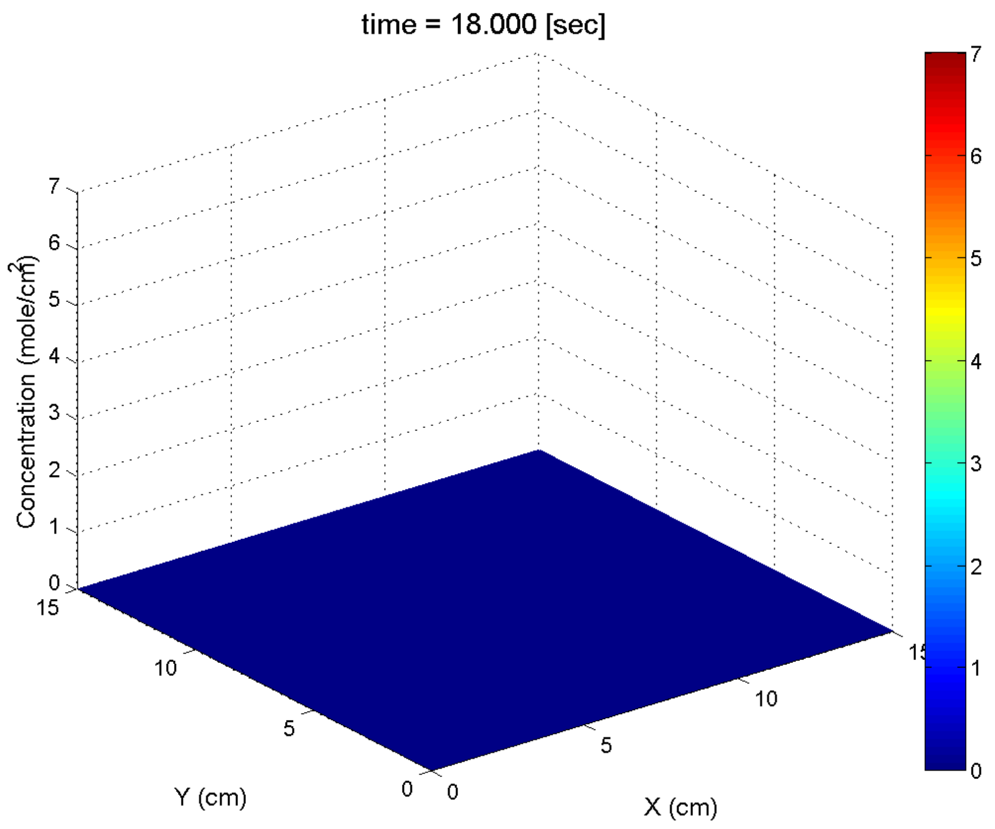
time = 10.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)


time = 12.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)

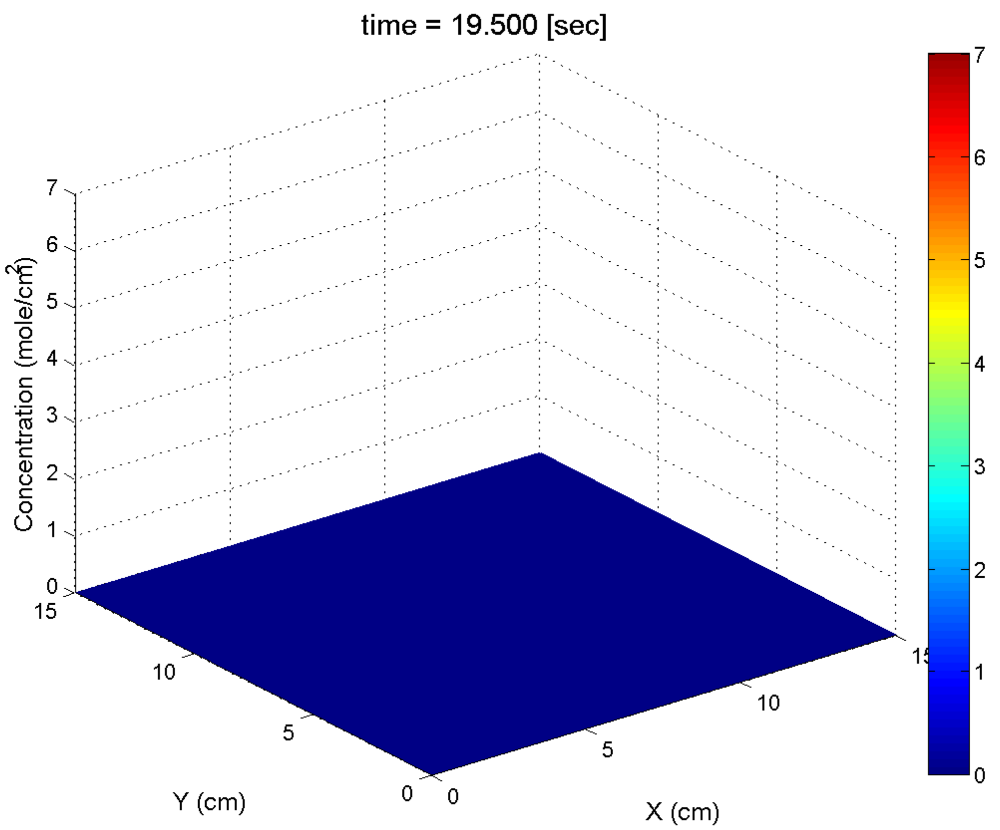

time = 13.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)


time = 15.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7

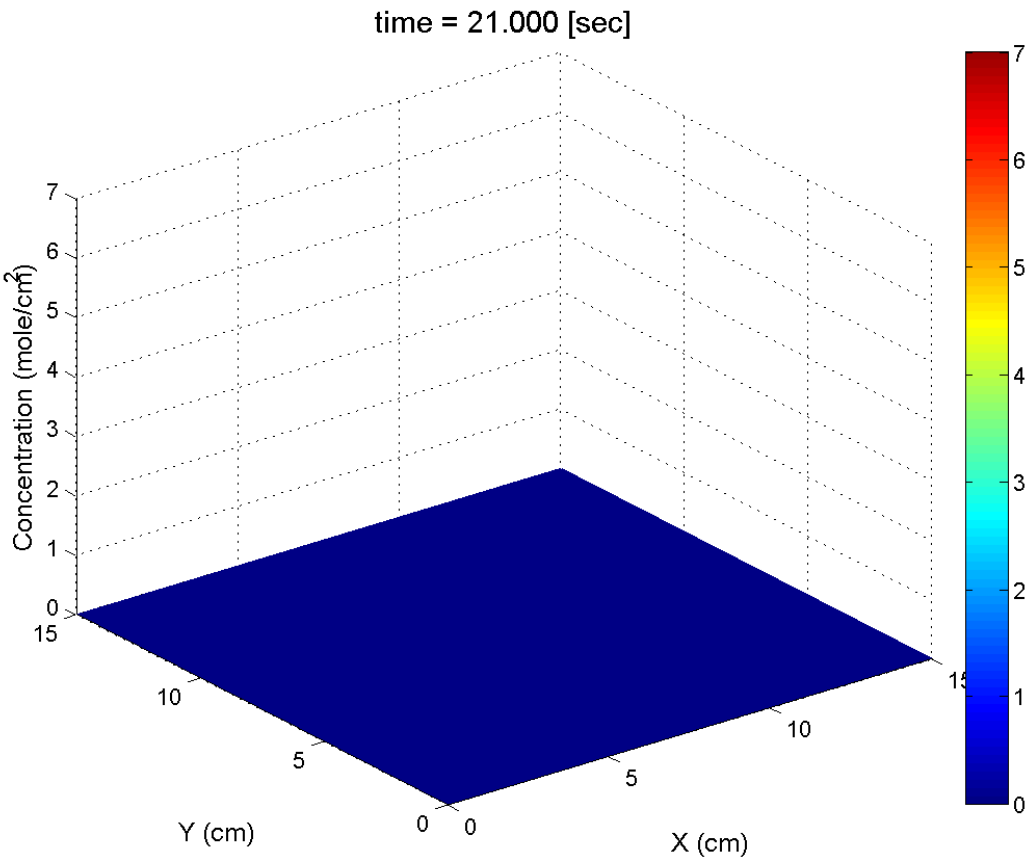

time = 16.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7

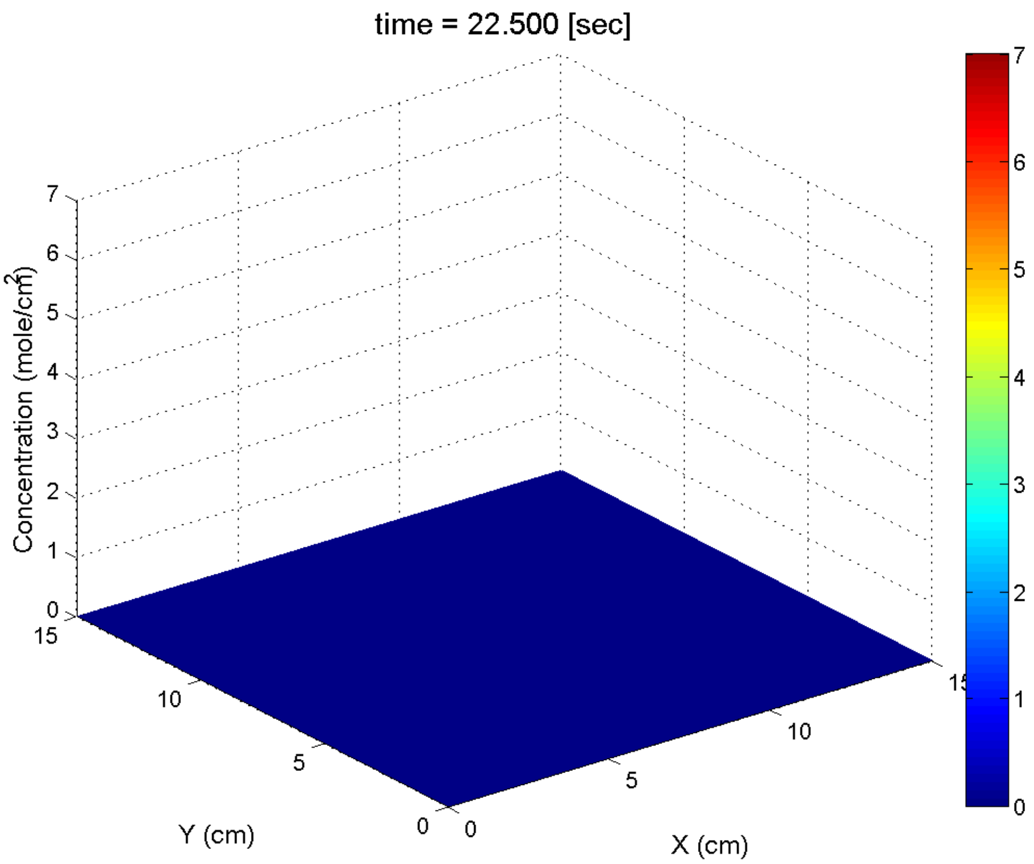


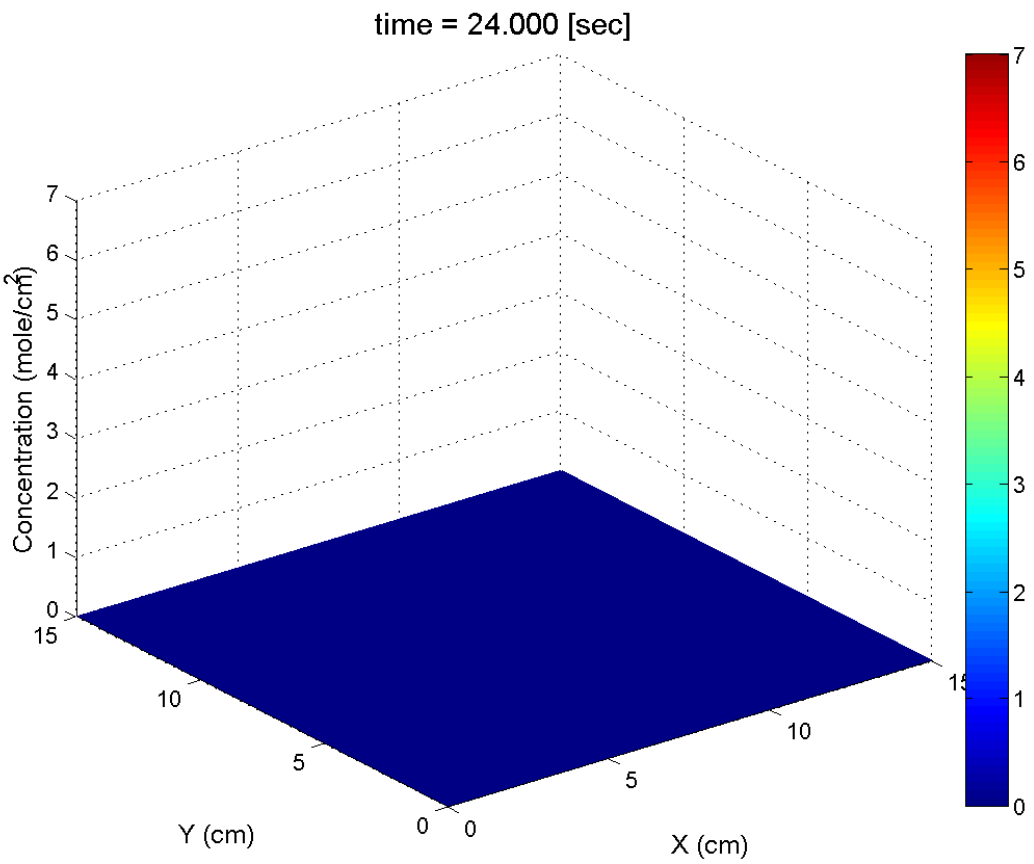
time = 18.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)



time = 19.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)


time = 21.000 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10
15


time = 22.500 [sec]
Concentration (mole/cm2)
Y (cm)
X (cm)
0
1
2
3
4
5
6
7
15
10
5
0
0
5
10
15



Total conclusion:

Concluding our project, we want to say, that we have used all knowledge which we got from the whole semester. We have learned how to find the concentrations and masses of each matters. Then we have remembered how to create the mathematical models of reactions and animate them using MATLAB. Moreover, we have learnt to use diffusion and convection in models and to animate them. We considered one- and two-dimensional spaces for wide view of chemical reactions.