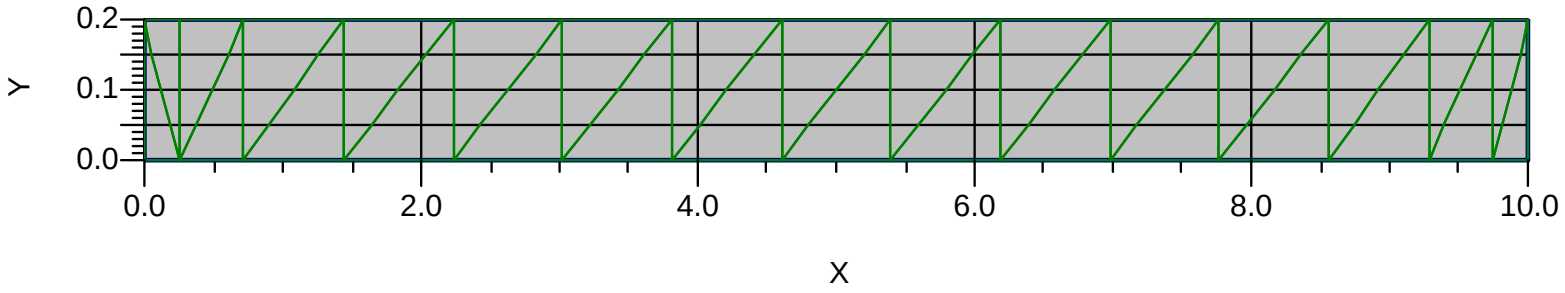
Macsyma Program Example: Chromatogram

- Grid Model
- Variation of the Superficial Velocity
- Variation of the Initial Concentration
- Concentration across the Column
- Conclusion

Grid Model

The given area is divided in 30 Cells with 93 Nodes.



Macsyma Program

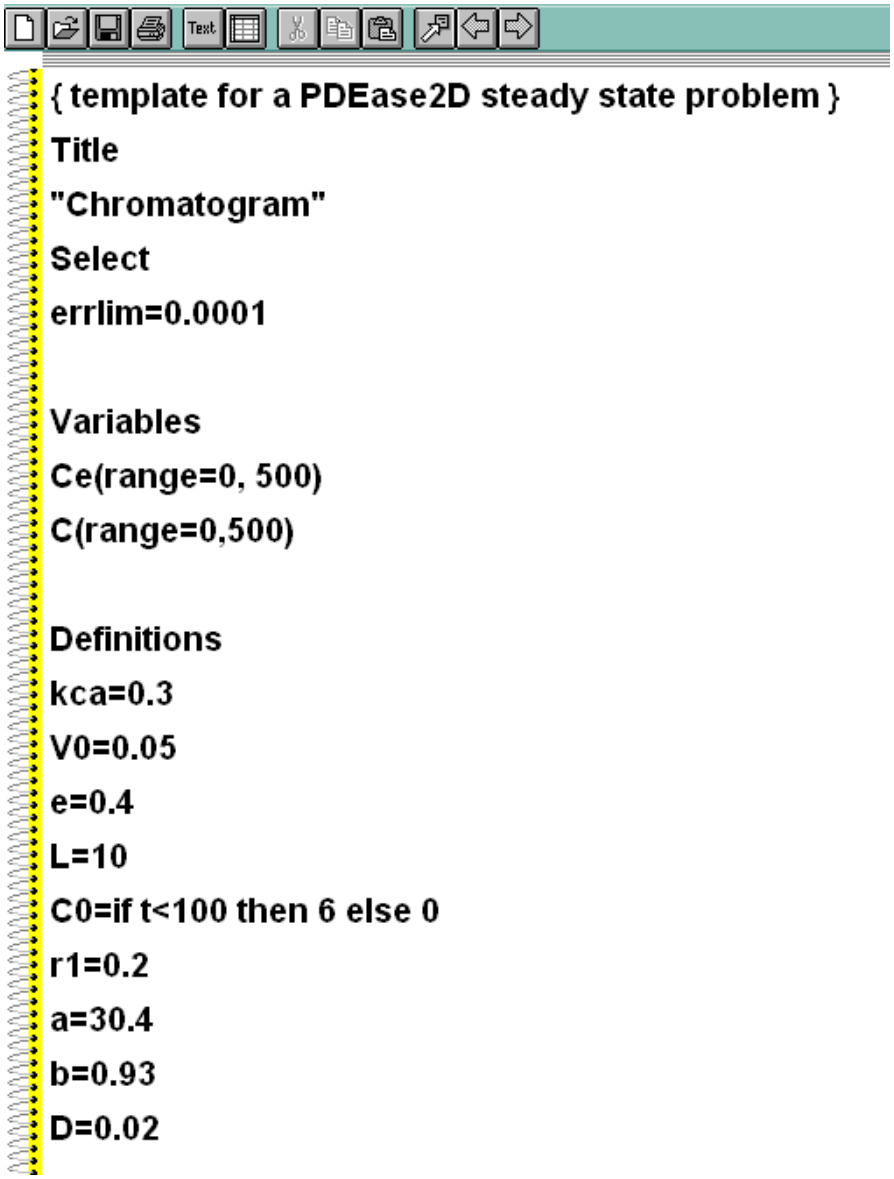
Time dependent problem statement (Line 1).

Title of the program is displayed in the line 2.

In the command Select (Line 4) the error limits are determined. Additionally the labeling of axis can be determined in this section.

Variables of the program are determined with their respective range (Line 7).

Un Definitions the constant parameters are determined with their respective constant values (Line 11 to 20).

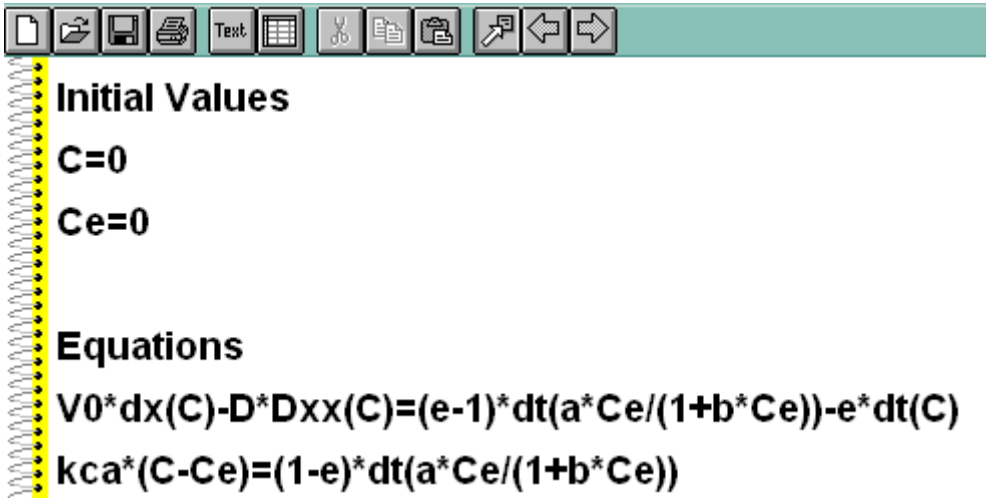


Macsyma Program

Initial boundary conditions are set for problem variables.

Partial differential equations are displayed below the command line Equations.

The example PDEs in the usual form of writing are expressed as in Eq 1 and 2:

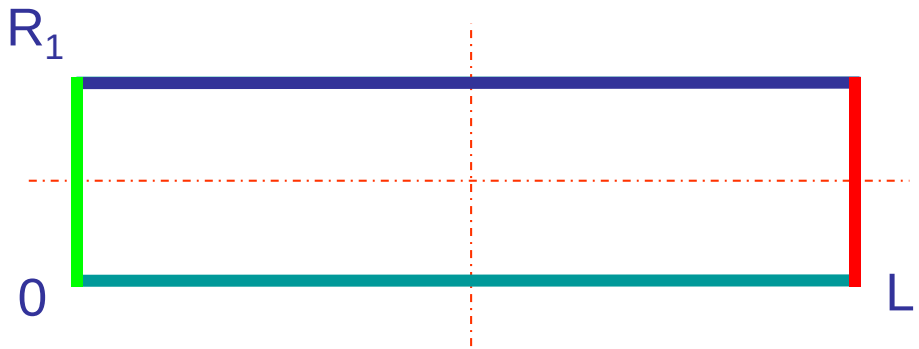


$$V_0 \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = (\varepsilon - 1) \frac{\partial}{\partial t} \left(\frac{a \cdot C_e}{1 + b \cdot C_e} \right) - \varepsilon \frac{\partial C}{\partial t} \qquad (1)$$

$$K_{CA}(C - C_e) = (\varepsilon - 1) \frac{\partial}{\partial t} \left(\frac{a \cdot C_e}{1 + b \cdot C_e} \right) \qquad (2)$$

Macsyma Program

Under Boundaries the physical geometry of the problem are described.



value (variable)

describe the boundary conditions

natural (variable)

gives the value of the first derivative of the respective variable for the value of the function normal at the point of interest.

```
Boundaries
  region 1
start(0,0)
value(C)=C0
value(Ce)=0
line to (0,r1)
natural(C)=0
natural(Ce)=0
line to (L,r1)
natural(C)=0
natural(Ce)=0
line to (L,0)
natural(C)=0
natural(Ce)=0
line to finish

Time
0 by 10 to 5000
```

Macsyma Program

Results can be viewed in various forms. For dynamic processes the animation of the process can be helpful. The cycle number gives the time step to reach the shape of curve along the reactor length (0 to L) at the center of the reactor ($R_1/2$).

The history (variable) command gives the result in diagram shape for certain position inside the reactor given by the coordinates (x, y).

Of the interest is the concentration C at the rear position of the reactor at the position (L, r1/2).

```
Plots
for cycle=6
elevation(C) from (0,r1/2) to (L,r1/2)
animate as "Concentration"

Histories
history(C) at (L/2,r1/2)as "Concentration"
dv file
history(C) at (L,r1/2) as "Concentration"
dv file

End
```

Time Dependent Variable‘s Diagram

Command line for display of the history is :

history (variable)

with information about the spot of interest (x,y)

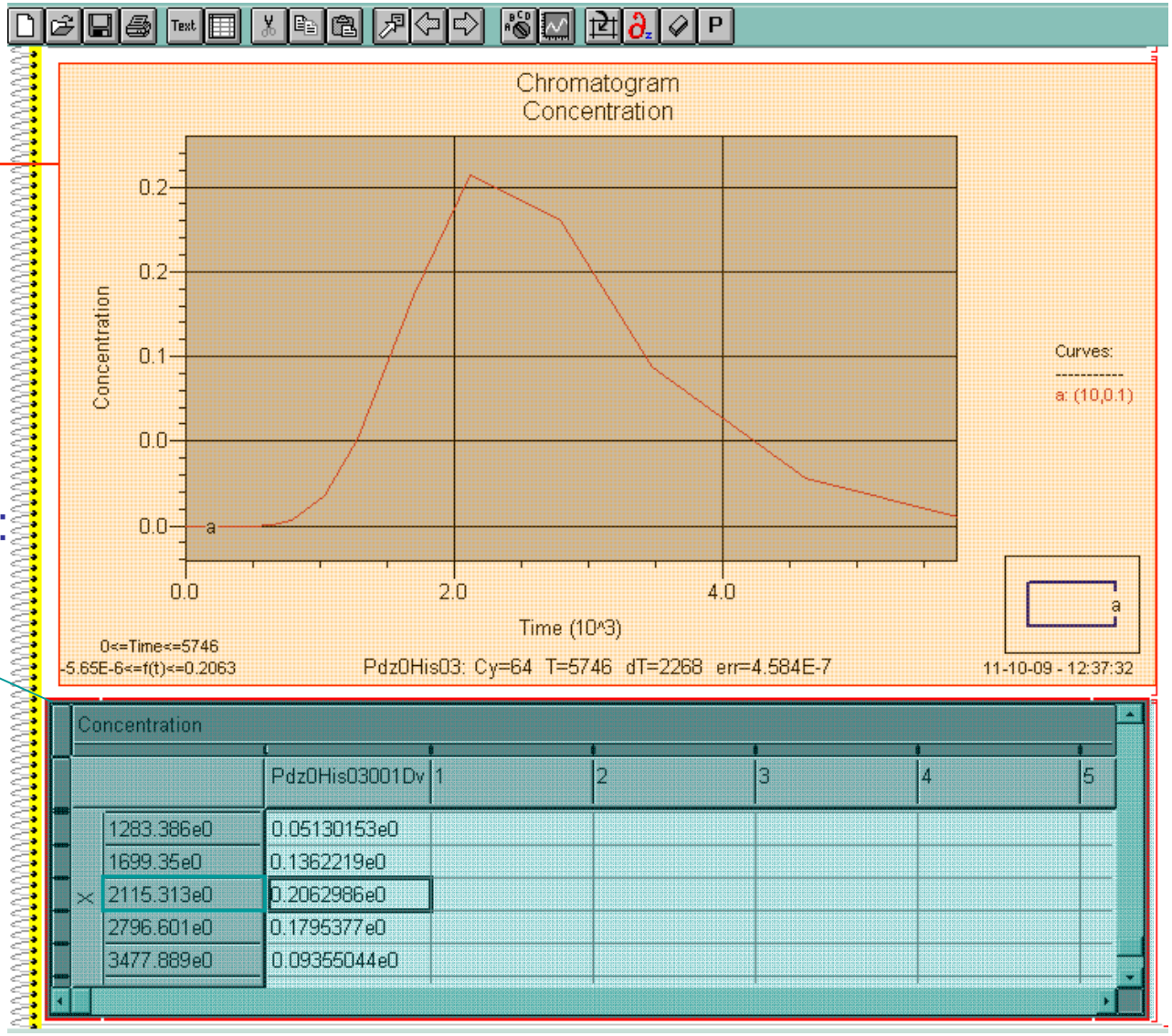
The data which are displayed can be displayed using the command of **d**ata**v**iewer:

dv

And the command for displaying the file is

file

which will make the file in the respective folder as ***Pdz0His01.dat***



Text File Data

Pdz0His03.txt - Notepad

File Edit Format View Help

```
PDEase2D v3.0 (Small Node - 32 Equation)

Problem Title: Chromatogram
   Start time: 15:13:19 - 11-10-2009 (ß)

Cycle=98 | Time=3521 | dT=2573 | Nodes=163 | Cells=60 | PDE Err=6.904E-9


PLOTTED FUNCTION: Concentration
a : 10,0.1
  Time                a
-------------------------------------------------------------------}
 0.00000E+0000    0.00000E+0000
 2.44141E-0003   -6.76333E-0017
 4.88281E-0003   -2.53201E-0017
 6.53376E-0003   -1.28648E-0018
```

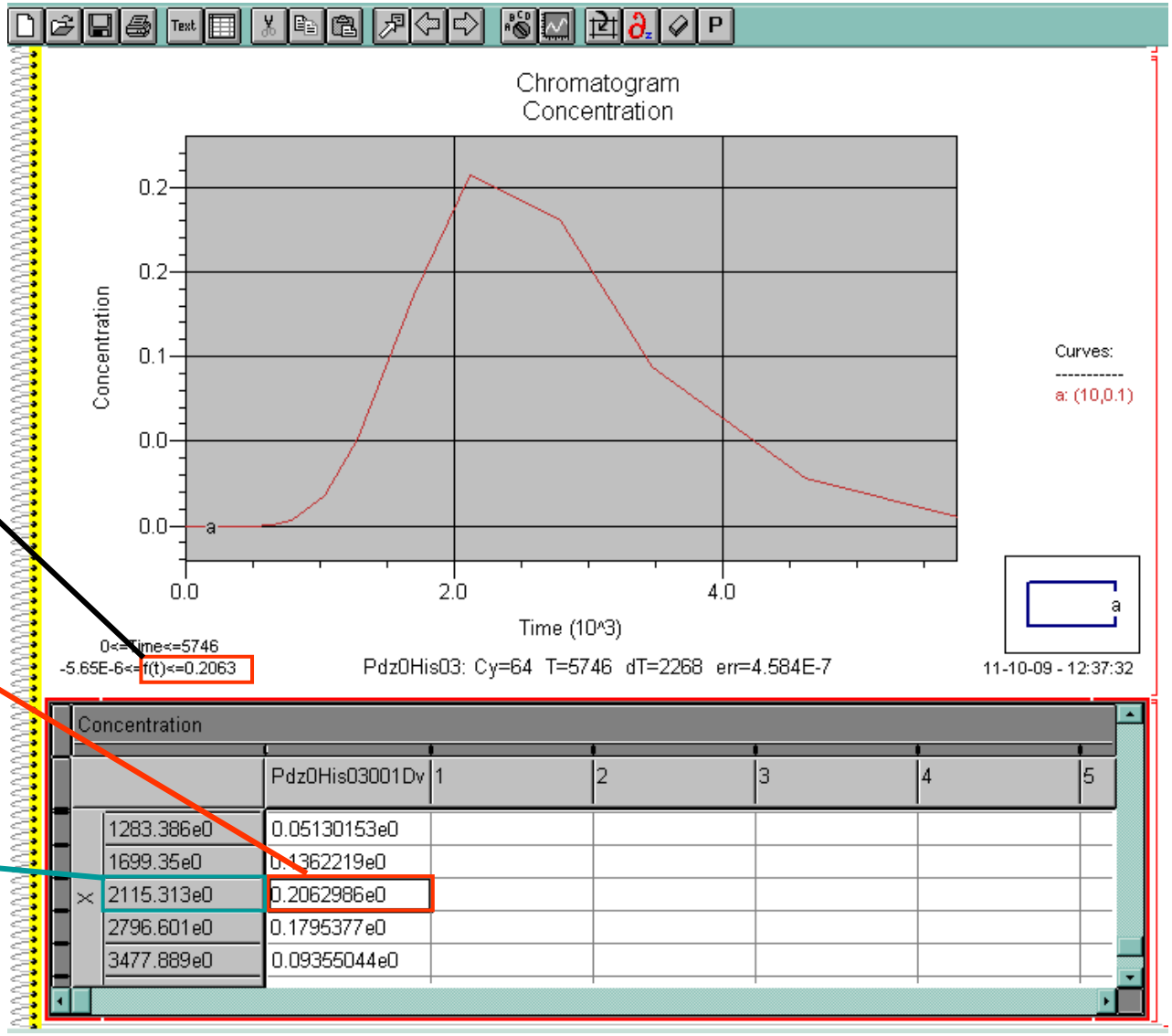
```
 8.38271E+0001    5.99931E+0000
 8.69683E+0001    5.99963E+0000
 8.95422E+0001    6.00026E+0000
 9.21162E+0001    5.99919E+0000
 9.44328E+0001    6.00098E+0000
 9.67494E+0001    5.99864E+0000
 9.77918E+0001    6.00185E+0000
 9.88343E+0001    5.99779E+0000
 9.93034E+0001    6.00249E+0000
 9.97725E+0001    5.99752E+0000
 9.98781E+0001    6.00323E+0000
 9.99836E+0001    5.99588E+0000
 9.99895E+0001    5.99833E+0000
 9.99955E+0001    5.99903E+0000
 9.99968E+0001    5.99909E+0000
 9.99981E+0001    5.99914E+0000
 9.99994E+0001    5.99918E+0000
```

Data Aquisition

Peak Concentration

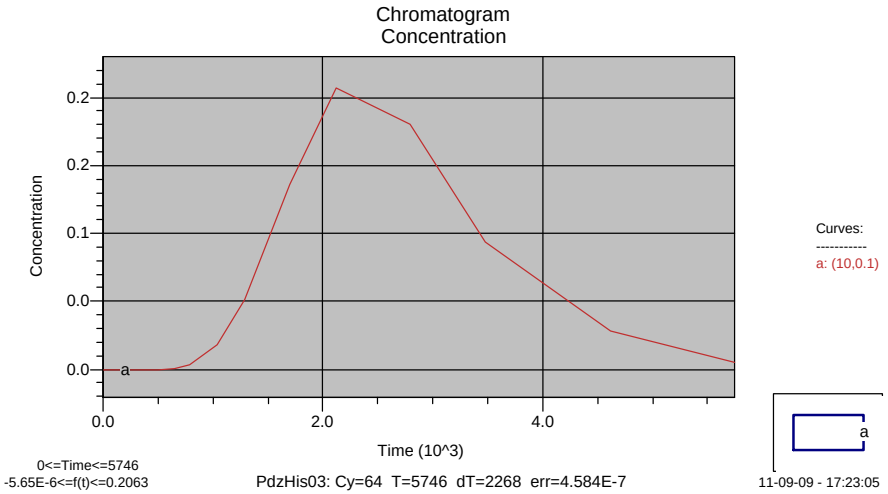
Peak Concentration

Retention Time

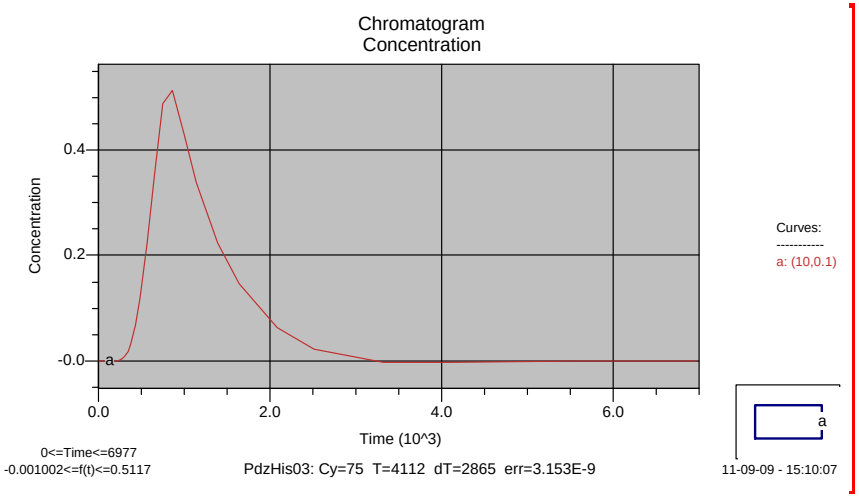


Variation of Superficial Velocity V_0

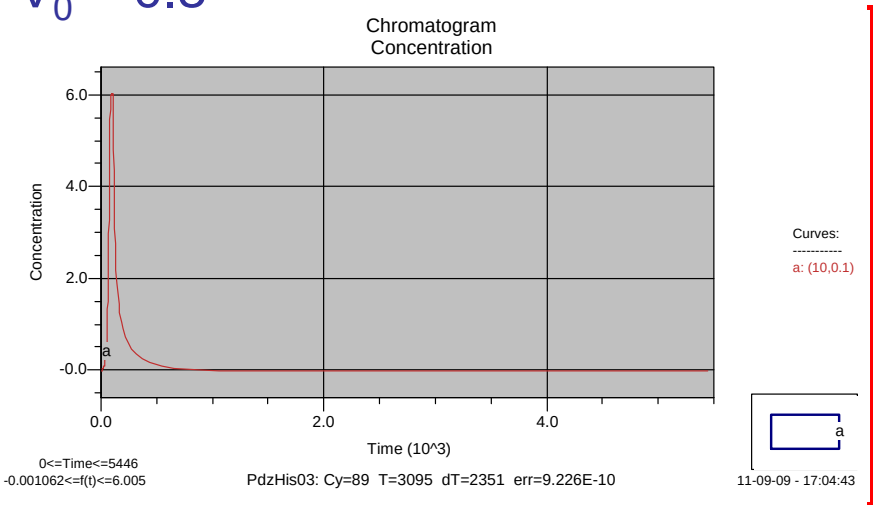
$V_0 = 0.05$



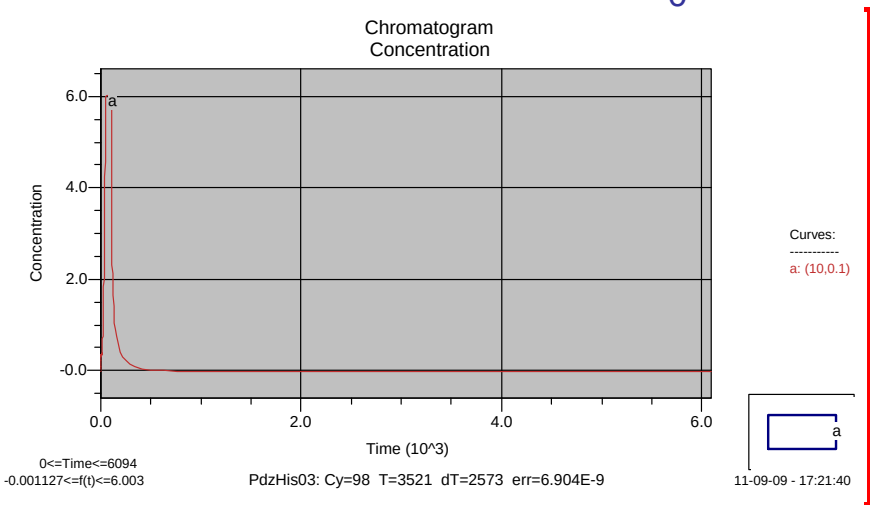
$V_0 = 0.1$



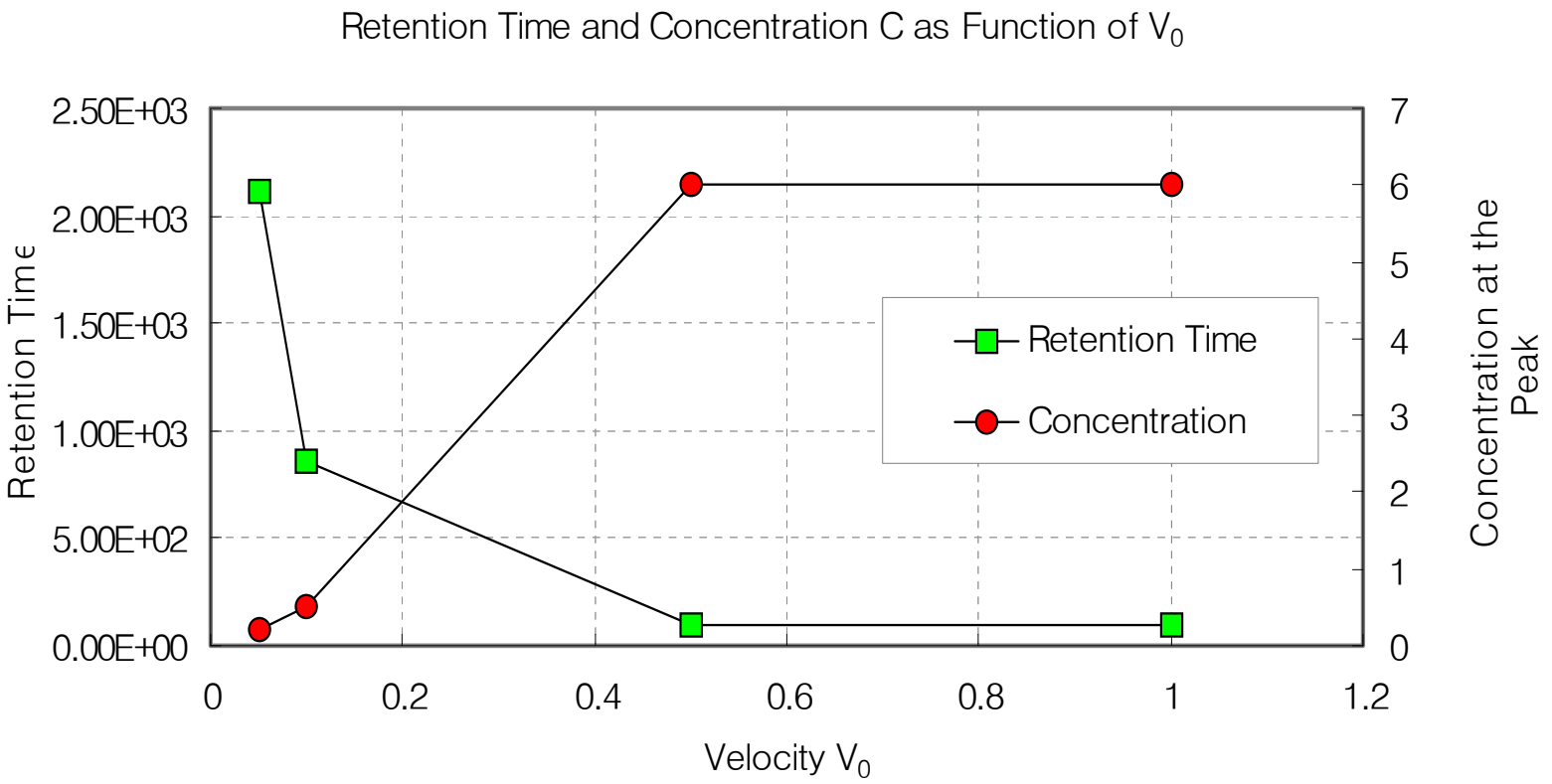
$V_0 = 0.5$



$V_0 = 1.0$

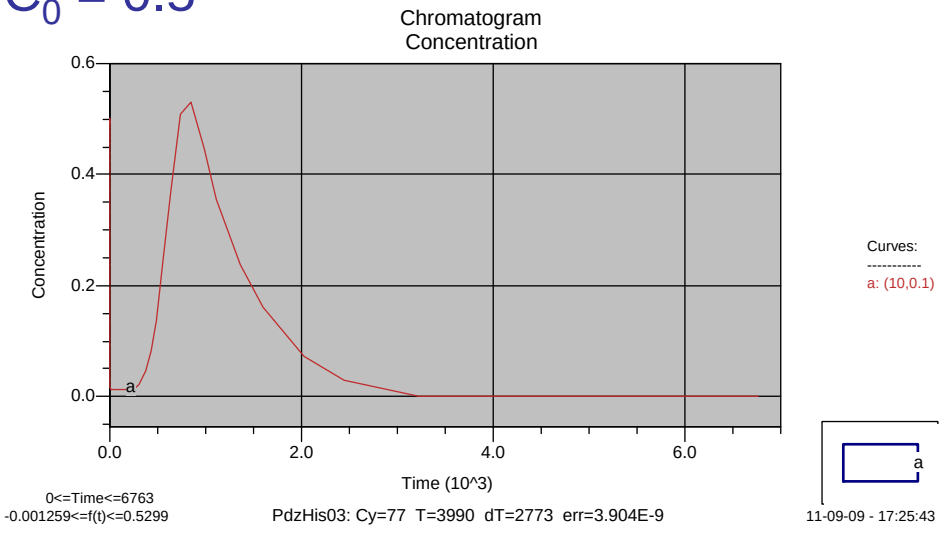


Variation of Velocity V_0

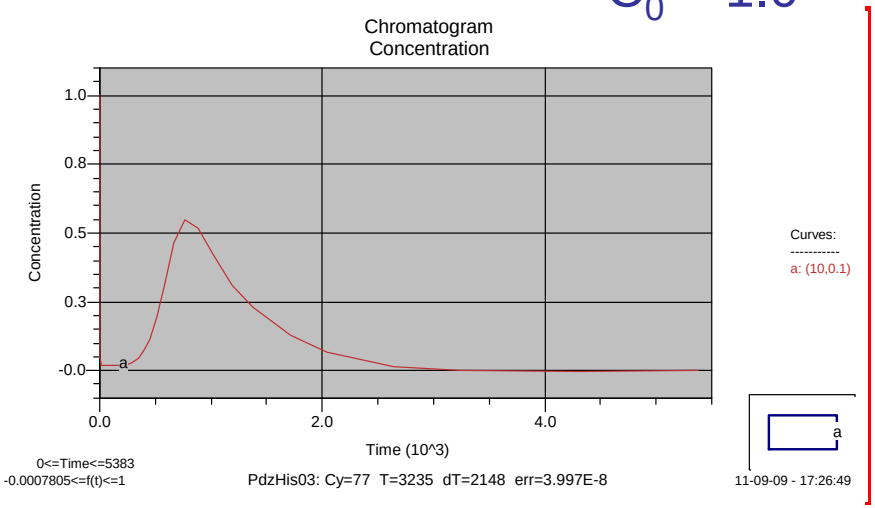


Variation of Initial Concentration C_0

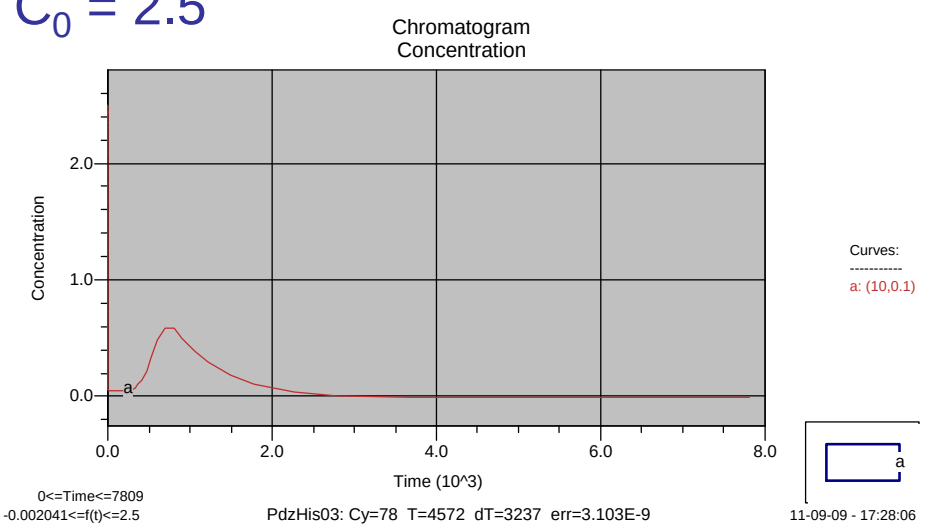
$C_0 = 0.5$



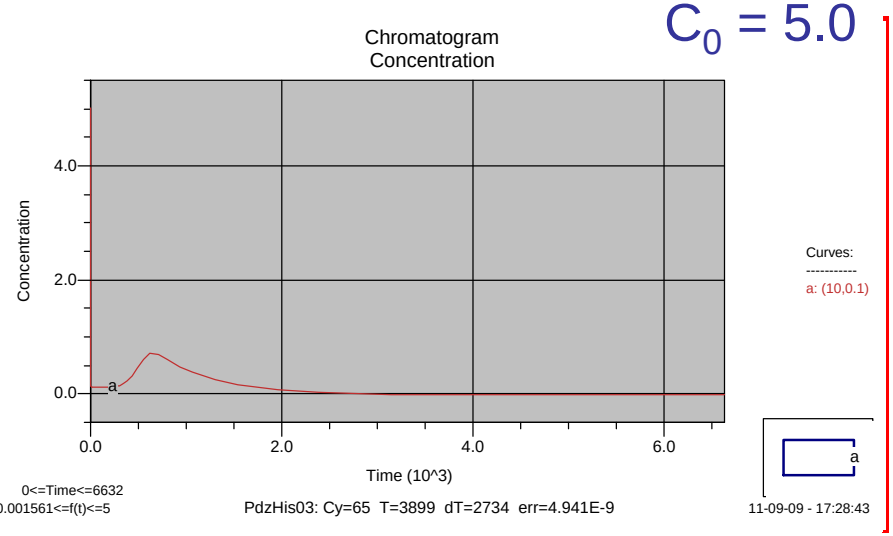
$C_0 = 1.0$



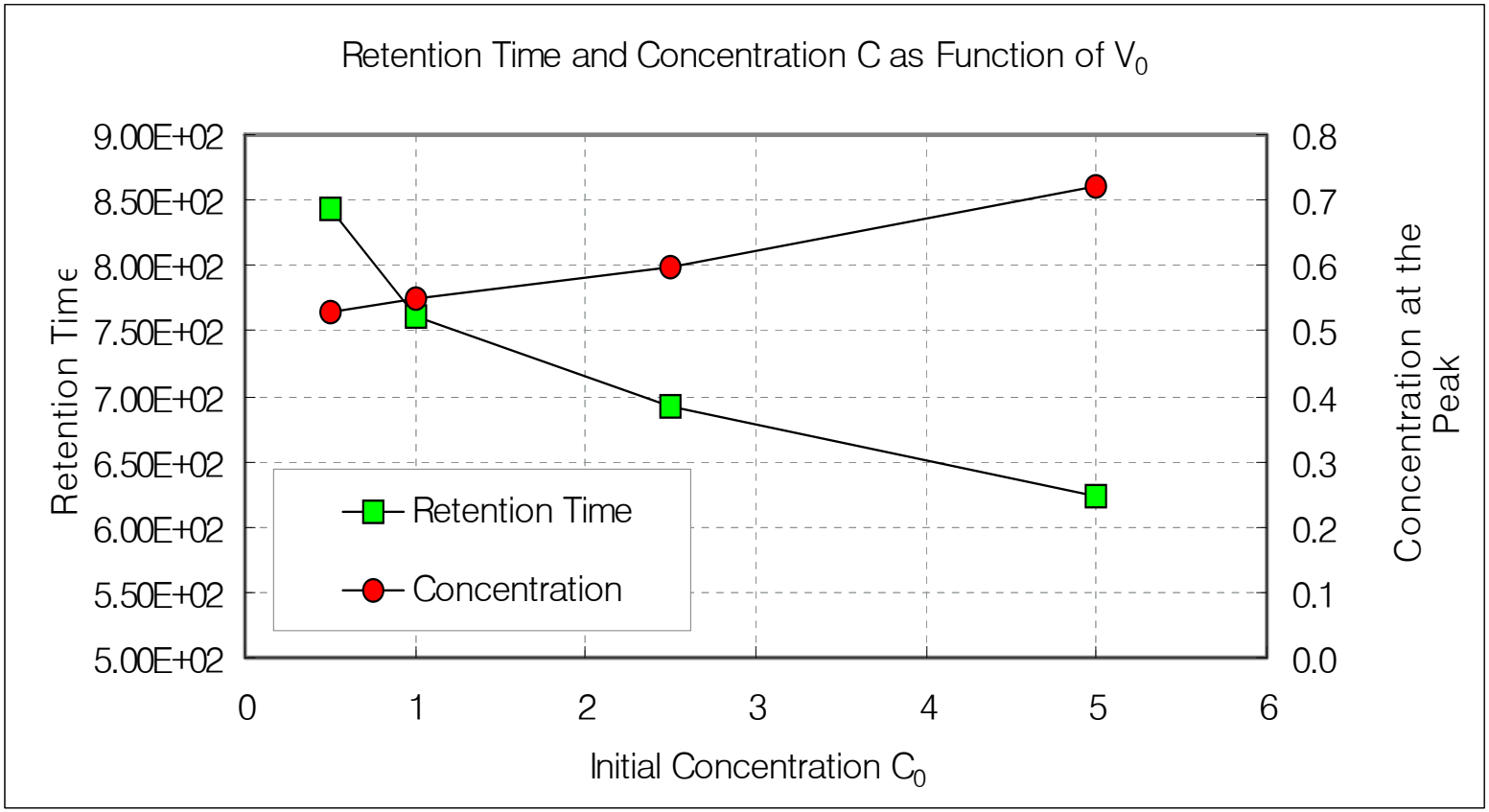
$C_0 = 2.5$



$C_0 = 5.0$



Variation of Initial Concentration C_0



Concentration Along R_1

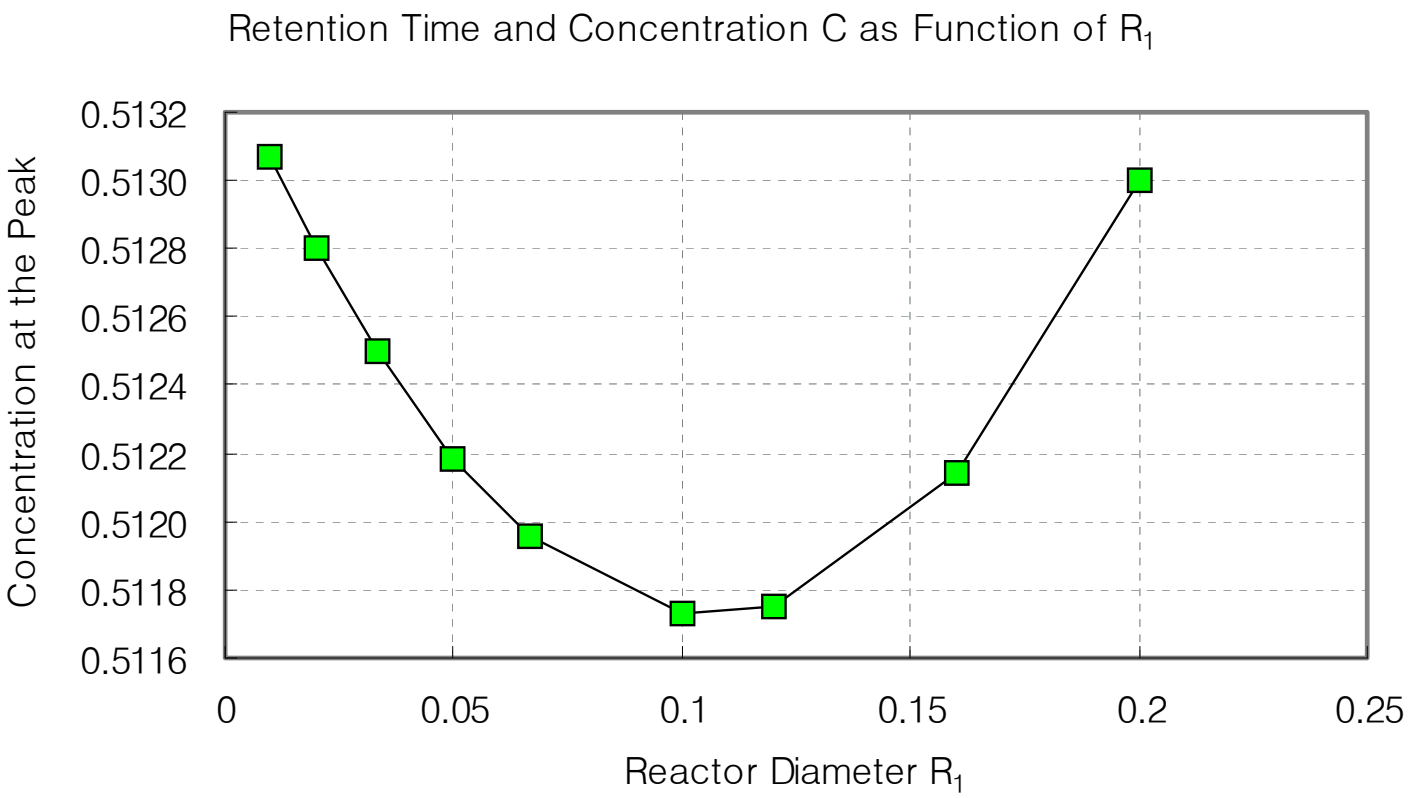
Histories

history(C) at (L/2,r1*0.05)as "Concentration"

dv file

history(C) at (L,r1*0.05) as "Concentration"

dv file



Conclusion

15

- The effect of the **superficial velocity** V_0 on the concentration alongside the length L seems to not that high for the values up to 0.5cm/sec. For the values greater than 0.5 the time is scale is almost the same and the change in concentration are not significant. The difference in the time scale is for values 0.1cm/sec and 1.0cm/sec one order of magnitude. In the case of V_0 = 1.0cm/sec the detection time is much shorter with a high peak in contrast with other cases for the same initial concentration.

- **Initial concentration** C_0 effect is slightly detectable on the concentration scale. The concentration distribution along the length L if the value is varied from 1 to 5 mg/ml is followed without any significant change in concentration and retention time. The difference between the initial value and the peak of concentration along the length is though bigger the greater the inlet concentration is. For the value 0.5 mg/ml the concentration has a peak at the almost same level and the curve has strong tendency to reach the tailing shape.