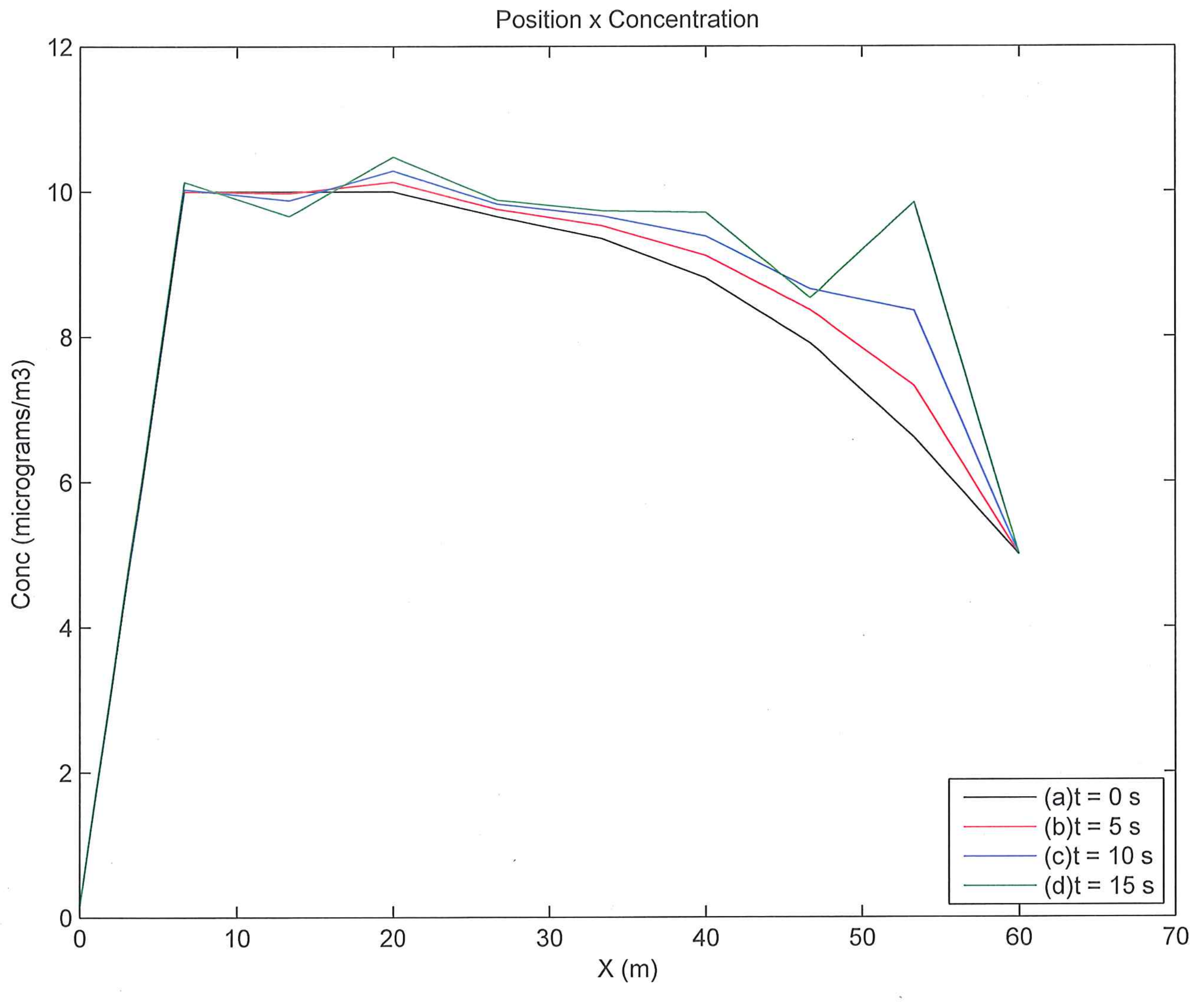
P1: Solving PDE

(a) Matlab script available @ MyA.
Plot is attached.

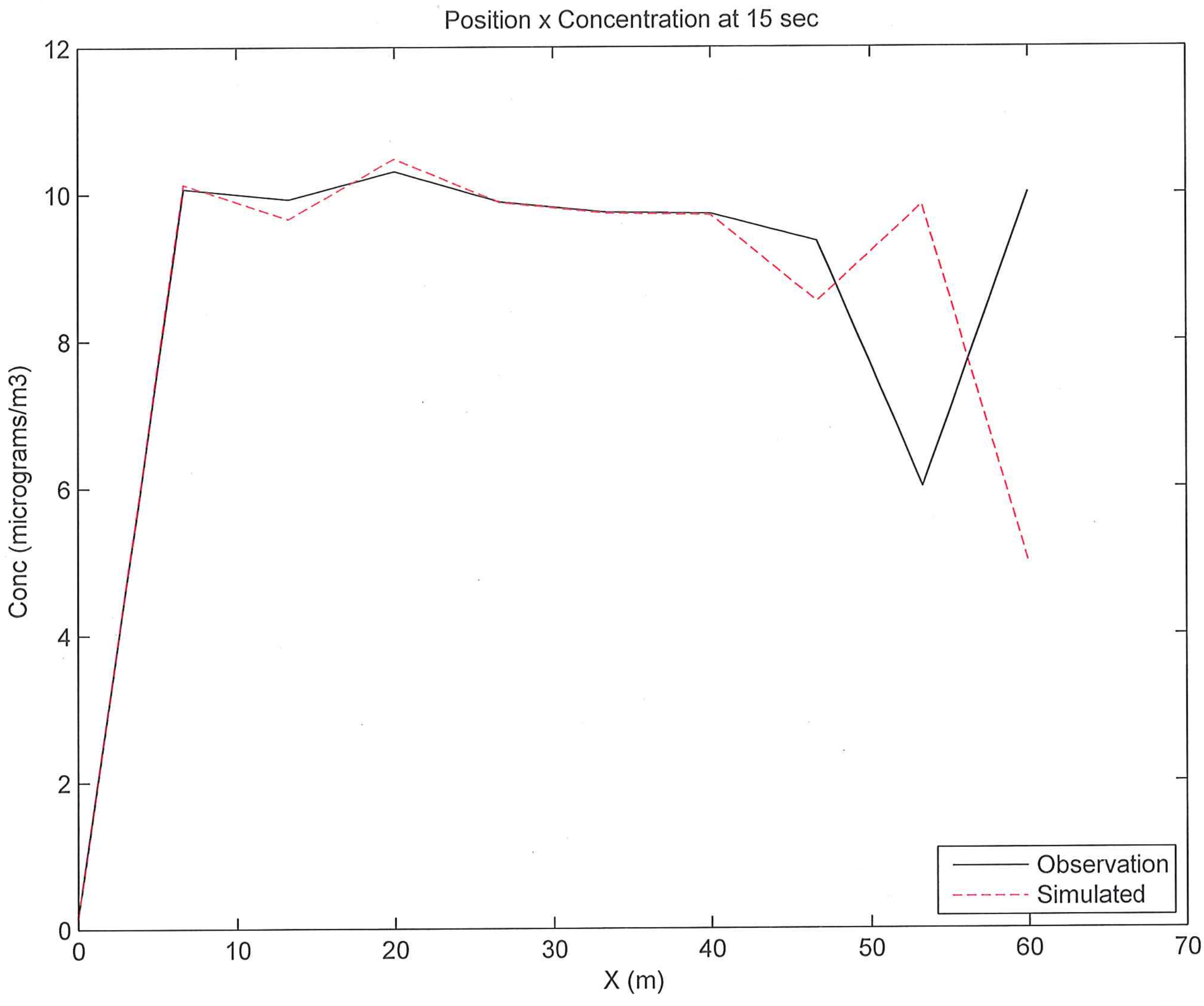
(b) Two arrays containing simulated and observation data can be compared via L_2-norm:

$$L_2 = \left[\frac{\sum_{i=1}^{n} \left[C_i^{obs} - C_i^{sim} \right]^2}{\sum_{i=1}^{n} \left(C_i^{obs} \right)^2} \right]^{1/2} = 2.23 \times 10^{-1}$$

The relatively large L_2-norm is a clear indication that the two sets of discrete data do not match (as can also be observed in the attached plot).


Position x Concentration
Conc (micrograms/m3)
X (m)
0
2
4
6
8
10
12
0
10
20
30
40
50
60
70
(a)t = 0 s
(b)t = 5 s
(c)t = 10 s
(d)t = 15 s

3


Position x Concentration at 15 sec
Conc (micrograms/m3)
X (m)
0
2
4
6
8
10
12
0
10
20
30
40
50
60
70
Observation
Simulated

P2 : Pseudo-code for Gauss-Jordan Method

For $Ax = b$ $\therefore$ $\underbrace{A^{-1}A}_{I} x = A^{-1} b$

In reduced form:

$$\left(\begin{array}{cccc|c} a_{11} & a_{12} & \dots & a_{1n} & b_1 \\ a_{21} & a_{22} & \dots & a_{2n} & b_2 \\ & & \ddots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} & b_n \end{array}\right) \Rightarrow \left(\begin{array}{ccccc|c} 1 & 0 & 0 & \dots & 0 & b_1^* \\ 0 & 1 & 0 & \dots & 0 & b_2^* \\ & & \ddots & & & \vdots \\ 0 & 0 & 0 & \dots & 1 & b_n^* \end{array}\right)$$

when $x_i = b_i^*$

Given $\left.\begin{array}{l} [A] = a_{ij} \\ [b] = b_i \end{array}\right\} \begin{array}{l} A(1:n, 1:n) \\ b(1:n) \end{array}$

$b(1:n)$ is allocated as a last column of matrix A, i.e., $A(1:n, 1:n+1)$, thus

$$A(1:n, n+1) = b(1:n)$$

The Gauss-Jordan algorithm becomes (as pseudocode):

```
Given A(1:m, 1:m+1)
For i = 1:m

    For j = i+1:m+1
        A(i,j) = A(i,j) / A(i,i)
    End

    For k = 1:m
        If (k ≠ i)
            For j = i+1:m+1
                A(k,j) = A(k,j) - A(k,i) A(i,j)
            End
        End If
    End

End
```

P3:

(a) A^{-1} (Gauss-Jordan method)

$$
\begin{array}{cccc|cccc|l}
\multicolumn{4}{c|}{\overbrace{\qquad\qquad\qquad}^{A}} & \multicolumn{4}{c|}{\overbrace{\qquad\qquad\qquad}^{I}} & \\
5 & 0 & 3 & 1 & 1 & 0 & 0 & 0 & \leftarrow (\times 1/5) \\
4 & 19 & 10 & 3 & 0 & 1 & 0 & 0 & \\
1 & 4 & 8 & -1 & 0 & 0 & 1 & 0 & \\
0 & 3 & 1 & 7 & 0 & 0 & 0 & 1 &
\end{array}
$$

$$
\begin{array}{cccc|cccc|l}
1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 & \\
4 & 19 & 10 & 3 & 0 & 1 & 0 & 0 & \times(-4)+ \\
1 & 4 & 8 & -1 & 0 & 0 & 1 & 0 & \times(-1)+ \\
0 & 3 & 1 & 7 & 0 & 0 & 0 & 1 &
\end{array}
$$

$$
\begin{array}{cccc|cccc|l}
1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 & \\
0 & 19 & 38/5 & 11/5 & -4/5 & 1 & 0 & 0 & \leftarrow \times(1/19) \\
0 & 4 & 37/5 & -6/5 & -1/5 & 0 & 1 & 0 & \\
0 & 3 & 1 & 7 & 0 & 0 & 0 & 1 &
\end{array}
$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 \\ 0 & 1 & 2/5 & 11/95 & -4/95 & 1/19 & 0 & 0 \\ 0 & 4 & 37/5 & -6/5 & -1/5 & 0 & 1 & 0 \\ 0 & 3 & 1 & 7 & 0 & 0 & 0 & 1 \end{array}\right) \begin{array}{l} \\ \times(-4)+ \\ \times(-3)+ \\ \\ \end{array}$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 \\ 0 & 1 & 2/5 & 11/95 & -4/95 & 1/19 & 0 & 0 \\ 0 & 0 & 29/5 & -158/95 & -3/95 & -4/19 & 1 & 0 \\ 0 & 0 & -1/5 & 632/95 & 12/95 & -3/19 & 0 & 1 \end{array}\right) \begin{array}{l} \\ \\ \leftarrow \times(5/29) \\ \\ \end{array}$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 \\ 0 & 1 & 2/5 & 11/95 & -4/95 & 1/19 & 0 & 0 \\ 0 & 0 & 1 & -158/551 & -3/551 & -20/551 & 5/29 & 0 \\ 0 & 0 & -1/5 & 632/95 & 12/95 & -3/19 & 0 & 1 \end{array}\right) \begin{array}{l} \\ \\ \times(1/5)+ \\ \\ \end{array}$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 \\ 0 & 1 & 2/5 & 11/95 & -4/95 & 1/19 & 0 & 0 \\ 0 & 0 & 1 & -158/551 & -3/551 & -20/551 & 5/29 & 0 \\ 0 & 0 & 0 & 3634/551 & 69/551 & -91/551 & 1/29 & 1 \end{array}\right) \begin{array}{l} \\ \\ \\ \leftarrow \times(551/3634) \end{array}$$

$$\left(\begin{array}{cccc|cccc}
1 & 0 & 3/5 & 1/5 & 1/5 & 0 & 0 & 0 \\
0 & 1 & 2/5 & 11/95 & -4/95 & 1/19 & 0 & 0 \\
0 & 0 & 1 & -158/551 & -3/551 & -20/551 & 5/29 & 0 \\
0 & 0 & 0 & 1 & 3/158 & -91/3634 & 19/3634 & 551/3634
\end{array}\right)
\begin{array}{l}
\times(-1/5)+ \\
\times(-11/95)+ \\
\times(158/551)+ \\

\end{array}$$

$$\left(\begin{array}{cccc|cccc}
1 & 0 & 3/5 & 0 & 31/158 & 91/18170 & -19/18170 & -551/18170 \\
0 & 1 & 2/5 & 0 & -7/158 & 1009/18170 & -11/18170 & -319/18170 \\
0 & 0 & 1 & 0 & 0 & -1/23 & 4/23 & 1/23 \\
0 & 0 & 0 & 1 & 3/158 & -91/3634 & 19/3634 & 551/3634
\end{array}\right)
\begin{array}{l}
\times(-3/5)+ \\
\times(-2/5)+ \\
 \\

\end{array}$$

$$\underbrace{\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}}_{I}
\;\Bigg|\;
\underbrace{\begin{array}{cccc}
31/158 & 113/3634 & -383/3634 & -205/3634 \\
-7/158 & 265/3634 & -255/3634 & -127/3634 \\
0 & -1/23 & 4/23 & 1/23 \\
3/158 & -91/3634 & 19/3634 & 551/3634
\end{array}}_{A^{-1}}$$

$$A^{-1} = \begin{pmatrix} 31/158 & 113/3634 & -383/3634 & -205/3634 \\ -7/158 & 265/3634 & -255/3634 & -127/3634 \\ 0 & -1/23 & 4/23 & 1/23 \\ 3/158 & -91/3634 & 19/3634 & 551/3634 \end{pmatrix} =$$

$$= \begin{pmatrix} 0.19620 & 0.03110 & -0.10539 & -0.05641 \\ -0.04430 & 0.07292 & -0.07017 & -0.03495 \\ 0 & -0.04348 & 0.17391 & 0.04348 \\ 0.01899 & -0.02504 & 0.00523 & 0.15162 \end{pmatrix}$$

(b) Gaussian Elimination

$$\left(\begin{array}{cccc|c} 5 & 0 & 3 & 1 & 8 \\ 4 & 19 & 10 & 3 & 25 \\ 1 & 4 & 8 & -1 & 18 \\ 0 & 3 & 1 & 7 & 72 \end{array}\right) \begin{array}{l} \leftarrow \times(1/5) \\ \\ \\ \\ \end{array} \sim \left(\begin{array}{cccc|c} 1 & 0 & 3/5 & 1/5 & 8/5 \\ 4 & 19 & 10 & 3 & 25 \\ 1 & 4 & 8 & -1 & 18 \\ 0 & 3 & 1 & 7 & 72 \end{array}\right) \begin{array}{l} \\ \times(-4)+ \\ \times(-1)+ \\ \\ \end{array} \sim$$

$$\left(\begin{array}{cccc|c} 1 & 0 & 3/5 & 1/5 & 8/5 \\ 0 & 19 & 38/5 & 11/5 & 93/5 \\ 0 & 4 & 37/5 & -6/5 & 82/5 \\ 0 & 3 & 1 & 7 & 72 \end{array}\right) \begin{array}{l} \\ \\ \times(-4/19)+ \\ \times(-3/19)+ \end{array} \sim \left(\begin{array}{cccc|c} 1 & 0 & 3/5 & 1/5 & 8/5 \\ 0 & 19 & 38/5 & 11/5 & 93/5 \\ 0 & 0 & 29/5 & -158/95 & 1186/95 \\ 0 & 0 & -1/5 & 632/95 & 6561/95 \end{array}\right) \begin{array}{l} \\ \\ \\ \times(1/29)+ \end{array} \sim$$

$$\left(\begin{array}{cccc|c} 1 & 0 & 3/5 & 1/5 & 8/5 \\ 0 & 19 & 38/5 & 11/5 & 93/5 \\ 0 & 0 & 29/5 & -158/95 & 1186/95 \\ 0 & 0 & 0 & 3634/551 & 38291/551 \end{array}\right)$$

$$\underbrace{\phantom{\begin{array}{cccc} 0 & 0 & 0 & 3634/551 \end{array}}}_{U}$$

Now using backward substitution:

$$\frac{3634}{551} X_4 = \frac{38291}{551} \quad \therefore \quad \boxed{X_4 = \frac{38291}{3634} \cong 10.5369}$$

$\frac{29}{5} X_3 - \frac{158}{95} X_4 = \frac{1186}{95} \therefore \boxed{X_3 = \frac{119}{23} \cong 5.1739}$

$19 X_2 + \frac{38}{5} X_3 + \frac{11}{5} X_4 = \frac{93}{5} \therefore \boxed{X_2 = -\frac{8397}{3634} \cong -2.3107}$

$X_1 + \frac{3}{5} X_3 + \frac{1}{5} X_4 = 8/5 \therefore \boxed{X_1 = -\frac{13125}{3634} \cong -3.6117}$

(c) Matlab script available @ MyA

Using $X = (1\ 1\ 1\ 1)^T$ as initial guess and tolerance of 10^{-5}:

(i) Gauss-Seidel: $X_{GS} = (-3.6117\ \ -2.3107\ \ 5.1739\ \ 10.5369)^T$

number of iterations: 13

(ii) SOR ($\omega = 0.4$): $X_{SOR} = (-3.6114\ \ -2.3105\ \ 5.1737\ \ 10.5368)^T$

number of iterations: 43