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CL249: ASSIGNMENT 9

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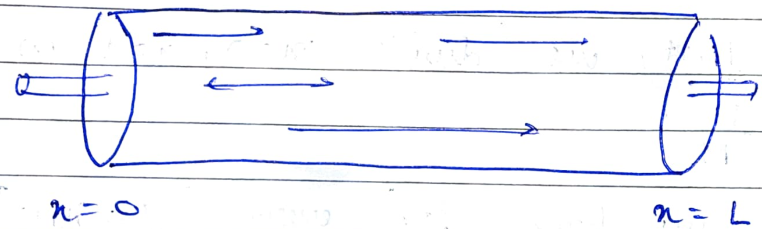
PROBLEM

We have to solve the following diff. eqn which describes the steady state conc. of substance that reacts with 1st order kinetics in an axially-dispersed plug flow reactor.



$$D\frac{d^2C}{dx^2} - u\frac{dc}{dx} = kc$$

D = diffusion const = 5000 m^2/hr
C = conc. of subs.
u = Axial velocity = 100 m/hr
K = Rate const = $2h^{-1}$
C_{inlet} = 100 mol/L

(1) $U C_{inlet} = u C_{x=0} - D\frac{dc}{dx}\Big|_{x=0}$

(2) $\frac{dc}{dx}\Big|_{x=L} = 0$

L = length = 100 m

We have to submit plot of y vs x for diff. h.

Description of method

Boundary value problem

we have a diff. eqn

$$D \frac{d^2c}{dx^2} - v\frac{dc}{dx} = kc$$

first, we divide $x=0$, $x=1$ in N parts

$h = \frac{L}{N}$;

then we have for every $[x_{i-1}, x_{i+1}]$

$$\frac{d^2c}{dx^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2}$$

$$\frac{dc}{dx} = \frac{C_{i+1} - C_{i-1}}{2h}$$

$$D\left(\frac{C_{i+1}}{h^2} - \frac{2C_i}{h^2} + \frac{C_{i-1}}{h^2}\right) - v\left[\frac{C_{i+1} - C_{i-1}}{2h}\right] = kC_i$$

$$2D(C_{i+1} - 2C_i + C_{i-1}) - hv(C_{i+1} - C_{i-1}) = 2h^2kC_i$$

$$(2D + hv)C_{i-1} - (2h^2k + 4D)C_i + (2D - hv)C_{i+1} = 0 \quad \text{--- (1)}$$

and Bound. cond.

$$uC_{in} = uC_1 - D\left(\frac{C_2 - C_0}{2h}\right)$$

$$2hUC_{in} = 2hUC_1 - DC_2 + DC_0 \quad \text{--- (2)}$$

and

$$\frac{C_{n+2} - C_n}{2h} = 0 \quad \text{--- (3)}$$

we can define matrix in which

$$
\begin{bmatrix} D & -2hv-D & 0 & \cdots & 0 \\ 0 & 2D+hv & -2h^2k-4D & -2D+hv & \\ & & \cdots & & \\ & & \cdots & & \\ 0 & 0 & \cdots 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \vdots \\ C_{n+1} \end{bmatrix} = \begin{bmatrix} 2h\,v\,C_{in} \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}
$$

solve this using gauss elim

Pseudo code

main.m

loop in N to increase values

$N = 2^i$

divide X in parts

get y from solun.

$\text{error} = \dfrac{y - y_{pre}}{y}$

get maximum error

if max err > tol

normal plot

else bold plot

solve.m

define constants

take inputs

A, B = zeros

loop to define general matrix

$A(i, i+1) = $ —

define boundary cond. in the matrix

solve using gauss elim

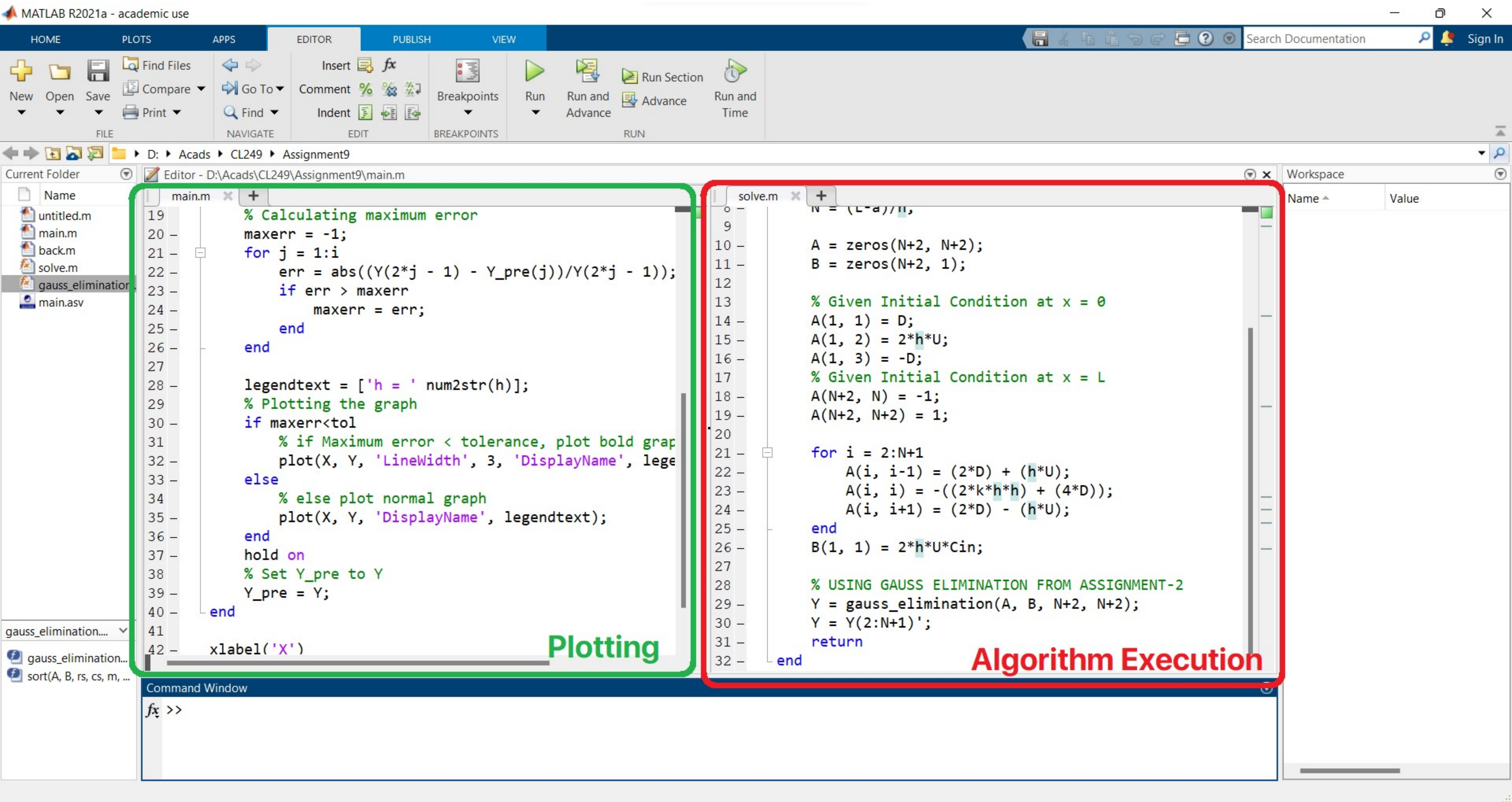
return value

```
% Boundary
a = 0;
b = 100;

% Tolerance
tol = 10^-4;

% Defining Y_pre to store previous Y matrix for error calculation
% Size = 4 due to first iteration of the loop
Y_pre = zeros(1, 4);
for i = 2:10
    % Increasing N exponentially
    N = 2^i;
    h = (b-a)/N;
    % X interval
    X = linspace(a, b, N);
    % Getting Y through solver
    Y = solve(a, b, h);
    % Calculating maximum error
    maxerr = -1;
    for j = 1:i
        err = abs((Y(2*j - 1) - Y_pre(j))/Y(2*j - 1));
        if err > maxerr
            maxerr = err;
        end
    end

    legendtext = ['h = ' num2str(h)];
    % Plotting the graph
    if maxerr<tol
        % if Maximum error < tolerance, plot bold graph to highlight
        plot(X, Y, 'LineWidth', 3, 'DisplayName', legendtext);
    else
        % else plot normal graph
        plot(X, Y, 'DisplayName', legendtext);
    end
    hold on
    % Set Y_pre to Y
    Y_pre = Y;
end

xlabel('X')
ylabel('Concentration')
title('Plot of Concentration (x) vs Distance from origin (x)')
legend
```

```
function Y = solve(a, b, h)
    Cin = 100;
    L = b;
    k = 2;
    U = 100;
    D = 5000;

    N = (L-a)/h;

    A = zeros(N+2, N+2);
    B = zeros(N+2, 1);

    % Given Initial Condition at x = 0
    A(1, 1) = D;
    A(1, 2) = 2*h*U;
    A(1, 3) = -D;
    % Given Initial Condition at x = L
    A(N+2, N) = -1;
    A(N+2, N+2) = 1;

    for i = 2:N+1
        A(i, i-1) = (2*D) + (h*U);
        A(i, i) = -((2*k*h*h) + (4*D));
        A(i, i+1) = (2*D) - (h*U);
    end
    B(1, 1) = 2*h*U*Cin;

    % USING GAUSS ELIMINATION FROM ASSIGNMENT-2
    Y = gauss_elimination(A, B, N+2, N+2);
    Y = Y(2:N+1)';
    return
end
```

```
function X = gauss_elimination(A, B, m, n)
    operations = 0;
    X = zeros(n,1); % Initialize X

    % Sorting initially
    [A, B] = sort(A, B, 1, 1, m, n);

    for c = 1:n
        % Sorting A and B (max. diagonal element)
        [A, B] = sort(A, B, c, c, m, n);
        for r = m:-1:c+1
            if (A(r,c) ~= 0)
                factor = A(r, c)/A(c, c); % 1 operation
                A(r,:) = A(r, :) - (factor*A(c, :)); % 2*n operations
                B(r) = B(r) - (factor*B(c)); % 2 operations
                operations = operations + (2*n) + 3;
            end
        end
    end

    % Back-Substitution
    X(n) = (B(n)/A(n,n));
    operations = operations + 1;
    for i = m-1:-1:1
        sum = 0;
        for j = n:-1:i+1
            sum = sum + (X(j)*A(i, j));
            operations = operations + 2;
        end
        X(i) = (B(i) - sum)/A(i, i);
        operations = operations + 2;
    end

end

% Sorting Function
function [mat1, mat2] = sort(A, B, rs, cs, m, n)
    for s = rs:m-1
        for r = rs:m-1
            if abs(A(r, cs)) < abs(A(r+1, cs))
                temp1 = A(r, :);
                A(r, :) = A(r+1, :);
                A(r+1, :) = temp1;
                temp2 = B(r);
                B(r) = B(r+1);
                B(r+1) = temp2;
            end
        end
    end
    mat1 = A;
```

```
    mat2 = B;
end
```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Breakpoints
BREAKPOINTS
Run
Run and Advance
Run Section
Advance
Run and Time
RUN
D: ▸ Acads ▸ CL249 ▸ Assignment9
Current Folder
Name
untitled.m
main.m
back.m
solve.m
gauss_elimination
main.asv
Editor - D:\Acads\CL249\Assignment9\main.m
main.m
% Calculating maximum error
maxerr = -1;
for j = 1:i
err = abs((Y(2*j - 1) - Y_pre(j))/Y(2*j - 1));
if err > maxerr
maxerr = err;
end
end
legendtext = ['h = ' num2str(h)];
% Plotting the graph
if maxerr<tol
% if Maximum error < tolerance, plot bold grap
plot(X, Y, 'LineWidth', 3, 'DisplayName', lege
else
% else plot normal graph
plot(X, Y, 'DisplayName', legendtext);
end
hold on
% Set Y_pre to Y
Y_pre = Y;
end
xlabel('X')
Plotting
solve.m
A = zeros(N+2, N+2);
B = zeros(N+2, 1);
% Given Initial Condition at x = 0
A(1, 1) = D;
A(1, 2) = 2*h*U;
A(1, 3) = -D;
% Given Initial Condition at x = L
A(N+2, N) = -1;
A(N+2, N+2) = 1;
for i = 2:N+1
A(i, i-1) = (2*D) + (h*U);
A(i, i) = -((2*k*h*h) + (4*D));
A(i, i+1) = (2*D) - (h*U);
end
B(1, 1) = 2*h*U*Cin;
% USING GAUSS ELIMINATION FROM ASSIGNMENT-2
Y = gauss_elimination(A, B, N+2, N+2);
Y = Y(2:N+1)';
return
end
Algorithm Execution
Workspace
Name
Value
gauss_elimination...
gauss_elimination...
sort(A, B, rs, cs, m, ...
Command Window
fx >>

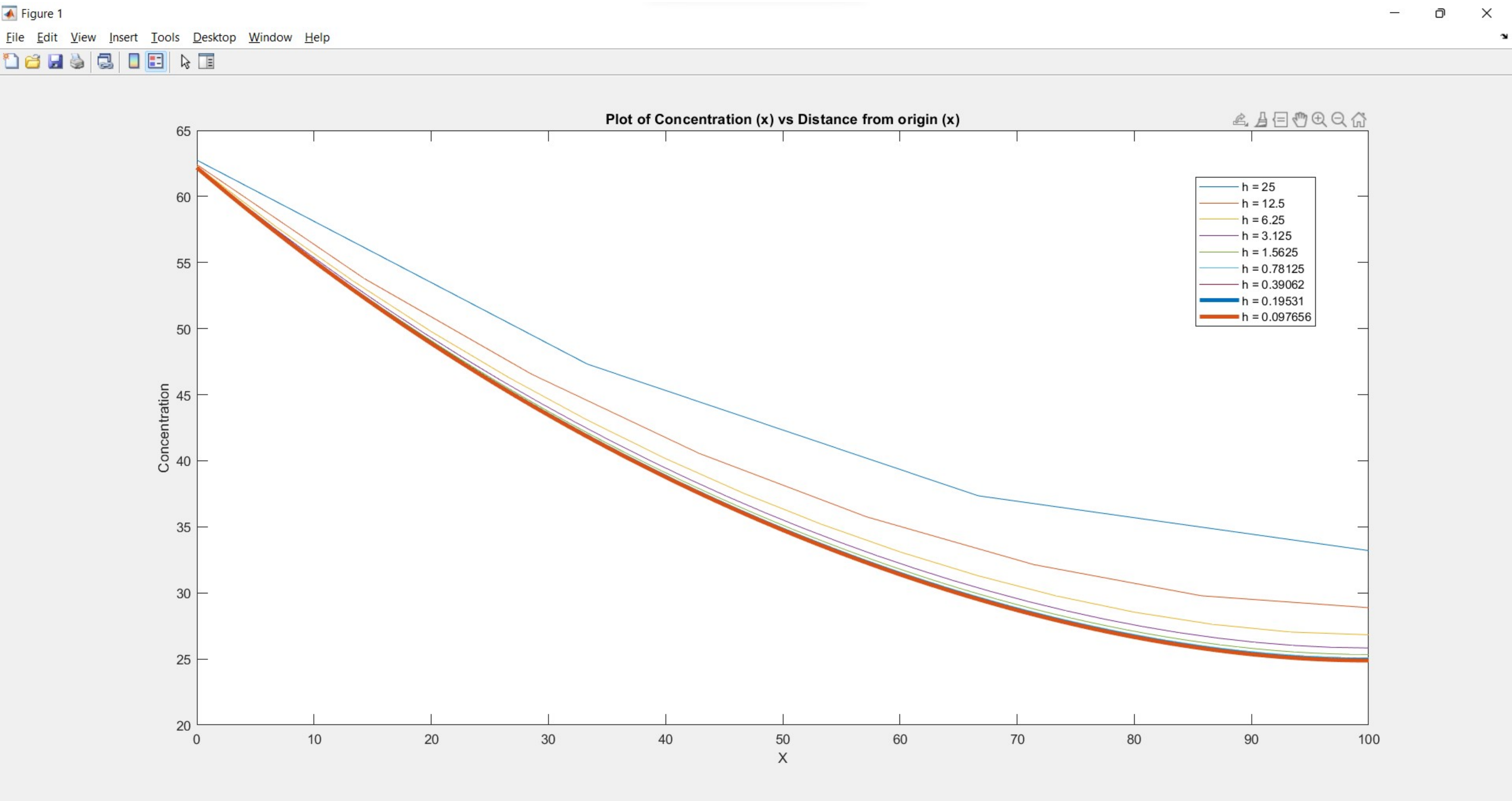
Figure 1
File Edit View Insert Tools Desktop Window Help
Plot of Concentration (x) vs Distance from origin (x)
Concentration
X
h = 25
h = 12.5
h = 6.25
h = 3.125
h = 1.5625
h = 0.78125
h = 0.39062
h = 0.19531
h = 0.097656
65
60
55
50
45
40
35
30
25
20
0
10
20
30
40
50
60
70
80
90
100