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CL249 - Computational Methods Lab
Assignment 1 : Solution of non-linear Eq^n

Submitted By:

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PROBLEM STATEMENT:

Due to climate change, heavy rainfall is occuring in many parts of the world. The CO_2 released in the atmosphere plays a significant role. One mitigation approach is to capture and store gaseous CO_2 under geological systems at higher pressure. For efficient design of such systems, the amount of volume per mole of CO_2 (V) at sub-surface conditions van der Waals equation of state is used, given as:

$$\left(P + \frac{a}{V^2}\right)\left(V - b\right) = RT$$

Given data:

$a = 3.592$, $b = 0.04267$, $R = 0.082056$. Generate a P-V isotherem for subsurface conditions of $T = 345K$ and $P = 1$ to 100 atm.

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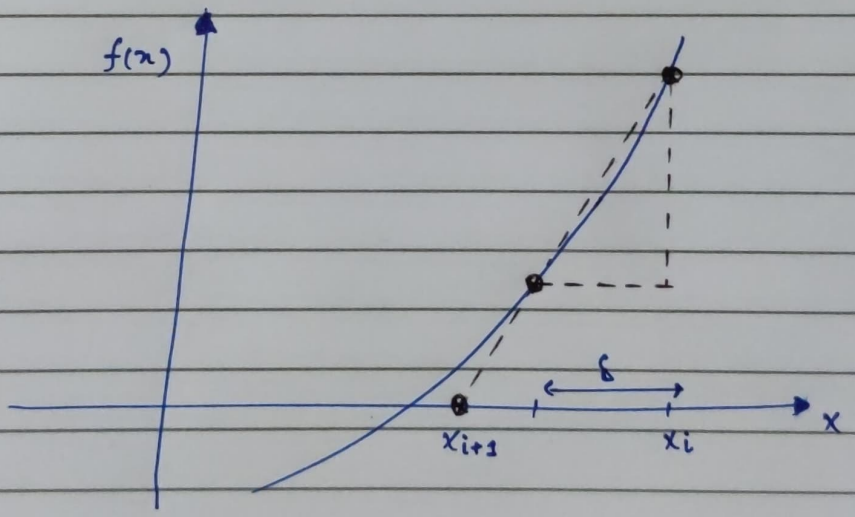
SOLUTION METHODOLOGY

⇒ Modified Secant Method

Unlike Secant method, this requires only one initial guess for its functing. The second parameter of the secant method is replaced by a fractional constant (δ).

Secant method ⇒ $$x_{i+1} = x_i - \frac{f(x_i) \times (x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

Modified Secant Method ⇒ $$x_{i+1} = x_i - \frac{f(x_i) \times \delta}{f(x_i + \delta) - f(x_i)}$$



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PSEUDOCODE FOR MODIFIED SECANT METHOD

1. Start
2. Declaration of fn $y = f(x)$ and delta (δ)
3. User Input initial guess (x_0)
4. User Input error limit (epsilon)
5. $$x_1 = x_0 - \frac{f(x_0+\delta)\cdot \delta}{f(x_0+\delta) - f(x_0)}$$
6. while $abs\left(\frac{x_1 - x_0}{x_1}\right) > epsilon$ {:

$x_0 = x_1$ }

$$x_1 = x_0 - \frac{f(x_0+\delta)\cdot \delta}{f(x_0+\delta) - f(x_0)}$$

7. Root = x_1
8. Stop

```
function y=f(P,V)
a=3.592;
b=0.04267;
R=0.082056;
T=345;
% y as a function of V.
y = P*(V.^3) - (P*b + R*T)*(V.^2) + a*V - a*b;
end
```

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```
function V = MSM(P,Vo,del, epsilon)
% Modified Secant Method

for i= 1:length(P)
    V1 = Vo - (f(P(i),Vo)*del)/(f(P(i),Vo+del) - f(P(i),Vo)); %
 Modified Secant Method formula
    while abs((V1-Vo)/V1) > epsilon % Break (anti) condition
            Vo = V1;
            V1 = Vo - (f(P(i),Vo)*del)/(f(P(i),Vo+del) - f(P(i),Vo));
    end
V(i) =V1; % storing value as vector for each P
end

end
```

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```
clc;
clear;

%Vector P with values from 1 to 100 in 0.1 gap.
P= 1:0.1:100;

% Taking input of initial guess and error limit.
Vo = input('Enter your first guess for volume:');
epsilon = input('Enter value of epsilon:');

% For best accuracy, take epsilon = 1e-4

% delta value for modified secant method.
del = 0.01;

%storing resultant vector V from MSM function
V = MSM(P,Vo,del,epsilon);


figure
plot(V,P)
title('P-V Isotherm at T=345K')
xlabel('V ->')
ylabel('P lying between 1 to 100 ->')
```

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1 ITERATION

$$y = Pv^3 - (Pb + RT)v^2 + av - ab$$

BEGIN

$V_0 = 50$ delta (δ) $= 0.01$

Let $P = 1$

$\Rightarrow y(50) = 5.4299 \times 10^4$ $\Rightarrow y(50+\delta) = 5.4346 \times 10^4$

$$\therefore V_1 = V_0 - \frac{y(50+\delta)\,\delta}{y(50+\delta) - y(50)}$$

$$V_1 = 38.437$$

ITERATION 1

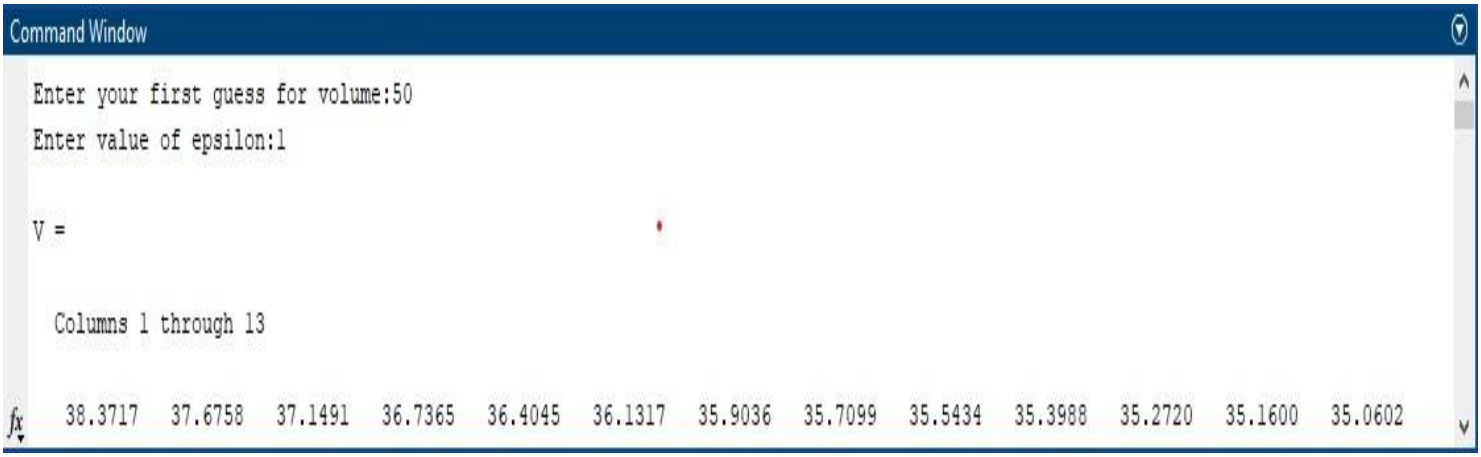
$V_0 = 38.437$ $y(V_0) = 1.5038 \times 10^4$

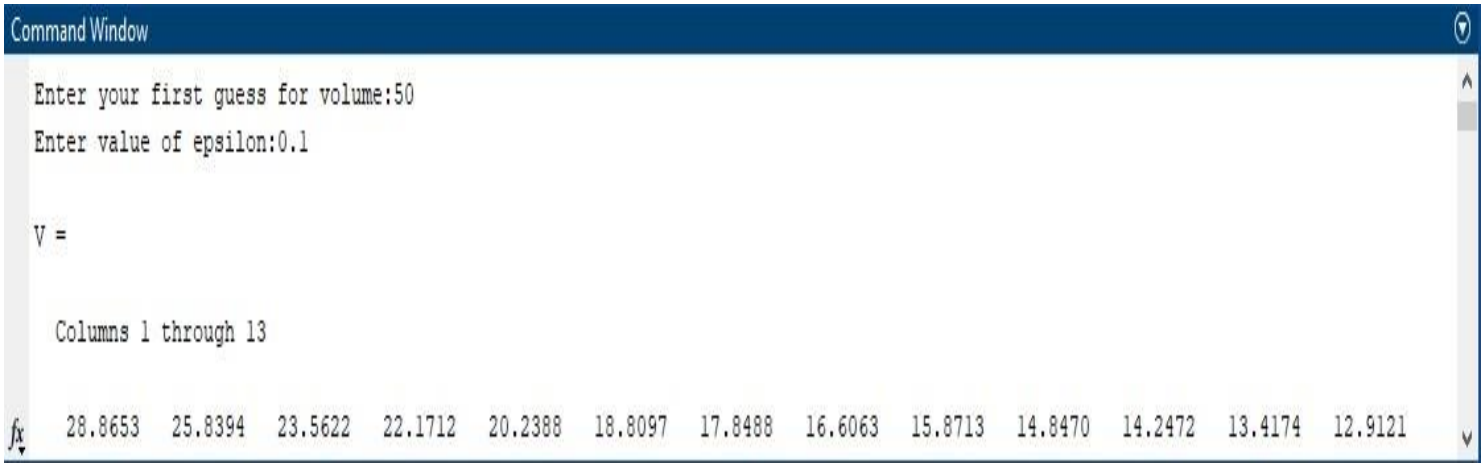
$y(V_0+\delta) = 1.5060 \times 10^4$

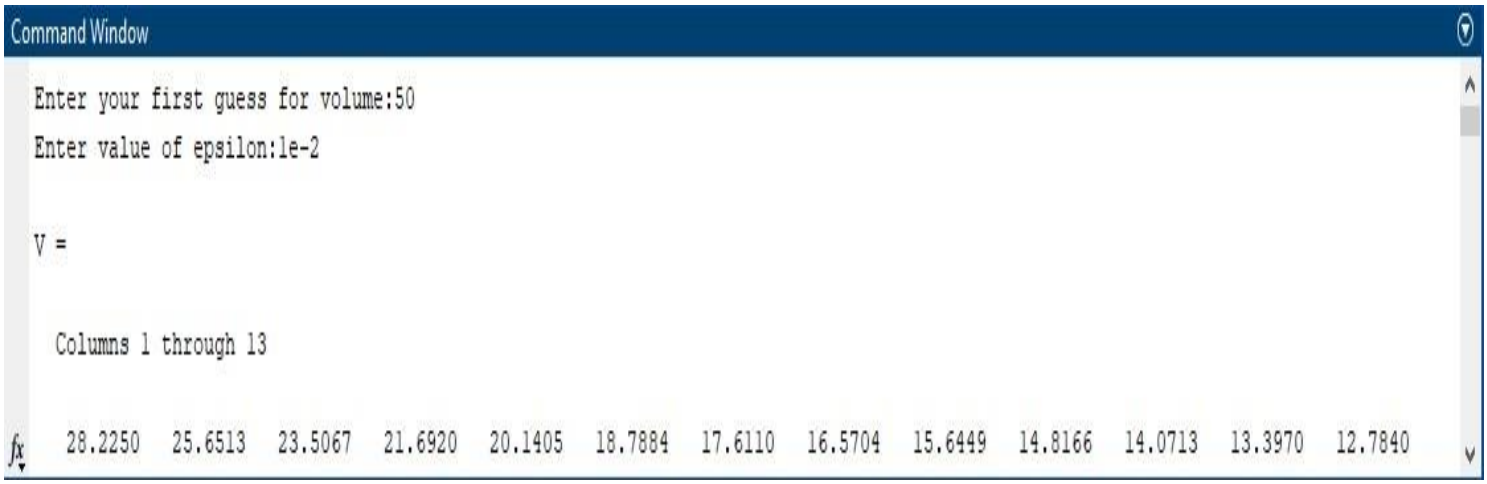
$$V_1 = V_0 - \frac{y(V_0+\delta)\,\delta}{y(V_0+\delta) - y(V_0)}$$

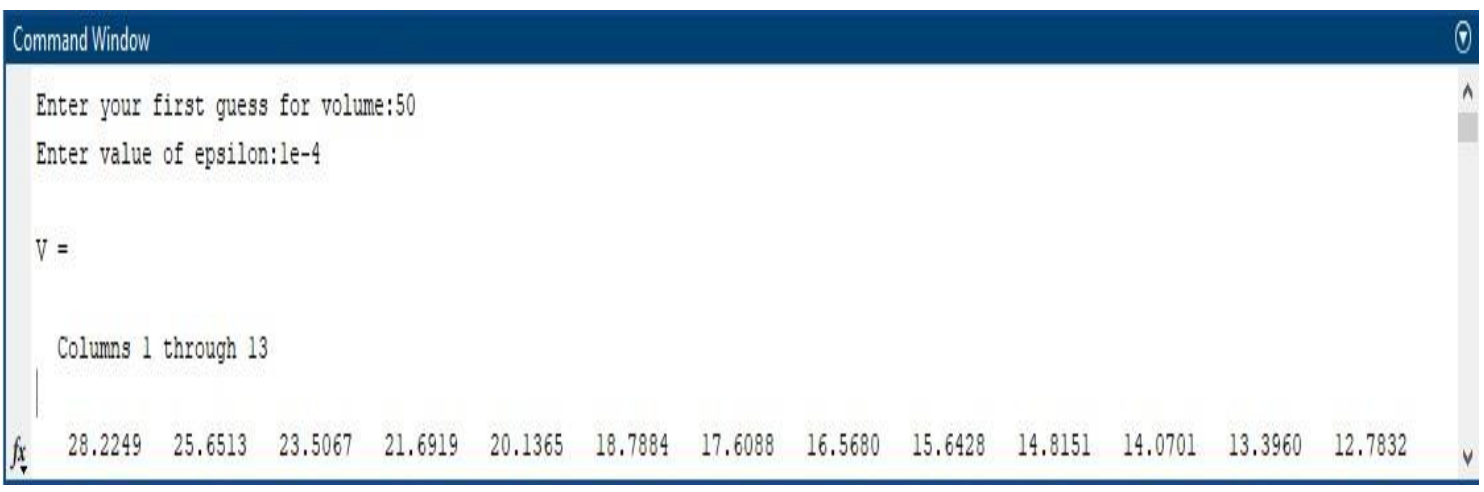
$$V_1 = 31.591$$

Values of V for P=1:0.1:100 on different values of epsilon.

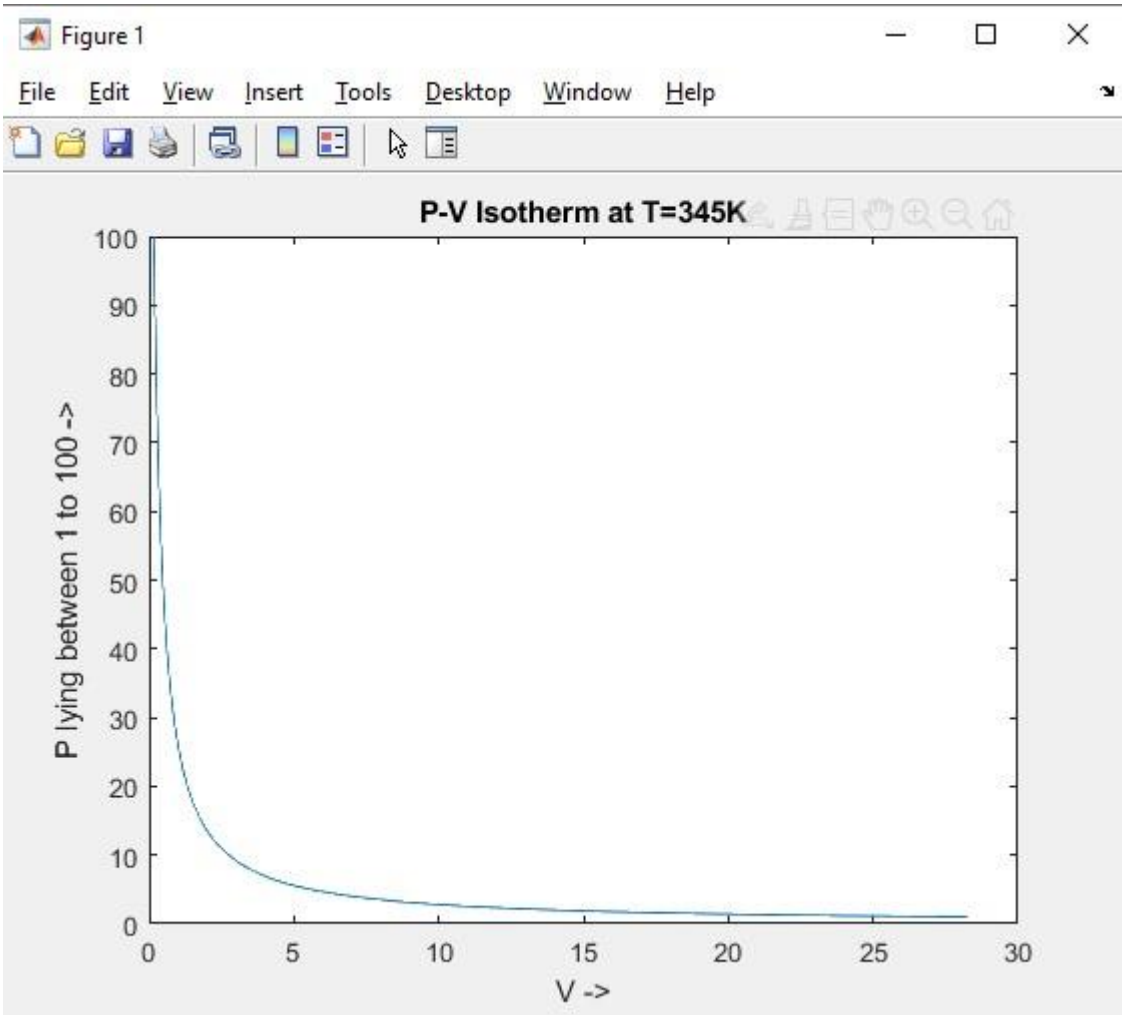








Final plot for epsilon = 1e-4 and smaller:



Comments and Remarks:

The assignment helped in self-learning the Modified Secant Method. It was a good assignment for an introduction to MATLAB.

The graph crosses (28.2249,1), i.e. the volume of CO_2 at atmospheric pressure is 28.2249 liters, which is a little deviated from ideal gas volume of 22.4 liters. As the pressure mounts, volume occupied per mole of CO_2 decreases rapidly. Thus, the graph obtained is almost **hyperbolic**.