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%% CHEN 320 - 202 Homework 2
% Problem: 1
% Author: Nathaniel Thomas
% Date: 09/16/2022
% Due: 09/18/2022

%% Problem 1(a):
% Reaction:  $2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2$ 

T = 2000; % Temperature, K
P = 1; % Pressure, atm
k = 62.4E6; % Equilibrium constant, atm
n_CO = 2; % Basis of CO, gmoles
n_O2 = 1; % Basis of O_2, gmoles
n_N2 = 3.76; % Basis of N_2, gmoles

syms x

% Function handle for final expression
k_func = ((x.^2).*(6.76 - 0.5.*x)) - (k.*(1 - 0.5.*x).*(2-x).^2);

% Function handle for derivative of final expression
k_func_diff = diff(k_func);

% Convert to Matlab Functions
k_func = matlabFunction(k_func);
k_func_diff = matlabFunction(k_func_diff);

x_i = 0.1; % Initial guess for moles of CO reacted, gmoles
x_i1 = x_i - k_func(x_i)./k_func_diff(x_i);

% Newton's Method
% Control loop. Stop after [tol] is reached.

tol=10^-4; itr_max=100; % Input tolerance and maximum iterations
% Input starting point
for i=1:itr_max % Begin iterative solution
    fx = k_func(x_i); % Calculate function value
    dfx=k_func_diff(x_i); % Calculate df/dx
    x_i1=x_i-fx/dfx; % Apply Newton's method
    Rerr=(x_i1-x_i)./x_i1; % Calculate relative error
    % Print out intermediate results
    fprintf(' i=%d x=%f f(x)=%f relative error=%f\n',i,x_i1,fx,Rerr)
    x_i=x_i1; % Transfer xnew to x0 for next iteration
    if abs(Rerr)<tol % Check for convergence
        break
    end
end

if i>itr_max-1 % Check for maximum iteration limit
    fprintf('Maximum iterations exceeded without convergence\n')
else
end

fprintf("The mole fraction is: %.3f\n", x_i1);

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% Newton's method cannot converge due to the extremely steep slope at the x
% = 0.1 point.

%% Problem 1(b)
% Illinois Method
tol=10^-4; itr_max=100;           % Input tolerance and maximum iterations
x0=0.1;                           % Input starting point
f = k_func;                       % Define function as an anonymous function
%
% Bound the root with a positive and negative function value
%
dx=0.1*x0;                       % Set step size dx for bounding the root
if dx<10^-8;dx=10^-8;end         % Clamp dx to 10^-8 if less than this
x1=x0+dx;                        % Increment x by dx
                                % Move in the desired direction
if abs((x1))>abs(f(x0));dx=-dx;end
while f(x0)*f(x1)>0              % Check for a bounded root
    x0=x1;                      % Transfer x1 to x0
    x1=x0+dx;                   % If not bounded, continue incrementing
                                % x by dx
end
fprintf('The function has been bounded between x= %f and %f\n',x0,x1)
%
% Begin iterative solution of bounded root using Illinois method
%
fun=f(x0);                      % Initialize fun
for i=1:itr_max
    % Apply estimate of the root
    xnew=x1-f(x1)*(x1-x0)/(f(x1)-fun);
    Rerr=(xnew-x1)/xnew;         % Calculate relative error
                                % Print out intermediate results
    fprintf(' i=%d  x=%f  f(x)=%f  relative error=%f\n',i,xnew,f(x1),Rerr)
                                % Check for convergence
    if abs(Rerr)<tol,break,end
    if (f(x1)*f(xnew))<0        % Check for alternating sign of function
                                % values
        x0=x1;                % Transfer value of xnew to x1 for next
                                % iteration
        x1=xnew;               % Transfer value of xnew to x1 for next
                                % iteration
        fun=f(x0);             % Use use regula falsi method when the
                                % sign of the function alternates
    else
        x1=xnew;               % Transfer value of xnew to x1 for next
                                % iteration
        fun=0.5*f(x0);         % Use Illinois method modification when
                                % the sign does not alternate
    end
end
end
if i>itr_max-1                  % Check for maximum iteration limit
    fprintf('Maximum iterations exceeded without convergence\n')
else
end
fprintf('The mole fraction is: %.3f\n', x1);

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%% Problem 1(c)

% Use fzero() to find a solution:
xi = 0.1;
res = fzero(k_func, xi);
fprintf("The mole fraction is: %.3f\n", res);

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Output for Problem 1:

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i=1 x=0.733333 f(x)=-214000799.932900 relative error=0.863636
i=2 x=1.155556 f(x)=-63407641.412415 relative error=0.365385
i=3 x=1.437037 f(x)=-18787445.308173 relative error=0.195876
i=4 x=1.624691 f(x)=-5566645.804434 relative error=0.115501
i=5 x=1.749792 f(x)=-1649371.438717 relative error=0.071495
i=6 x=1.833192 f(x)=-488697.260161 relative error=0.045494
i=7 x=1.888786 f(x)=-144793.605028 relative error=0.029434
i=8 x=1.925839 f(x)=-42896.096288 relative error=0.019240
i=9 x=1.950517 f(x)=-12704.157057 relative error=0.012652
i=10 x=1.966914 f(x)=-3758.345885 relative error=0.008336
i=11 x=1.977722 f(x)=-1107.718269 relative error=0.005465
i=12 x=1.984659 f(x)=-322.394145 relative error=0.003495
i=13 x=1.988737 f(x)=-89.927391 relative error=0.002051
i=14 x=1.990568 f(x)=-21.768238 relative error=0.000919
i=15 x=1.990968 f(x)=-3.339993 relative error=0.000201
i=16 x=1.990986 f(x)=-0.139315 relative error=0.000009

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The mole fraction is: 1.991

The function has been bounded between x= 1.990000 and 2.000000

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i=1 x=1.992665 f(x)=23.040000 relative error=-0.003681
i=2 x=1.990756 f(x)=10.571923 relative error=-0.000959
i=3 x=1.991034 f(x)=-1.801762 relative error=0.000140
i=4 x=1.990987 f(x)=0.361375 relative error=-0.000023

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The mole fraction is: 1.991

The mole fraction is: 1.991

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%% CHEN 320 - 202 Homework 2
% Problem: 2
% Author: Nathaniel Thomas
% Date: 09/16/2022
% Due: 09/18/2022

%% Problem 2
r = 15 / 2; % Radius of the spherical tank, ft
V = 500; % Volume of liquid in the tank, ft^3
% Function for determining height
f = @(h) V - (pi .* h.^2 * (3 .* r - h))./3;

% Start with a guess of the tank's radius
h = r;
h = fzero(f, h);

fprintf("The height of liquid in the tank is %.3f ft.\n", h);

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Problem 2 output:

The height of liquid in the tank is 5.263 ft.

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%% CHEN 320 - 202 Homework 2
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% Problem: 3
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%% Problem 3
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Q = 850; % Desired heat flux, Btu/(h ft^2)
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h = 1.0; % Convective heat transfer coefficient, Btu/(h ft^2 degF)
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T = 100 + 459.67; % Surrounding temperature, F
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e = 0.9; % Emmissivity, Dimensionless
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o = 1.174E-9; % Btu/(h ft R^4)
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% Function for determining the average surface temperature
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f = @(Ts) h*(Ts - T) + e * o * (Ts^4 - T^4) - Q;
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Ts = T*2; % Guess that the average surface is double the surroundings
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Ts = fzero(f, Ts);
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fprintf("The average surface temperature is %.3f degF \n", Ts - 459.67);
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Problem 3 output:
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The average surface temperature is 420.252 degF
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