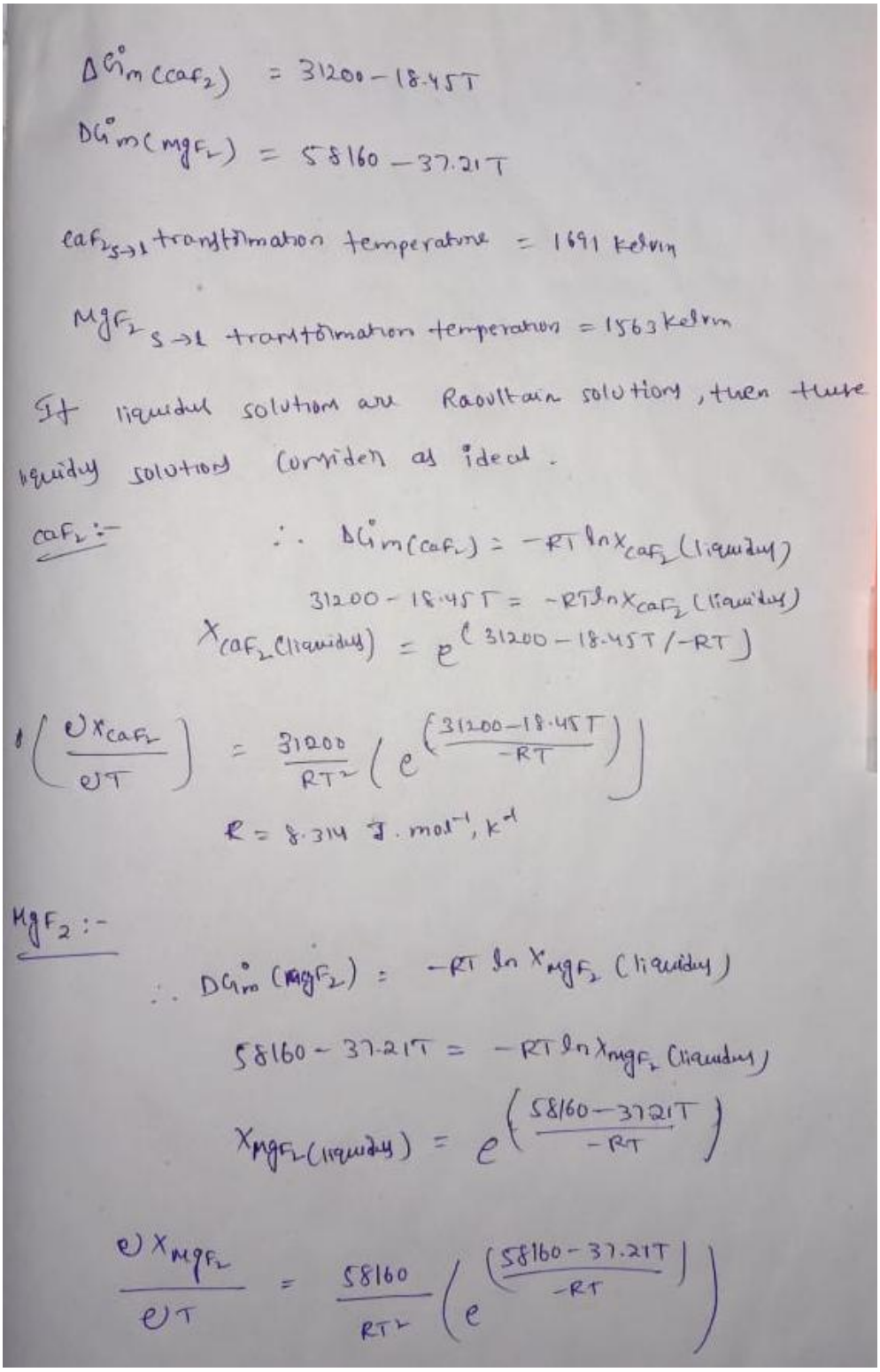
Assignment2: NMM

1). Equations for Liquids lines:



2). Finding Eutectic Temperature by using newton.m

Program Commands:

```
function [rx,ry] = newton(x0,itmax,tol)
% You need to enter your equation in the last part of
% this code. That is, for f(x)=0, you need to enter
% your function f and its derivative fprime(x)
% As an example, this code solves the equation exp(-x)-x=0 by Newton's method.
```

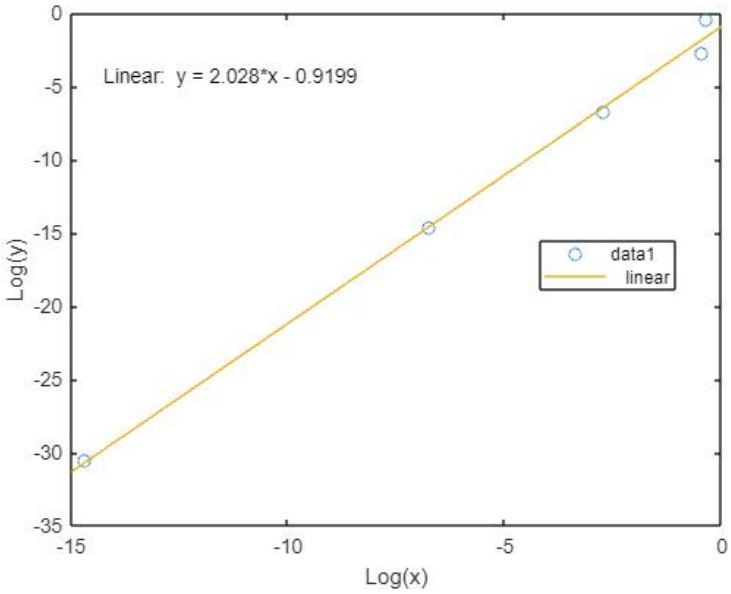
```
% To solve your own equation, you can delete those lines (Line 54 and 56) and enter your own
equations and it's first derivative.
% You don't need to change anything else in the code.
% After typing your equation and the derivative, this code should be called in MATLAB as
newton(..., ..., ...) where the three arguments refer to
% the initial guess value, maximum iterations, and tolerance value respectively.
%
%Initialize variables
%
x=zeros(itmax+1,1);r=zeros(itmax+1,1);
x(1,1)=x0; r(1,1)=f(x0);
fprintf('\n');
%
%Set up the iterative scheme
%
for k=1:itmax
x(k+1,1)=x(k,1)-f(x(k,1))/fprime(x(k,1));
r(k+1,1)=f(x(k+1,1));
if abs(r(k+1,1))<=tol
disp(['Method has converged after ',num2str(k),' iterations.'])
break
end
end
if abs(r(k+1,1))>tol
disp(['Method has NOT converged after ',num2str(k),' iterations.'])
end
%
%Some print statements
%
fprintf('\n');
disp(' iter value of x value of f(x)')
for i=1:k+1
fprintf('%4.0f',i-1)
fprintf('%19.14f',x(i,1))
fprintf('%19.14f',r(i,1))
fprintf('\n');
end
fprintf('\n');
%
%Residual values of the function to be passed as output to the function
%
rx=zeros(k,1);ry=zeros(k,1);
for i=1:k
rx(i,1)=abs(r(i,1));
ry(i,1)=abs(r(i+1,1));
end
%
% Subroutines to enter your function and its derivative
%
function y=f(x)
y=(exp((31200-18.45062093*x)./(-8.31446261815324*x)))+(exp((58160-37.21049264*x)./(-
8.31446261815324*x)))-1;
function yp=fprime(x)
yp=(((31200)./(8.31446261815324*x.^2))*exp((31200-18.45062093*x)./(-
8.31446261815324*x)))+((((58160)./(8.31446261815324*x.^2))*exp((58160-37.21049264*x)./(-
8.31446261815324*x))));
```

Command Window Execution Statement:

A) Initial Guess value is 1000 kelvin

```
  >>[x,y]=newton(1000,10,0.0000000001)

Method has converged after 5 iterations.

iter value of x value of f(x)
```

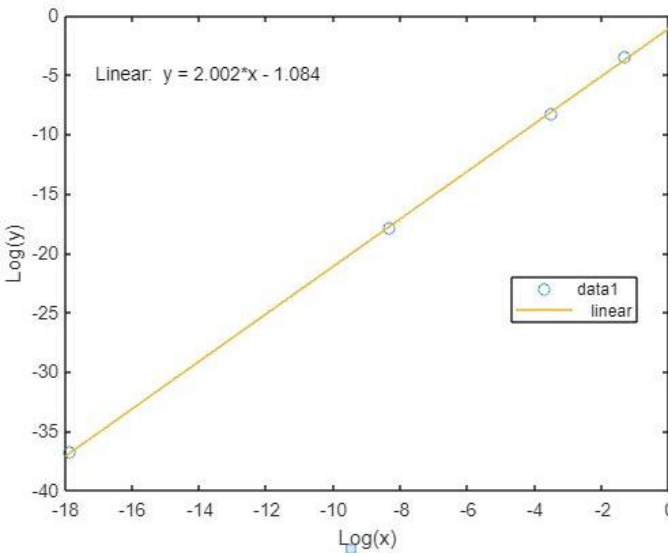
```
01000.00000000000000 -0.70371079174431
11512.60594569427008 0.63120995105120
21350.60092722583522 0.06630978821847
31329.02222385252981 0.00119744884944
41328.61794638082461 0.00000042018468
51328.61780442027407 0.00000000000005

x =
0.7037
0.6312
0.0663
0.0012
0.0000

y =
0.6312
0.0663
0.0012
0.0000
0.0000
```




```
>>plot(log(x),log(y),'o')
```

B) Second (Improve Guess value is 1231 kelvin

```
>> [x,y]=newton(1231,10,0.0000000001)

Method has converged after 4 iterations.

iter value of x value of f(x)
01231.00000000000000 -0.26452624528948
11338.47658676612332 0.02943060455895
21328.70082145190372 0.00024573722169
31328.61781040542769 0.00000001771532
41328.61780442025656 -0.00000000000000

x =
0.2645
0.0294
0.0002
0.0000


y =
0.0294
0.0002
0.0000
0.0000
```



Quadratic Convergence

```
>>plot(log(x),log(y),'o')
```

Therefore Eutectic Temperature is **1328.6178** kelvin

Note: newton.m file and quadratic convergence.fig also added in folder.

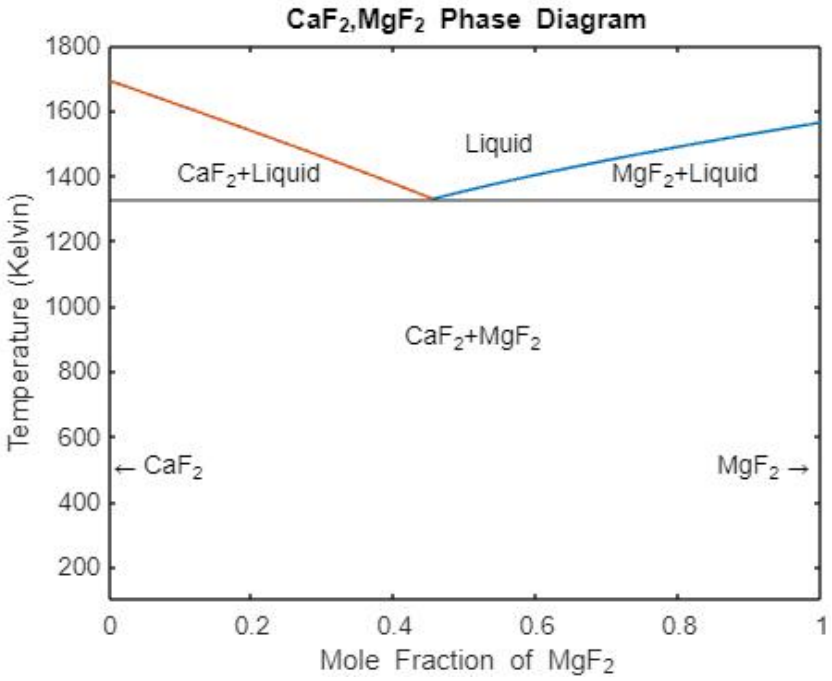
Eutectic Composition:

```
  >>T=1328.61780442027407
  T =
  1.3286e+03
  >>MolefractionCaF2=(exp((31200-18.45062093*T)./(-8.31446261815324*T)))

MolefractionCaF2 =
0.5459

  >>MolefractionMgF2=(exp((58160-37.21049264*T)./(-8.31446261815324*T)))

MolefractionMgF2 =
0.4541
```

3). Construction of Eutectic Phase Diagram

Program Commands:

```
%Eutectic Phase digarm
r1=[1328:23.5:1563];
t3=(exp((58160-37.21049264*r1)./(-8.31446261815324*r1)));
r2=[1328:36.3:1691];
t4=(exp((31200-18.45062093*r2)./(-8.31446261815324*r2)));
f=1-t4;
plot(t3,r1);
hold on
plot(f,r2);
yline(1328);
ylim([800,1800]);
xlabel('Mole Fraction of MgF_2');
ylabel('Temperature (Kelvin)');
title('CaF_2,MgF_2 Phase Diagram');
text(0,900,'\leftarrowCaF_2');
text(0.85,900,'MgF_2\rightarrow');
str='liquid';
text(0.5,1500,str);
str1='CaF_2+Liquid';
text(0.09,1400,str1)
str2='MgF_2+Liquid';
text(0.70,1400,str2);
str3='CaF_2+MgF_2';
text(0.41,1198,str3);
```



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