MM6010 - Assignment 2

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1 Question 1

The Excess enthalpy of $Co_{10}Cu_{30}Fe_{60-y}Ni_y$ system is calculated. The excess enthalpy of the binary systems are calculated as mentioned in the code snippet given below.

```
% functions to implement different binary systems
function y = CoCu(x1,x2)
y = x1*x2*(39332 - 1356*(x1-x2) + 7953*(x1-x2)^2 - 1119*(x1-x2)^3);
end

function y = CoFe(x1,x3)
y = x1*x3*(-9312 - 1752*(x1-x3));
end

function y = CoNi(x1,x4)
y = x1*x4*(1331);
end

function y = CuFe(x2,x3)
y = x2*x3*(35626 - 1530*(x2-x3) + 12714*(x2-x3)^2 + 1177*(x2-x3)^3);
end

function y = CuNi(x2,x4)
y = x2*x4*(12049 - 1862*(x2-x4));
end

function y = FeNi(x3,x4)
y = x3*x4*(-18379 + 9228*(x3-x4));
end
```

The extrapolation is performed using different schemes as outlined in the code snippet given below.

```
% Muggianu Scheme
beta  = 1.0;
for m = 1:no_of_comp-1
    for n = m+1 : no_of_comp
        x_i = ( 1 + mole_frac(m) - mole_frac(n))/2;
        x_j = ( 1 + mole_frac(n) - mole_frac(m))/2;
        f = mole_frac(m)*mole_frac(n)/(x_i*x_j);
        del_H_muggianu = del_H_muggianu + func(m,n,x_i,x_j)*f*beta;
    end
end
% Kohler Scheme
beta  = 1.0;
for m = 1:no_of_comp-1
    for n = m+1 : no_of_comp
        lamda = (mole_frac(m) - mole_frac(n))/(mole_frac(m) + mole_frac(n));
        x_i = (( 1 + mole_frac(m) - mole_frac(n)) + lamda*( 1 - mole_frac(m) -
    mole_frac(n)))/2;
        x_j = (( 1 + mole_frac(n) - mole_frac(m)) + lamda*( 1 - mole_frac(n) -
    mole_frac(m)))/2;
        f = mole_frac(m)*mole_frac(n)/(x_i*x_j);
        del_H_kohler= del_H_kohler + func(m,n,x_i,x_j)*f*beta;
    end
end
% Colinet Scheme
for m = 1:no_of_comp-1
```

```
    for n = m+1 : no_of_comp
        lamda_colinet = [1,-1];
        beta_colinet  = [0.5,0.5];
        for o = 1:2
            x_i = (( 1 + mole_frac(m) - mole_frac(n)) + lamda_colinet(o)*( 1 -
    mole_frac(m) - mole_frac(n)))/2;
            x_j = (( 1 + mole_frac(n) - mole_frac(m)) + lamda_colinet(o)*( 1 -
    mole_frac(n) - mole_frac(m)))/2;
            f = mole_frac(m)*mole_frac(n)/(x_i*x_j);
            del_H_colinet = del_H_colinet + func(m,n,x_i,x_j)*f*beta_colinet(o);
        end
    end
end
```

The excess enthalpy is calculated for various atomic percentages of Ni. The plot of excess enthalpy is given in Fig. 1

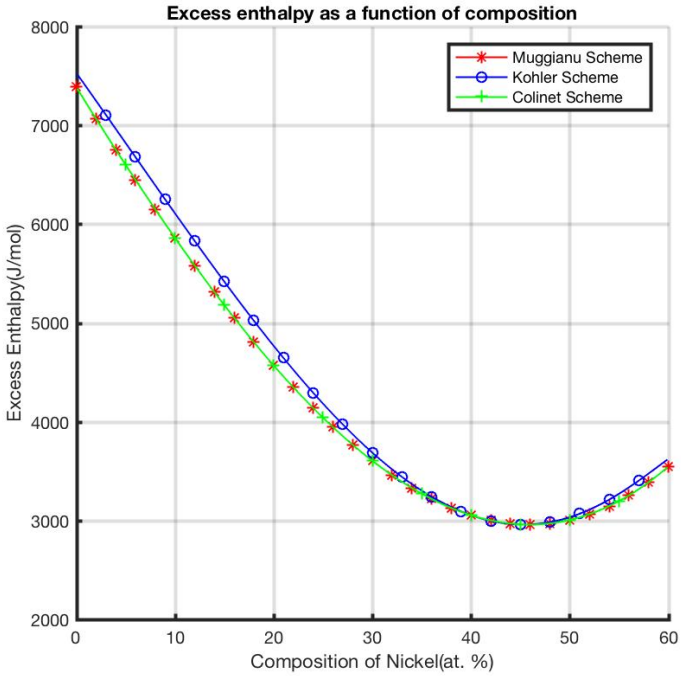

Figure 1: Excess enthalpy as function of composition of Ni

The calculation is repeated for equi-atomic composition and the output is given below.

```
Composition
    Co=0.25
    Cu=0.25
    Fe=0.25
    Ni=0.25
Excess Enthalpy in J/mol
    through Muggianu scheme = 3790.4375
    through Kohler   scheme = 3790.4375
    through Colinet  scheme = 3790.4375
```