NUMERICAL ANALYSIS

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조 혜 성

1.각 상에 대한 Ω계산(Excess Gibbs Energy 완성)

Enthalpy of formation

$$\Delta H_F^{\alpha} = X_{Tk}\Delta°G_{Tk}^{BCC\rightarrow\alpha} + (1 - X_{Tk})\Delta°G_{Ps}^{FCC\rightarrow\alpha} + X_{Tk}(1 - X_{Tk})\Omega$$

Enthalpy of mixing

$$\Delta H_M = X_{Tk}(1 - X_{Tk})\Omega$$

Activity

- $RTlna_{Tk} = \Delta°G_{Tk}^{BCC\rightarrow\alpha} + RTlnX_{Tk} + (1 - X_{Tk})^2(\Omega + \left(\frac{d\Omega}{dX_{Tk}}\right)X_{Tk})$
- $= \Delta°G_{Tk}^{BCC\rightarrow\alpha} + RTlnX_{Tk} + (1 - X_{Tk})^2(L_0 + 2X_{Tk}L_1)$
- $RTlna_{Ps} = \Delta°G_{Ps}^{FCC\rightarrow\alpha} + RTln(1 - X_{Tk}) + X_{Tk}{}^2(\Omega + \left(\frac{d\Omega}{d(1-X_{Tk})}\right)(1 - X_{Tk}))$
- $= \Delta°G_{Ps}^{FCC\rightarrow\alpha} + RTln(1 - X_{Tk}) + X_{Tk}{}^2(L_0 + (2X_{Tk} - 1)L_1)$

$\Omega = L_0$
→ regular solution

$\Omega = L_0 + L_1X_{Tk}$
→ sub-regular solution

L_0 =a+bT

L_1 =c+dT

Ps의 reference state: FCC
Tk의 reference state: BCC

1.각 상에 대한 Ω계산(Excess Gibbs Energy 완성)

$$\Delta H_m = x_{Tk}(1 - x_{Tk})(L_0 + L_1 x_{Tk})$$

$$\frac{\Delta H_m}{x_{Tk}(1 - x_{Tk})} = (L_0 + L_1 x_{Tk})$$

Activity of liquid at 1500K

선형 회귀분석 (Minimizing sum of squares of deviation)

$$y = a_0 + a_1 x + e$$

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2}$$

$$a_0 = \bar{y} - a_1 \bar{x}$$

$$r^2 = \frac{S_t - S_r}{S_t}$$

H_m → L0, L1
Activity → L0′, L1′

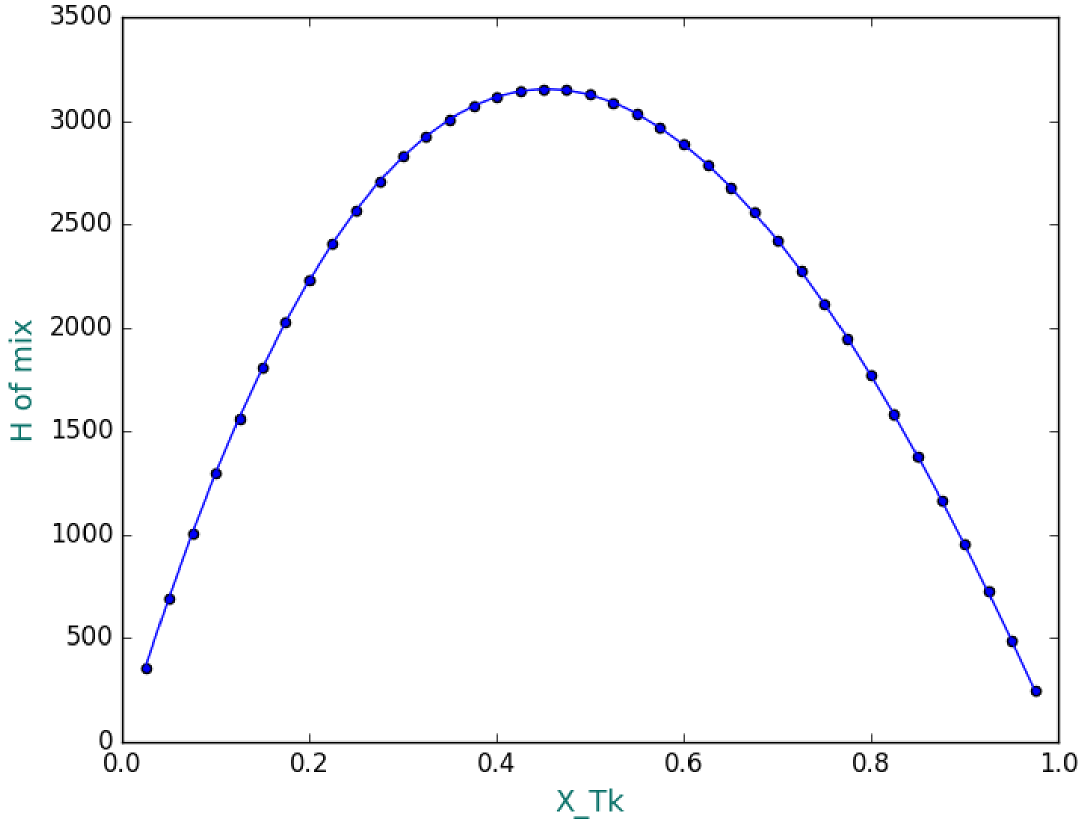
둘의 L0, L1 가 다르면 sub regular model 적용
L0′ = L0 + L01*T
L1′ = L1 + L11*T

1. Result

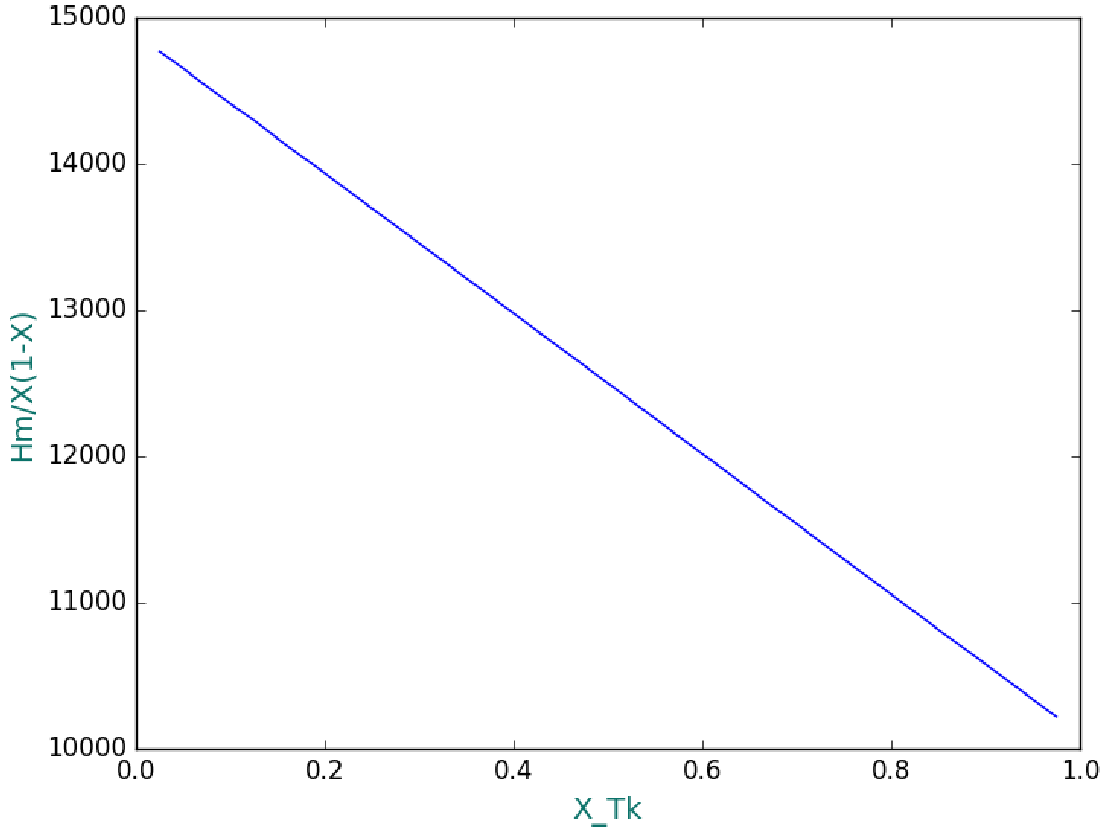
```python
def Sum(Hm, nHm, n):
    sumx, E, sumx2, sumy2, sumy, sumxy, E, R2, St, Sr = 0.0,
    x = []
    for i in range(0, n):
        sumx += Hm[i][0]
        sumx2+= Hm[i][0]**2
        sumy += nHm[i]
        sumy2+= nHm[i]**2
        sumxy+= Hm[i][0]*nHm[i]
    a1 = (n*sumxy - sumx * sumy)/(n*sumx2 - sumx**2)
    a0 = (sumy - a1*sumx)/n
    for i in range(0, n):
        E += (nHm[i] - a0 - a1*Hm[i][0])**2
    for i in range(0, n):
        St += (nHm[i] - sumy/n)**2
        Sr += (nHm[i]- a1*Hm[i][0] - a0)**2
    R2 = (St-Sr)/St
    R = math.sqrt(R2)
    Dev = math.sqrt(Sr/(n-2))
    x.append(sumx)
    x.append(sumx2)
    x.append(sumy)
    x.append(sumy2)
    x.append(sumxy)
    x.append(a0)
    x.append(a1)
    x.append(R)
    x.append(a1)
    x.append(R)
    x.append(E)
    x.append(Dev)
    if R <= 0.5:
        print "R too low, Not a correct model. Try Regular solution."
    return x
```

```
C:₩Users₩Sunny₩Desktop>python 0.py
<Enthalpy of Mixing at Liquid>
        Linearized Data:        y = 14894.23008578 + (-4794.92409497)x
        R =0.99999857, Dev = 2.345716

<Activity of Tk, Liquid>
        Linearized Data:        y = 2907.18296011 + 2(-4811.80163124)x
        R =0.99998720, Dev = 14.063918

Sub Regular! L parameters have dependence on T
!!!!    Omega = (14894.2301 + (-7.9914) *T) + (-4794.9241 + (-0.0113) *T) *X    !!!!

<Hf of Tk, in FCC>
        Linearized Data:        y = 12597.60930291 + (-7199.97751162)x
        R =0.99999872, Dev = 1.753449

<Activity of Tk, in FCC>
        Linearized Data:        y = 9596.83452729 + 2(-7192.03066260)x
        R =0.99999704, Dev = 5.315325

Sub Regular! L parameters have dependence on T
!!!!   Omega =  (12597.6093 + (-5.0013) *T) + (-7199.9775 + (0.0132) *T) *X    !!!!

<Hf of Tk, in BCC>
R too low, Not a correct model. Try Regular solution.
        Linearized Data:        y = 6999.01830703 + (1.64528143)x
        R =0.08437462, Dev = 2.393825

<Activity of Ps, in BCC>
R too low, Not a correct model. Try Regular solution.
        Linearized Data:        y = 4609.03035317 + (2x - 1)* -42.84914110
        R =0.37254061, Dev = 26.291772

<Regular Solution of BCC>
!!!!    Omega = 7000.3140 + (-4.0265) *T    !!!!
```

1. Result



H of mix
X_Tk
3500
3000
2500
2000
1500
1000
500
0
0.0
0.2
0.4
0.6
0.8
1.0



Hm/X(1-X)
X_Tk
15000
14000
13000
12000
11000
10000
0.0
0.2
0.4
0.6
0.8
1.0

1. Result

주어진 데이터를 선형화 하면
FCC는
Hf가 Xtk에 따라 변하는 Sub-regular,
BCC는 변하지 않는
Regular model
을 따름을 알 수 있음