$$\left.\frac{\partial G_m^{\alpha}}{\partial x_B}\right|_{x_B=x_B^{\alpha}} = \left.\frac{\partial G_m^{\beta}}{\partial x_B}\right|_{x_B=x_B^{\beta}} \text{ 이다.}$$

$$\frac{\partial G_m}{\partial x_B} = -{}^{\circ}G_A + {}^{\circ}G_B + RT(-\ln(1-x_B)+\ln x_B) + (1-2x_B)L$$

$$-{}^{\circ}G_A(\alpha) + {}^{\circ}G_B(\alpha) + RT(-\ln(1-x_B^{\alpha}) + \ln x_B^{\alpha}) + (1-2x_B^{\alpha})L^{\alpha}$$

$$= -{}^{\circ}G_A(\beta) + {}^{\circ}G_B(\beta) + RT(-\ln(1-x_B^{\beta}) + \ln x_B^{\beta}) + (1-2x_B^{\beta})L^{\beta}$$

$$({}^{\circ}G_A(\beta) - G_A^{\circ}(\alpha)) - ({}^{\circ}G_B(\beta) - {}^{\circ}G_B(\alpha)) + RT\left(\ln\frac{1-x_B^{\beta}}{x_B^{\beta}} - \ln\frac{1-x_B^{\alpha}}{x_B^{\alpha}}\right)$$

$$+ (1-2x_B^{\alpha})L^{\alpha} - (1-2x_B^{\beta})L^{\beta} = 0$$

$$= \Delta^{\circ}G_A^{\alpha\to\beta} - \Delta^{\circ}G_B^{\alpha\to\beta} + RT\left(\ln\frac{1-x_B^{\beta}}{x_B^{\beta}} - \ln\frac{1-x_B^{\alpha}}{x_B^{\alpha}}\right)$$

$$+ \left((1-2x_B^{\alpha})L^{\alpha} - (1-2x_B^{\beta})L^{\beta}\right) = 0$$

$$= \Delta^{\circ} G_A^{\alpha\to\beta} - \Delta^{\circ} G_B^{\alpha\to\beta} + RT\left(\ln\frac{x_A^{\beta}}{x_B^{\beta}} - \ln\frac{x_A^{\alpha}}{x_B^{\alpha}}\right)$$

$$+ \left((x_A^{\alpha} - x_B^{\alpha})L^{\alpha} - (x_A^{\beta} - x_B^{\beta})L^{\beta}\right) = 0 \quad \cdots ①$$

또한, 각 접선에 대한 부분도 같아야 한다,

$$\left(\bar{G}_A^{\alpha} = \bar{G}_A^{\beta},\ \bar{G}_B^{\alpha} = \bar{G}_B^{\beta} \right)$$

$$^{\circ}G_A(\alpha) + RT\ln x_A^{\alpha} + L^{\alpha} x_A^{\alpha 2} = {}^{\circ}G_A(\beta) + RT\ln x_A^{\beta} + L^{\beta} x_A^{\beta 2}$$

$$^{\circ}G_B(\alpha) + RT\ln x_B^{\alpha} + L^{\alpha} x_B^{\alpha 2} = {}^{\circ}G_B(\beta) + RT\ln x_B^{\beta} + L^{\beta} x_B^{\beta 2}$$

$$\Rightarrow \begin{cases} \Delta G_{m,A}^{\alpha\to\beta} + RT\ln\dfrac{x_A^{\beta}}{x_A^{\alpha}} + L^{\beta}(x_A^{\beta})^2 - L^{\alpha}(x_A^{\alpha})^2 = 0 \quad \cdots ② \\ \Delta G_{m,B}^{\alpha\to\beta} + RT\ln\dfrac{x_B^{\beta}}{x_B^{\alpha}} + L^{\beta}(x_B^{\beta})^2 - L^{\alpha}(x_B^{\alpha})^2 = 0 \quad \cdots ③ \end{cases}$$

식 ①, ②, ③ 이 바로 상평형 조건 식들이다,

그리고, 여기선 reference가 모두 소거되어, 필요없으므로 reference state와 관계없이 조성이 모두 결정된다.

5, $T = 1273K$

$G_m = x_A^\circ G_A + x_B^\circ G_B + RT(x_A \ln x_A + x_B \ln x_B) + G^{xs}$

① Ideal

ideal model이면, $G^{xs} = 0$이고,

$x_B = a_B$이므로 주어진 data값은 필요 없다.

② regular

$(1-x_B)x_B$
$+(1-x_A)x_B$
$= x_A + x_B$

regular model이면,

$G^{xs} = RT(x_A \ln a_A + x_B \ln a_B) = x_A x_B L$

$RT \ln a_B = RT \ln x_B + L(1-x_B)^2$ (∵ regular solution model이므로)

$RT \ln \frac{a_B}{x_B} = L(1-x_B)^2$

$L = \frac{RT}{(1-x_B)^2} \ln \frac{a_B}{x_B}$

데이터에 주어진 값인 $x_B = 0.5$, $a_B = 0.351$이므로

대입하면, $L = -14979$가 나오고,

$a_B = \gamma_B \exp\left(\frac{L(1-\gamma_B)^2}{RT}\right)$ 을 통해

γ_B에 대한 a_B의 값는

Xb	aB
0.1	0.0317784388
0.2	0.0808450159
0.3	0.14994852
0.4	0.240317597
0.5	0.351000078
0.6	0.478417508
0.7	0.616281932
0.8	0.755968919
0.9	0.887352133
1	1

엑셀과 같이 나타낼 수 있다.

③ Sub regular

$$RT\ln a_B = RT\ln \gamma_B + (1-\gamma_B)^2 L_0 + (1-\gamma_B)^2(1-4\gamma_B)L_1$$

$$L_0 + (1-4\gamma_B)L_1 = \frac{RT\ln \frac{a_B}{\gamma_B}}{(1-\gamma_B)^2}$$

$\gamma_B = 0.5$ $a_B = 0.3510$ 과

$\gamma_B = 0.6$ $a_B = 0.4782$ 를 대입하면,

$L_0 - L_1 = -1497$

$L_0 - 1.4L_1 = -1500$ 즉 $L_1 = 75$

$L_0 = -1490.4$

$\alpha_B = \gamma_B \exp\left(\frac{(1-x_B)^2(L_0 + (1-4x_B)L_1)}{RT}\right)$ 으로

x_B에 따른 α_B를 다시 구해보면,

Xb	aB
0.1	0.0320716335
0.2	0.0812861998
0.3	0.150365634
0.4	0.24056295
0.5	0.351000078
0.6	0.478200582
0.7	0.615967574
0.8	0.755711824
0.9	0.88725153
1	1

윗줄과 같이 나오게 된다

전체 data와 오차를 다시 계산해보면,

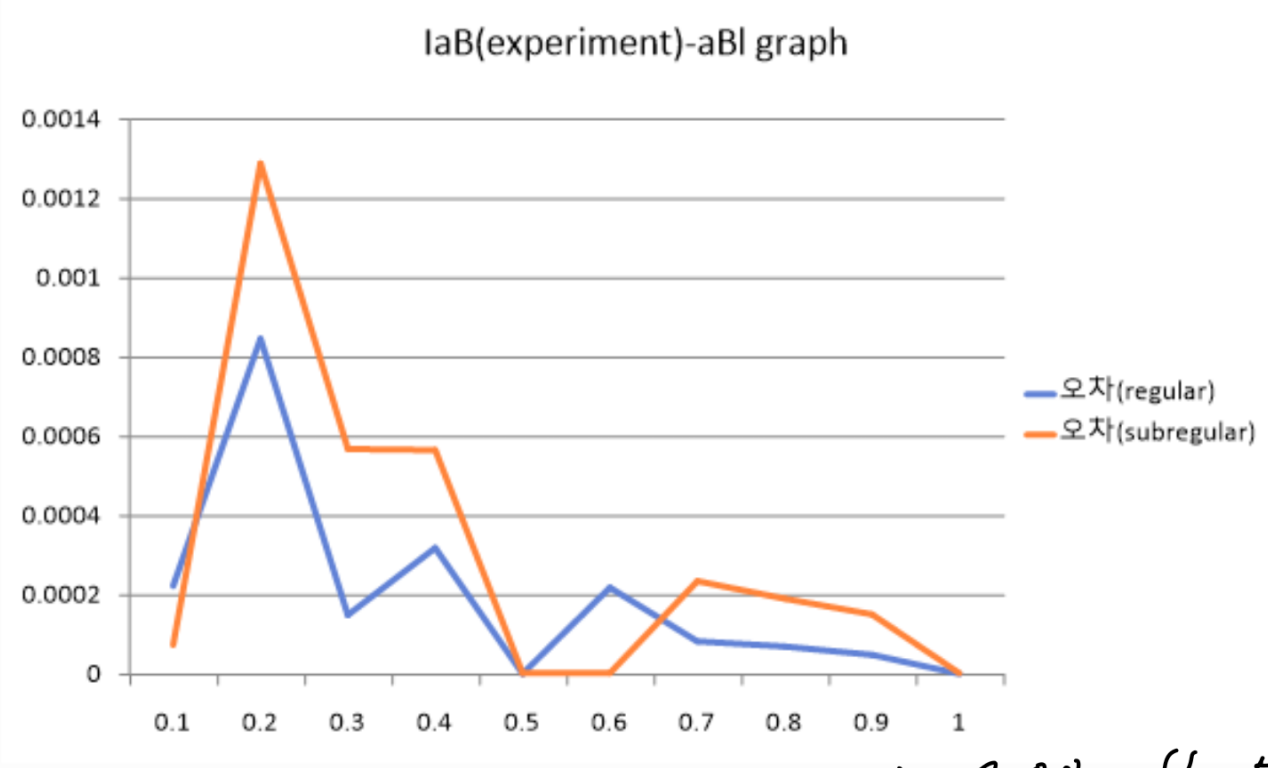
Xb	aB(experiment)	aB(regular)	오차(regular)	aB(subregular)	오차(subregular)
0.1	0.032	0.0317784388	0.000221561214	0.0320716335	7.16335E-5
0.2	0.08	0.0808450159	0.000845015911	0.0812861998	0.00128619979
0.3	0.1498	0.14994852	0.000148520297	0.150365634	0.000565633977
0.4	0.24	0.240317597	0.000317596805	0.24056295	0.000562950446
0.5	0.351	0.351000078	7.83356E-8	0.351000078	7.83356E-8
0.6	0.4782	0.478417508	0.00021750758	0.478200582	5.81684E-7
0.7	0.6162	0.616281932	8.19318E-5	0.615967574	0.000232425764
0.8	0.7559	0.755968919	6.89194E-5	0.755711824	0.000188175947
0.9	0.8874	0.887352133	4.78666E-5	0.88725153	0.000148470323
1	1	1	0	1	0

이런 data를 얻을 수 있고,

이 때 오차는

$|a_B(\text{experiment}) - a_B|$ 이다.

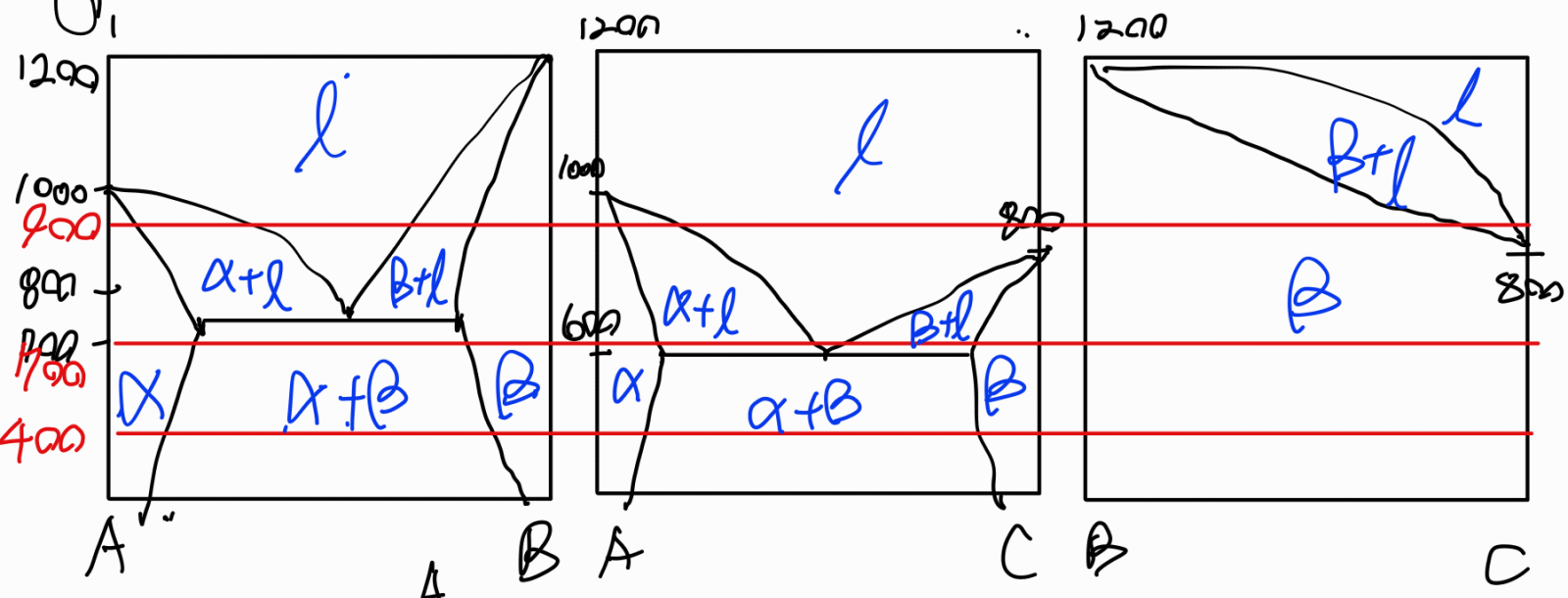
그래프로 plot해보자,

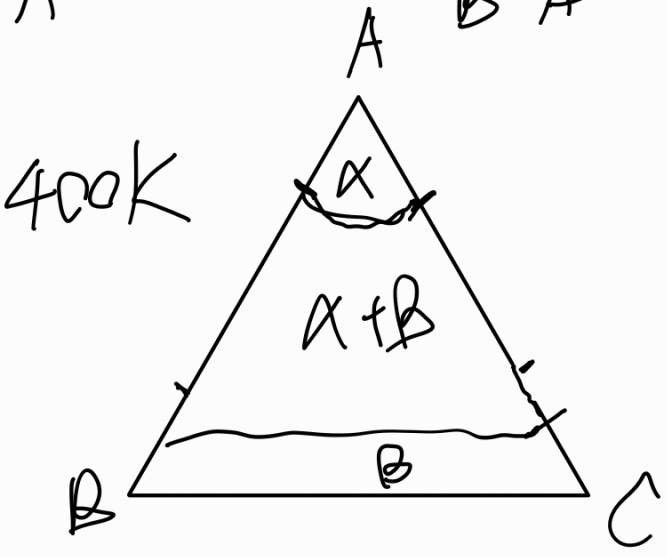


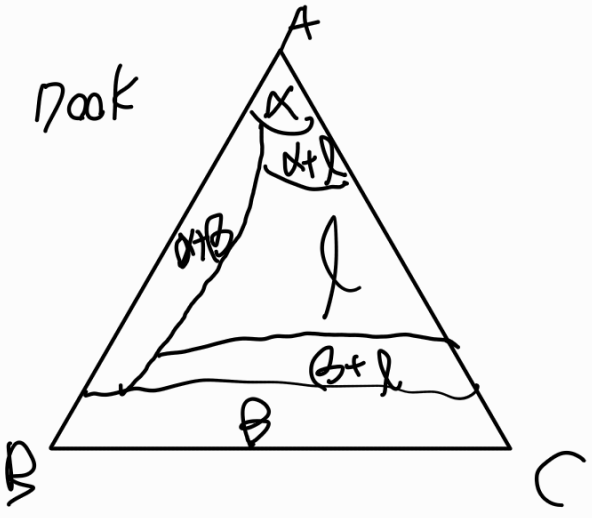
전체적인 오차는 regular일 때가 좋을 수 있다.

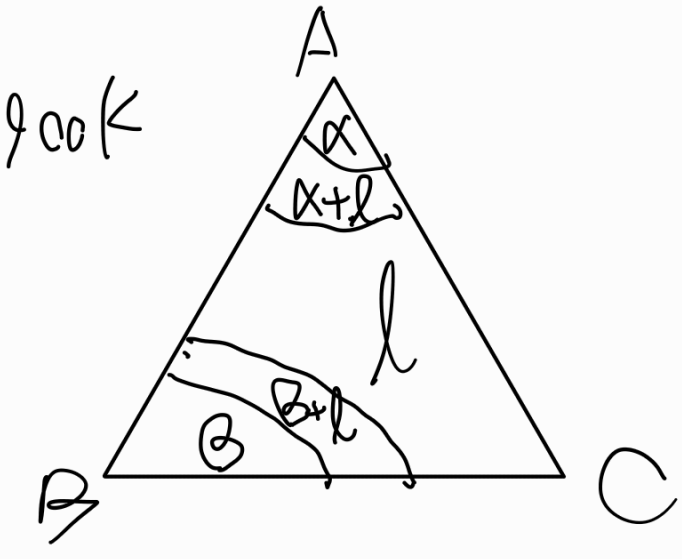
즉, regular model이 더 유용하다.

6.


1200
1000
900
800
700
600
400
l
α+l
β+l
α
α+β
β
A
B
C


A
400K
α
α+β
B
C


A
700K
α
α+l
α+β
l
β+l
β
B
C


A
900K
α
α+l
l
β+l
β
B
C