Numerical Analysis For Materials

Homework #6

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Dept: Material Science and Engineering

HW#6에서 가장 힘들었던 오류

시작 페이지 - Microsoft Visual Studio (관리자)

빠른 실행(Ctrl+Q)

파일(F) 편집(E) 보기(V) 디버그(D) 팀(M) 도구(T) 테스트(S) 분석(N) 창(W) 도움말(H)

Professional 2013

시작

새 프로젝트...

프로젝트 열기...

소스 제어에서 열기...

최근 항목

AMSE417_HW4

AMSE417_HW5_Lagrange

AMSW417_HW5

AMSE417_HW5_Lagrange

AMSE417_HW3

AMSW417_HW5

AMSE417_HW3

AMSE417_HW2_Newton's mtd

Untitle-1

HW3

프로젝트 로드 후 페이지를 열린 상태로 유지

시작할 때 페이지 표시

Visual Studio에 로그인

Visual Studio에서는 프로젝트를 계획하고, 팀과 공동 작업을 수행하고, 어디서든 온라인으로 코드를 관리할 수 있습니다.

자세히

Visual Studio에서는 자동으로 로그인 상태를 유지하고, 장치 간 설정을 동기화하고, 온라인 개발자 서비스에 연결합니다.

개인 정보 취급 방침

로그인(I)

제품 정보

Visual Studio

Professional 2013

라이선스: 30일 평가판(평가 목적으로만 사용)

라이선스가 만료되었습니다.

평가판이 만료되었습니다. 평가판을 연장하거나 온라인 계정이나 제품 키를 사용하는 라이선스를 구매하려면 로그인하십시오.

업데이트된 라이선스 확인

다른 Microsoft 또는 조직 계정이 있는 라이선스

제품 키가 있는 라이선스

Visual Studio를 구입할 준비가 되셨습니까? 온라인 주문

Visual Studio 종료(E)

오류 목록 출력

준비

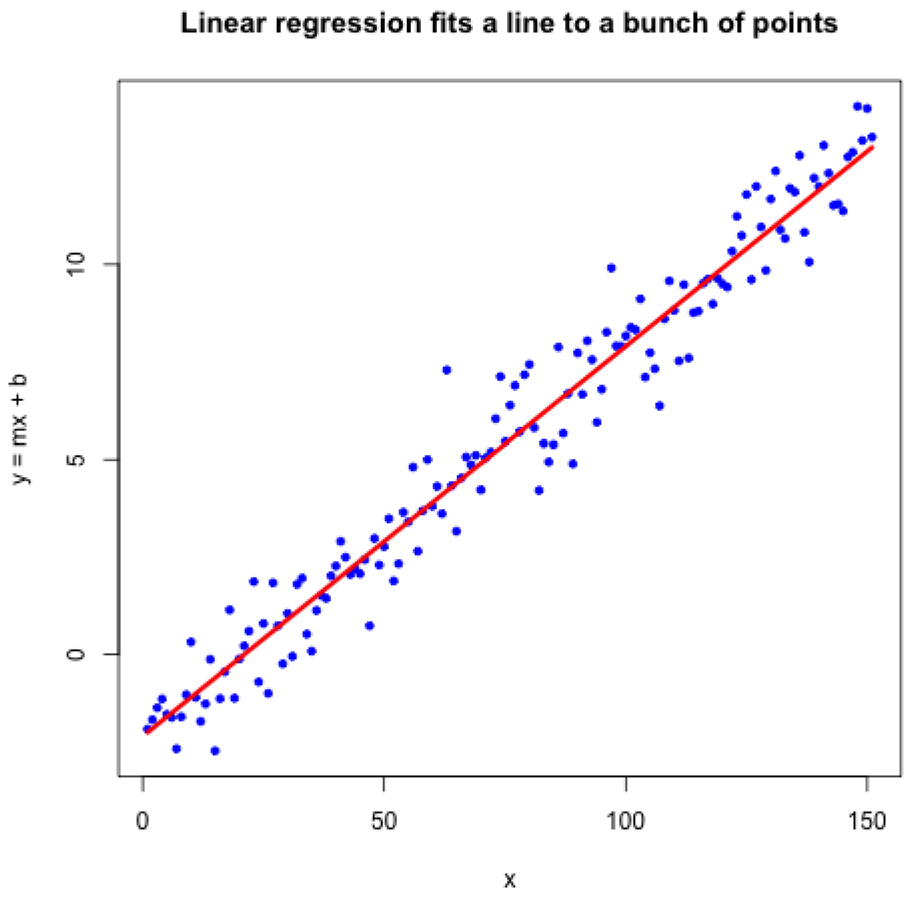
D - 0d 6h 13m

오전 3:17

Homework #6

Regression of Ps-Tk data

1. Idea to construct Regression



주어진 식이 어떻게 생겼든 간에 1차 함수의 꼴로 만들어보자!

수업시간 예제)

$y = x(1-x)(L_0 + L_1 x)$을 어떻게 분석할까?

-> 구해야 할 parameter가 있는 부분을 제외하고는 다 나눠버리자!

$$\frac{y}{x(1-x)} = L_0 + L_1 x$$

$$\updownarrow$$

$$Y = a + bX$$

1. Idea to construct Regression

* 주어진 각 data에 대한 관계식의 선형화

For sub-regular solution: $\boldsymbol{\Omega} = L_0 + L_1X_{Tk} + L_2X_{Tk}^2 + L_3X_{Tk}^3 \cong \boldsymbol{L_0} + \boldsymbol{L_1X_{Tk}}$

(from Thermodynamics of D. R. Gaskell)

액상에서의 Enthalpy of mixing: $\Delta H^M = \Omega X_{Tk}(1 - X_{Tk}) = (L_0 + L_1X_{Tk})X_{Tk}(1 - X_{Tk})$

$$\frac{\Delta H^M}{X_{Tk}(1 - X_{Tk})} = (\boldsymbol{L_0} + \boldsymbol{L_1}X_{Tk})$$

액상에서의 Activity of Tk: $RT\ln a_{Tk} = RT\ln X_{Tk} + (1 - X_{Tk})^2\left(\Omega + \frac{d\Omega}{dX_{Tk}}X_{Tk}\right)$

$$= RT\ln X_{Tk} + (1 - X_{Tk})^2(L_0 + 2L_1X_{Tk})$$

$$\frac{RT\ln a_{Tk} - RT\ln X_{Tk}}{(1 - X_{Tk})^2} = \boldsymbol{L_0} + \boldsymbol{L_1}(2X_{Tk})$$

1. Idea to construct Regression

* 주어진 각 data에 대한 관계식의 선형화

For sub-regular solution: $\boldsymbol{\Omega} = L_0 + L_1X_{Tk} + L_2X_{Tk}^2 + L_3X_{Tk}^3 \cong \boldsymbol{L_0} + \boldsymbol{L_1X_{Tk}}$

(from Thermodynamics of D. R. Gaskell)

FCC상에서의 Enthalpy of Formation: $\Delta H_f^{FCC} = X_{Tk}\Delta G_{Tk}^{BCC\to FCC} + \Omega X_{Tk}(1-X_{Tk})$

$$= 7500X_{Tk} + (L_0 + L_1X_{Tk})X_{Tk}(1-X_{Tk})$$

$$\frac{\Delta H_f^{FCC} - 7500X_{Tk}}{X_{Tk}(1-X_{Tk})} = (\boldsymbol{L_0} + \boldsymbol{L_1}X_{Tk})$$

BCC상에서의 Enthalpy of Formation: $\Delta H_f^{BCC} = (1-X_{Tk})\Delta G_{Ps}^{FCC\to FCC} + \Omega X_{Tk}(1-X_{Tk})$

$$= 4000(1-X_{Tk}) + (L_0 + L_1(1-X_{Tk}))X_{Tk}(1-X_{Tk})$$

$$\frac{\Delta H_f^{BCC} - 4000(1-X_{Tk})}{X_{Tk}(1-X_{Tk})} = (\boldsymbol{L_0} + \boldsymbol{L_1}(1-X_{Tk}))$$

1. Idea to construct Regression

* 주어진 각 data에 대한 관계식의 선형화

For sub-regular solution: $\boldsymbol{\Omega} = L_0 + L_1 X_{Tk} + L_2 X_{Tk}^2 + L_3 X_{Tk}^3 \cong \boldsymbol{L_0 + L_1 X_{Tk}}$

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FCC상에서의 Activity of Tk: $RT\ln a_{Tk} = \Delta G_{Tk}^{BCC\rightarrow FCC} + RT\ln X_{Tk} + (1 - X_{Tk})^2 \left(\Omega + \frac{d\Omega}{dX_{Tk}} X_{Tk}\right)$

$$= 7500 + RT\ln X_{Tk} + (1 - X_{Tk})^2 (L_0 + 2L_1 X_{Tk})$$

$$\frac{RT\ln a_{Tk} - RT\ln X_{Tk} - 7500}{(1 - X_{Tk})^2} = \boldsymbol{L_0} + \boldsymbol{L_1}(2X_{Tk})$$

BCC상에서의 Activity of Ps: $RT\ln a_{Ps} = \Delta G_{Tk}^{FCC\rightarrow BCC} + RT\ln(1 - X_{Tk}) + X_{Tk}^2 \left(\Omega + \frac{d\Omega}{dX_{Tk}} X_{Tk}\right)$

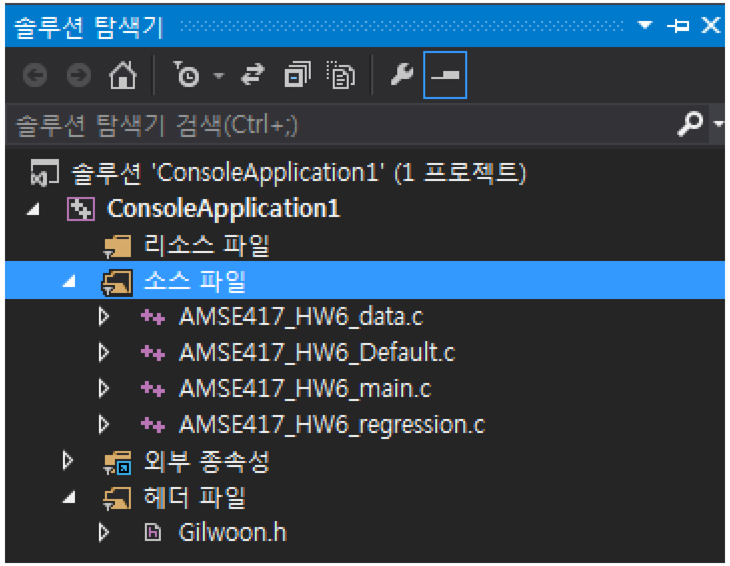
$$= 4000 + RT\ln(1 - X_{Tk}) + X_{Tk}^2 (L_0 + 2L_1(1 - X_{Tk}))$$

$$\frac{RT\ln a_{Ps} - RT\ln(1 - X_{Tk}) - 4000}{(X_{Tk})^2} = \boldsymbol{L_0} + \boldsymbol{L_1}(2(1 - X_{Tk}))$$

2. Programmed code

* Description of Program

1. Info. of Program



2. Characteristics of Program

- 헤더 및 각 기능 함수화
- 파일의 데이터 개수 입력 없이도 가능
- 파일명 입력 -> 각각의 함수로 연계

3. Part of regression

```
x_sum = 0;
y_sum = 0;
xy_sum = 0;
x_mean = 0;
y_mean = 0;
x_powersum = 0;
y_powersum = 0;
S_t = 0;
S_r = 0;
for (i = 0; i < count; i++)
{
x_sum += Data[i][0];
y_sum += Data[i][1];
x_powersum += pow(Data[i][0], 2);
y_powersum += pow(Data[i][1], 2);
xy_sum += (Data[i][0] * Data[i][1]);
}
x_mean = x_sum / count;
y_mean = y_sum / count;

L_1 = ((count*xy_sum) - (x_sum*y_sum)) / ((count*x_powersum) -
pow(x_sum, 2));
L_0 = y_mean - (L_1*x_mean);

for (i = 0; i < count; i++)
{
S_t += pow(y_mean - Data[i][1], 2);
S_r += pow(Data[i][1] - L_0 - L_1*Data[i][0], 2);
}
r = (S_t - S_r) / S_t;
printf("L_0: %f\nL_1: %f\nr^2: %f\n", L_0, L_1, r);
```

2. Programmed code

* Description of Program

4. Part of functions

```
#define _CRT_SECURE_NO_WARNINGS //Secure warning을 skip하는 명령문
#define R 8.3144621
#include<stdio.h>
#include<stdlib.h>
#include<math.h>
#include"Gilwoon.h"

void enthalpy(double **Data, double count)
{int i = 0;
for (i = 0; i < count; i++)
{Data[i][1] /= (Data[i][0] * (1 - Data[i][0]));}}

void activity(double **Data, double count)
{int i = 0;
for (i = 0; i < count; i++)
{Data[i][1] = (R * 1500 * log(Data[i][1]) - R * 1500 *
log(Data[i][0]))/pow((1-Data[i][0]), 2);
Data[i][0] *= 2;}}

void enthalpy_form_Tk(double **Data, double count)
{int i = 0;
for (i = 0; i < count; i++)
{Data[i][1] = (Data[i][1] - 7500 * Data[i][0]) / (Data[i][0] *
(1 - Data[i][0]));}}
```

```
void activity_600_Tk(double **Data, double count)
{int i = 0;
for (i = 0; i < count; i++)
{Data[i][1] = (R * 600 * log(Data[i][1]) - R * 600 *
log(Data[i][0]) -7500) / pow((1 - Data[i][0]), 2);
Data[i][0] *= 2;}}

void enthalpy_form_Ps(double **Data, double count)
{int i = 0;
for (i = 0; i < count; i++)
{Data[i][1] = (Data[i][1] - 4000 * (1 - Data[i][0])) /
(Data[i][0] * (1 - Data[i][0]));
Data[i][0] = (1 - Data[i][0]);}}

void activity_600_Ps(double **Data, double count)
{int i = 0;
for (i = 0; i < count; i++)
{Data[i][1] = (R * 600 * log(Data[i][1]) - R * 600 * log(1-
Data[i][0]) - 4000) / pow(Data[i][0], 2);
Data[i][0] = 2 * (1 - Data[i][0]);}}
```

Homework #6: Regression of Ps-Tk data

3. Result & Conclusion

1. 실행 결과

```
C:₩Windows₩system32₩cmd.exe
================================================================================
Program: Regression of Ps-Tk data
Date: 2015.04.21
Made by Gilwoon Lee
POSTECH, project 6 of [AMSE417] Numerical analysis for materials
Development environment: Visual Studio 2013
Code language: C
================================================================================

This programm will do Regression of Ps-Tk data.
==============================

* Enter file name(*.txt): enthalpy_mix.txt
# of data: 39
L_0: 14894.230619
L_1: -4794.925467
r^2: 0.999997
Enter 1 to repeat, 0 to exit: 1

* Enter file name(*.txt): activity_1500_Tk.txt
# of data: 39
L_0: 2907.166476
L_1: -4811.777322
r^2: 0.999975
Enter 1 to repeat, 0 to exit: 1

* Enter file name(*.txt): enthalpy_form_FCC.txt
# of data: 20
L_0: 12597.609462
L_1: -7199.977924
r^2: 0.999997
Enter 1 to repeat, 0 to exit: 1
```

```
* Enter file name(*.txt): enthalpy_form_BCC.txt
# of data: 16
L_0: 7000.661574
L_1: -1.638188
r^2: 0.007057
Enter 1 to repeat, 0 to exit: 1

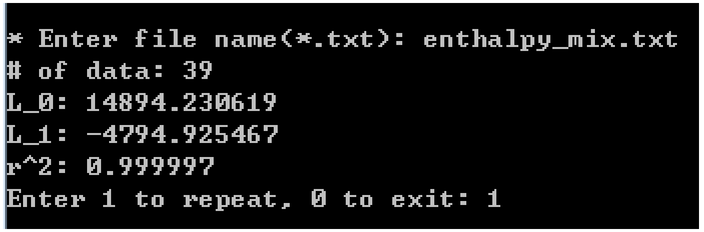
* Enter file name(*.txt): activity_600_Tk.txt
# of data: 20
L_0: 9596.838369
L_1: -7192.026746
r^2: 0.999994
Enter 1 to repeat, 0 to exit: 1

* Enter file name(*.txt): activity_600_Ps.txt
# of data: 16
L_0: 4566.182191
L_1: 42.853319
r^2: 0.138815
Enter 1 to repeat, 0 to exit: 0

==============================
계속하려면 아무 키나 누르십시오 . . . _
```

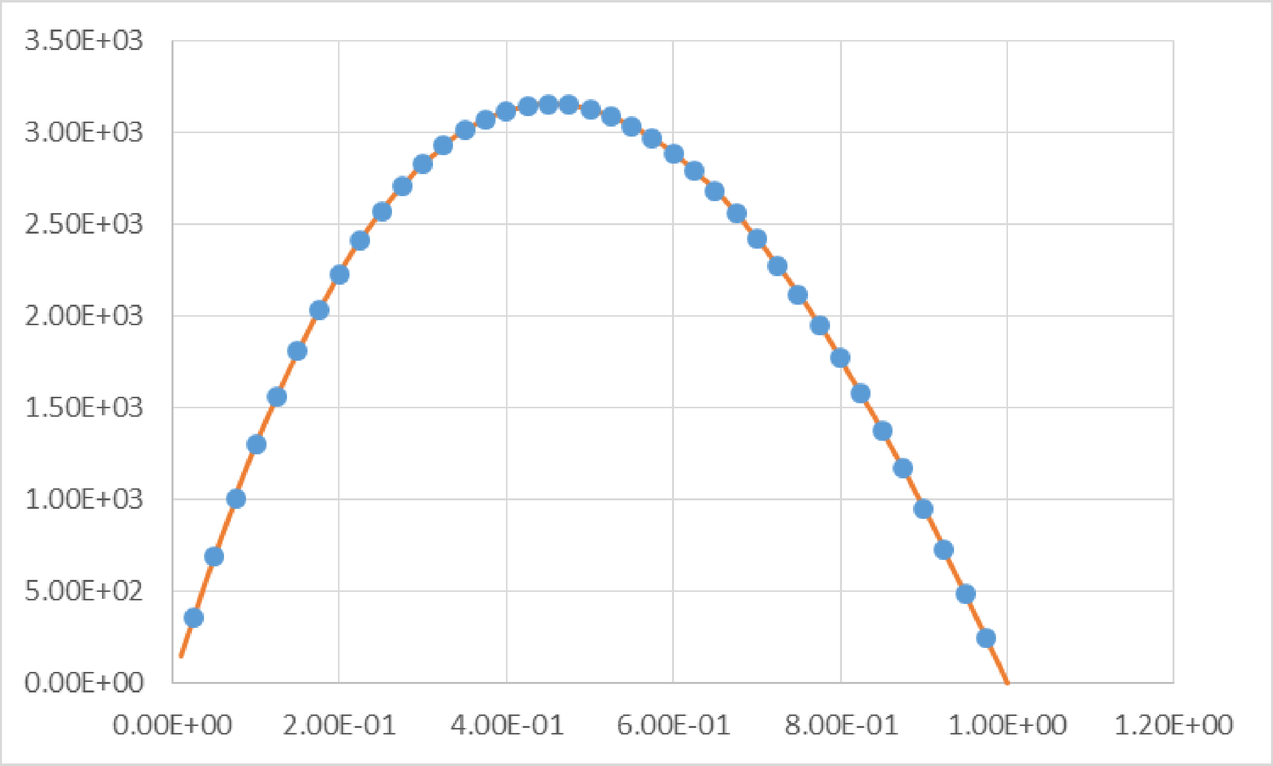
3. Result & Conclusion

2. Enthalpy mix(L)



액상에서의 Enthalpy of mixing: $\Delta H^M = \Omega X_{Tk}(1 - X_{Tk}) = (L_0 + L_1 X_{Tk}) X_{Tk}(1 - X_{Tk})$

$$\frac{\Delta H^M}{X_{Tk}(1 - X_{Tk})} = (\boldsymbol{L_0} + \boldsymbol{L_1} X_{Tk})$$



3. Result & Conclusion

2. Activity(L)

```
* Enter file name(*.txt): activity_1500_Tk.txt
# of data: 39
L_0: 2907.166476
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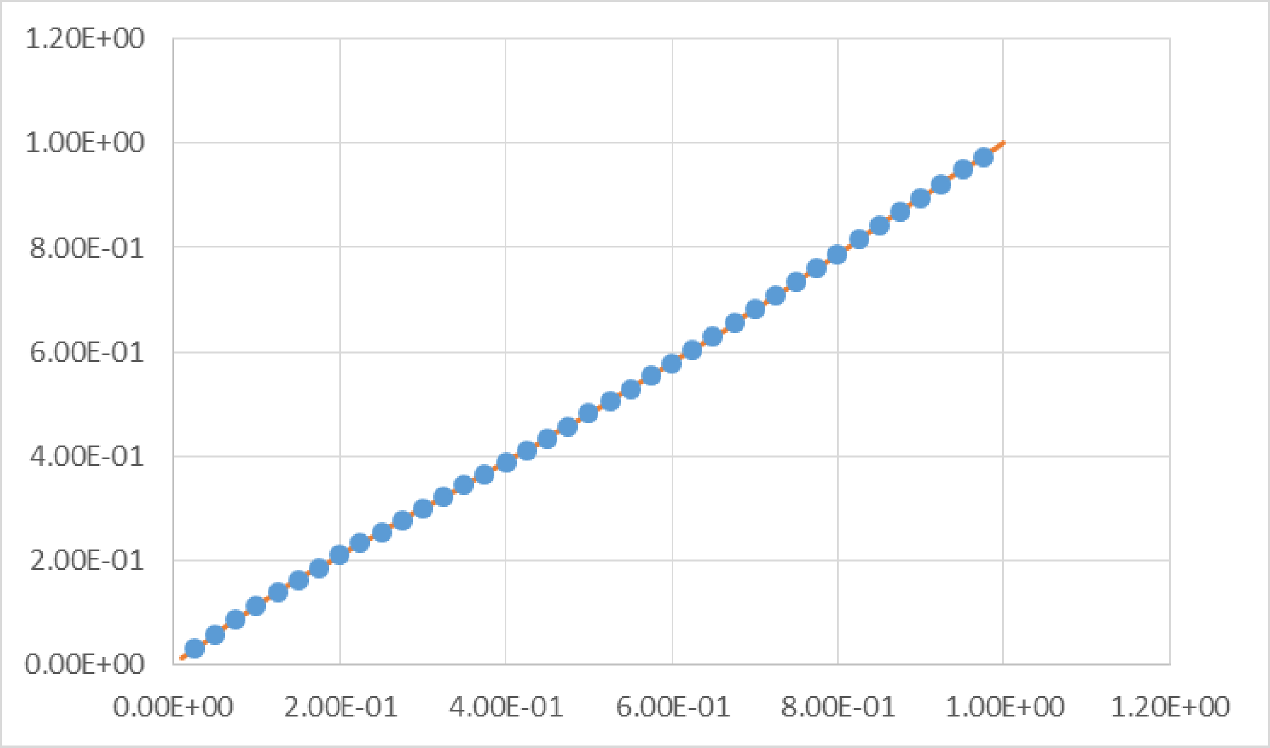
r^2: 0.999975
Enter 1 to repeat, 0 to exit: 1
```

액상에서의 Activity of Tk: $RT\ln a_{Tk} = RT\ln X_{Tk} + (1 - X_{Tk})^2\left(\Omega + \frac{d\Omega}{dX_{Tk}}X_{Tk}\right)$

$$= RT\ln X_{Tk} + (1 - X_{Tk})^2(L_0 + 2L_1X_{Tk})$$

$$\frac{RT\ln a_{Tk} - RT\ln X_{Tk}}{(1 - X_{Tk})^2} = \boldsymbol{L_0} + \boldsymbol{L_1}(2X_{Tk})$$



3. Result & Conclusion

3. Activity Ps, Tk

```
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L_0: 12597.609462
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# of data: 16
L_0: 7000.661574
L_1: -1.638188
r^2: 0.007057
Enter 1 to repeat, 0 to exit: 1
```

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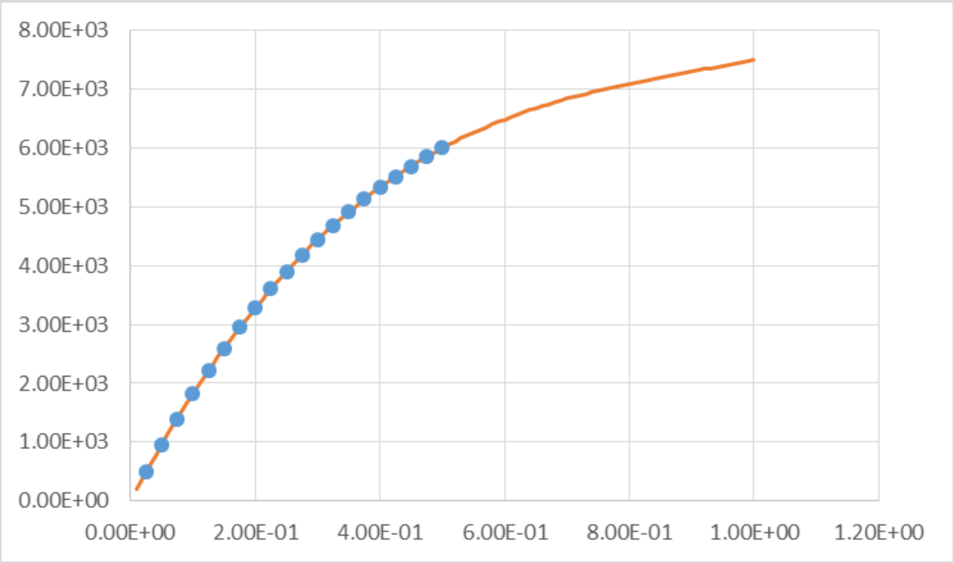
$$= 7500X_{Tk} + (L_0 + L_1X_{Tk})X_{Tk}(1-X_{Tk})$$

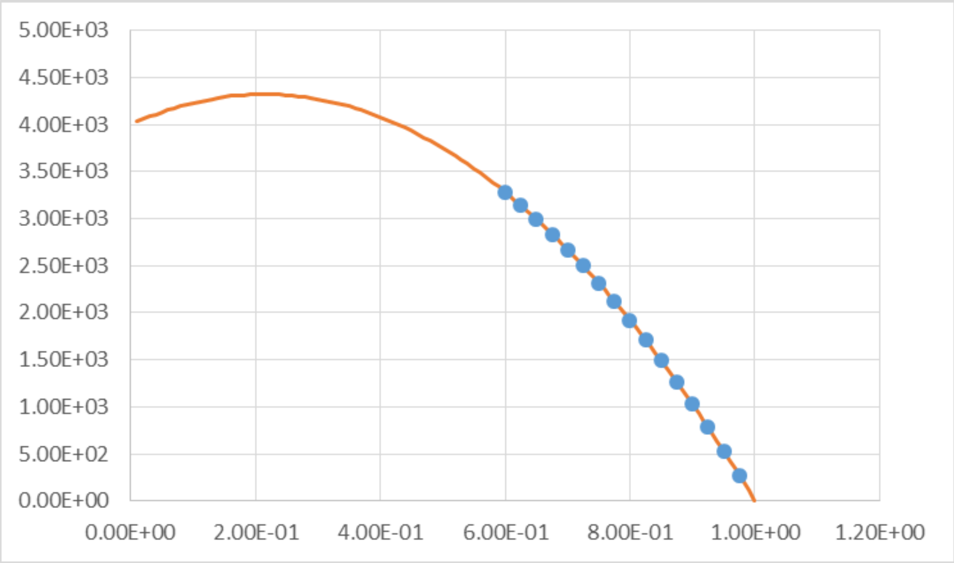
$$\frac{\Delta H_f^{FCC} - 7500X_{Tk}}{X_{Tk}(1-X_{Tk})} = (\boldsymbol{L_0} + \boldsymbol{L_1}X_{Tk})$$

BCC상에서의 Enthalpy of Formation: $\Delta H_f^{BCC} = (1-X_{Tk})\Delta G_{Ps}^{FCC\rightarrow FCC} + \Omega X_{Tk}(1-X_{Tk})$

$$= 4000(1-X_{Tk}) + (L_0 + L_1(1-X_{Tk}))X_{Tk}(1-X_{Tk})$$

$$\frac{\Delta H_f^{BCC} - 4000(1-X_{Tk})}{X_{Tk}(1-X_{Tk})} = (\boldsymbol{L_0} + \boldsymbol{L_1}(1-X_{Tk}))$$





3. Result & Conclusion

3. Formation(FCC, BCC)

```
* Enter file name(*.txt): activity_600_Tk.txt
# of data: 20
L_0: 9596.838369
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Enter 1 to repeat, 0 to exit: 1

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# of data: 16
L_0: 4566.182191
L_1: 42.853319
r^2: 0.138815
Enter 1 to repeat, 0 to exit: 0
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FCC상에서의 Activity of Tk: $RT\ln a_{Tk} = \Delta G_{Tk}^{BCC\rightarrow FCC} + RT\ln X_{Tk} + (1-X_{Tk})^2\left(\Omega + \frac{d\Omega}{dX_{Tk}}X_{Tk}\right)$

$$= 7500 + RT\ln X_{Tk} + (1-X_{Tk})^2(L_0 + 2L_1X_{Tk})$$

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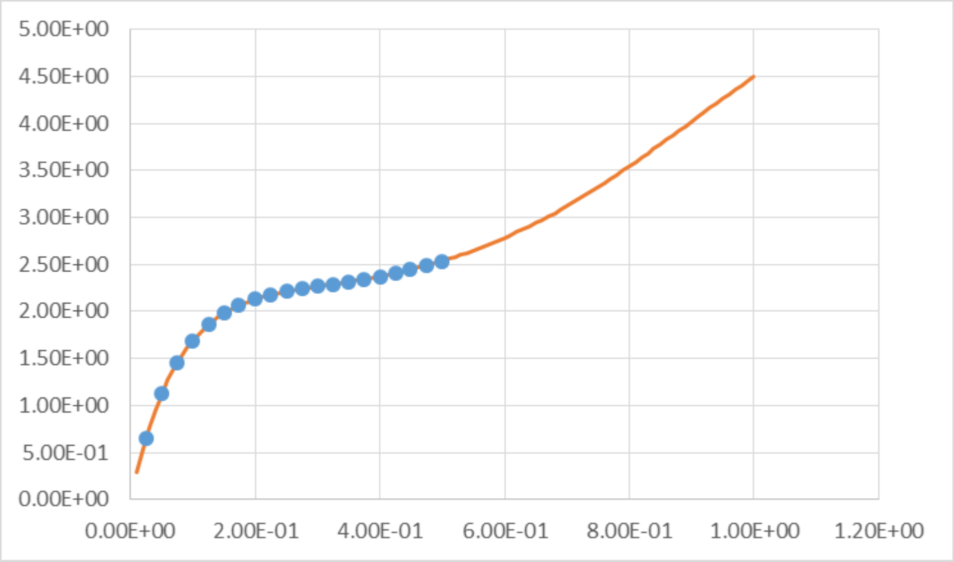
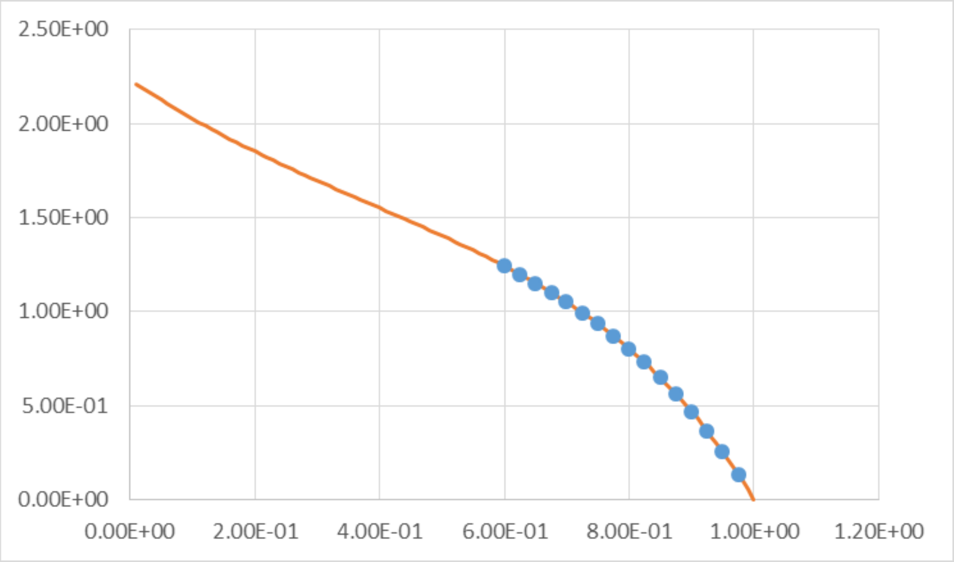
BCC상에서의 Activity of Ps: $RT\ln a_{Ps} = \Delta G_{Tk}^{FCC\rightarrow BCC} + RT\ln(1-X_{Tk}) + X_{Tk}^2\left(\Omega + \frac{d\Omega}{dX_{Tk}}X_{Tk}\right)$

$$= 4000 + RT\ln(1-X_{Tk}) + X_{Tk}^2(L_0 + 2L_1(1-X_{Tk}))$$

$$\frac{RT\ln a_{Ps} - RT\ln(1-X_{Tk}) - 4000}{(X_{Tk})^2} = \boldsymbol{L_0} + \boldsymbol{L_1}(2(1-X_{Tk}))$$





3. Conclusion

1) 각 데이터를 Regression을 통해서 구할 수 있고, 경향성이 많이 벗어나지 않음을 확인하였다.