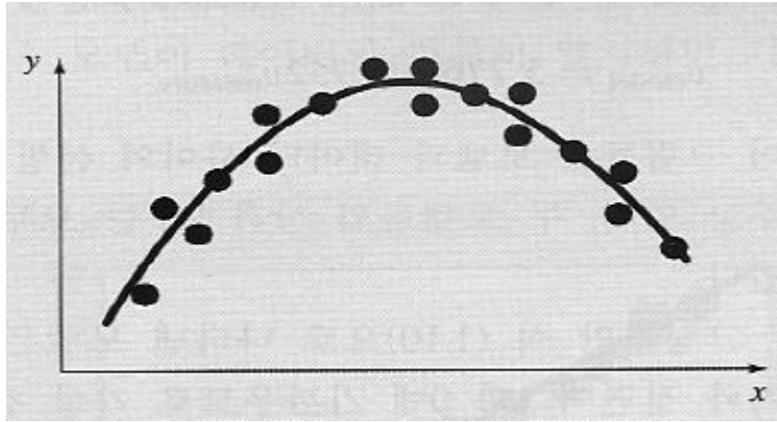


Numerical Method

Dept. Material Science & Engineering
Undergraduate Course (4th year)
Chang Jae Yu

Homework #6

Regression -> Enthalpy of Mixing



$$\Delta H_m^\alpha = X_A^0 H_A^{ref \rightarrow \alpha} + X_B^0 H_B^{ref \rightarrow \alpha} + X_A X_B (L_0^0 - (X_A - X_B) L_1^0)$$

$$\Delta H_{mix} = X_A X_B (L_0^0 - (X_A - X_B) L_1^0) = X_A (1 - X_A) (L_0^0 - (2X_A - 1) L_1^0)$$



$$\frac{\Delta H_{mix}}{X_A (1 - X_A)} = L_0^0 - (2X_A - 1) L_1^0$$

Minimizing sum of
squares of deviation

```
double sum_x = 0;
double sum_y = 0;
double sum_xy = 0;
double sum_x2 = 0;
for (i = 0; i < n; i++) {
    sum_x = sum_x + Data[i][0];
    sum_y = sum_y + Data[i][2];
    sum_xy = sum_xy + (Data[i][0] * Data[i][2]);
    sum_x2 = sum_x2 + (Data[i][0] * Data[i][0]);
}
```

```
double a0, a1;
a1 = ((n*sum_xy) - (sum_x * sum_y)) / ((n*sum_x2) - (sum_x * sum_x));
a0 = (sum_y - (sum_x * a1)) / n;
```

```
FILE *mat1 = fopen("result_linear.txt", "w");
fprintf(mat1, "x y\n");
for (i = 0; i < 39; i++) {
    fprintf(mat1, "%lf ", Data[i][0]);
    fprintf(mat1, "%lf\n", Data[i][2]);
}
```

Debug	2016-04-11 오후...	파일 폴더
1	2016-04-11 오후...	C Source
data	2016-04-11 오후...	텍스트 문서
HW6	2016-04-11 오후...	VC++ Project
HW6.vcxproj	2016-04-11 오후...	VC++ Project Fil...
result_curve	2016-04-11 오후...	텍스트 문서
result_linear	2016-04-11 오후...	텍스트 문서

Homework #6

```
<Homework #6> Regression <Minimizing Sum of Squares of Deviation>
Open the file 'data.txt'

y / x(1-x) = <-4794.925467>x + <14894.230619>
Sum of Square : 203.587186
Value of R : 0.999582

y = x(1-x) * <<-4794.925467>x + <14894.230619>>
Sum of Square : 5.648705
Value of R : 0.999932
계속하려면 아무 키나 누르십시오 . . .
```

$$L_0^0 - (2X_A - 1)L_1^0 = -4794.9255X_A + 14894.2306$$

$$L_1^0 = 2397.4628$$

$$L_0^0 = 12496.768$$

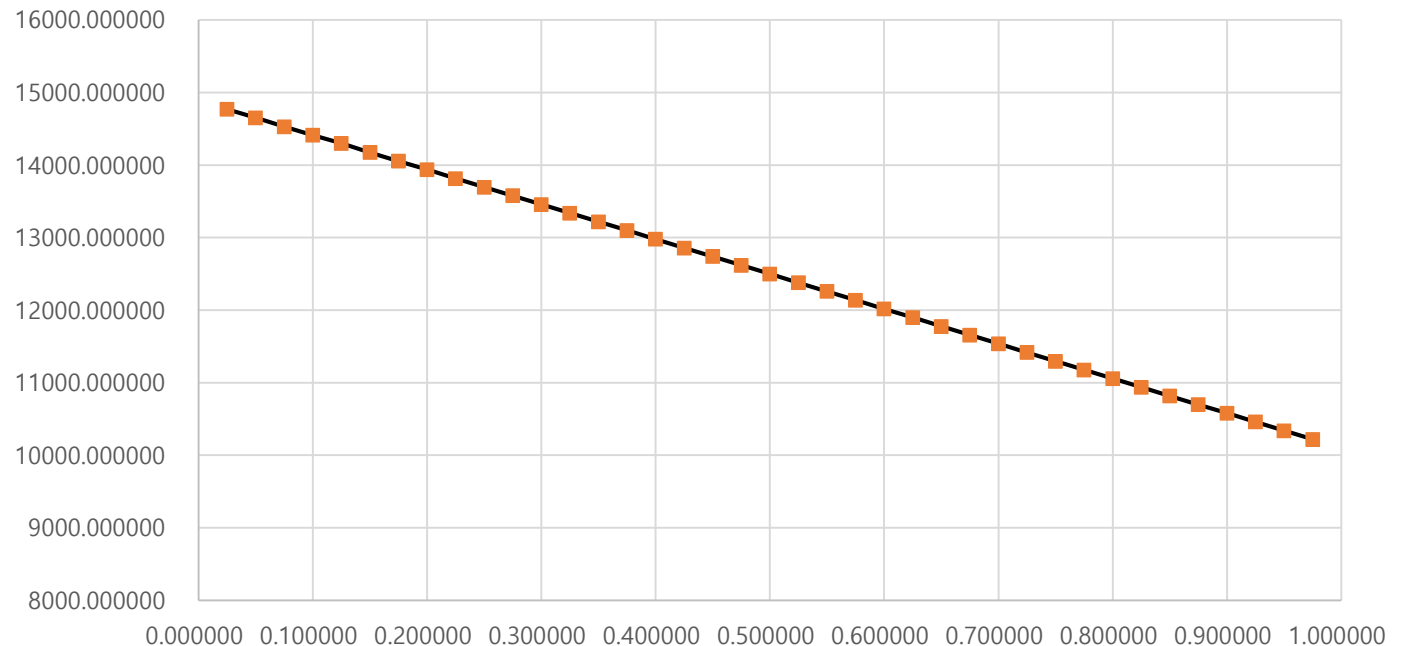
Sub-regular Regular

$$\frac{\Delta H_{mix}}{X_A(1 - X_A)} = L_0^0 - (2X_A - 1)L_1^0$$
$$= -4794.9255X_A + 14894.2306$$

Sum of Square : 203.587186

Value of R : 0.999582

Enthalpy of Mixing / X (1-X)



Homework #6

```
<Homework #6> Regression <Minimizing Sum of Squares of Deviation>  
Open the file 'data.txt'
```

```
y / x(1-x) = <-4794.925467>x + <14894.230619>
```

```
Sum of Square : 203.587186
```

```
Value of R : 0.999582
```

```
y = x(1-x) * <<-4794.925467>x + <14894.230619>>
```

```
Sum of Square : 5.648705
```

```
Value of R : 0.999932
```

```
계속하려면 아무 키나 누르십시오 . . .
```

$$L_0^0 - (2X_A - 1)L_1^0 = -4794.9255X_A + 14894.2306$$

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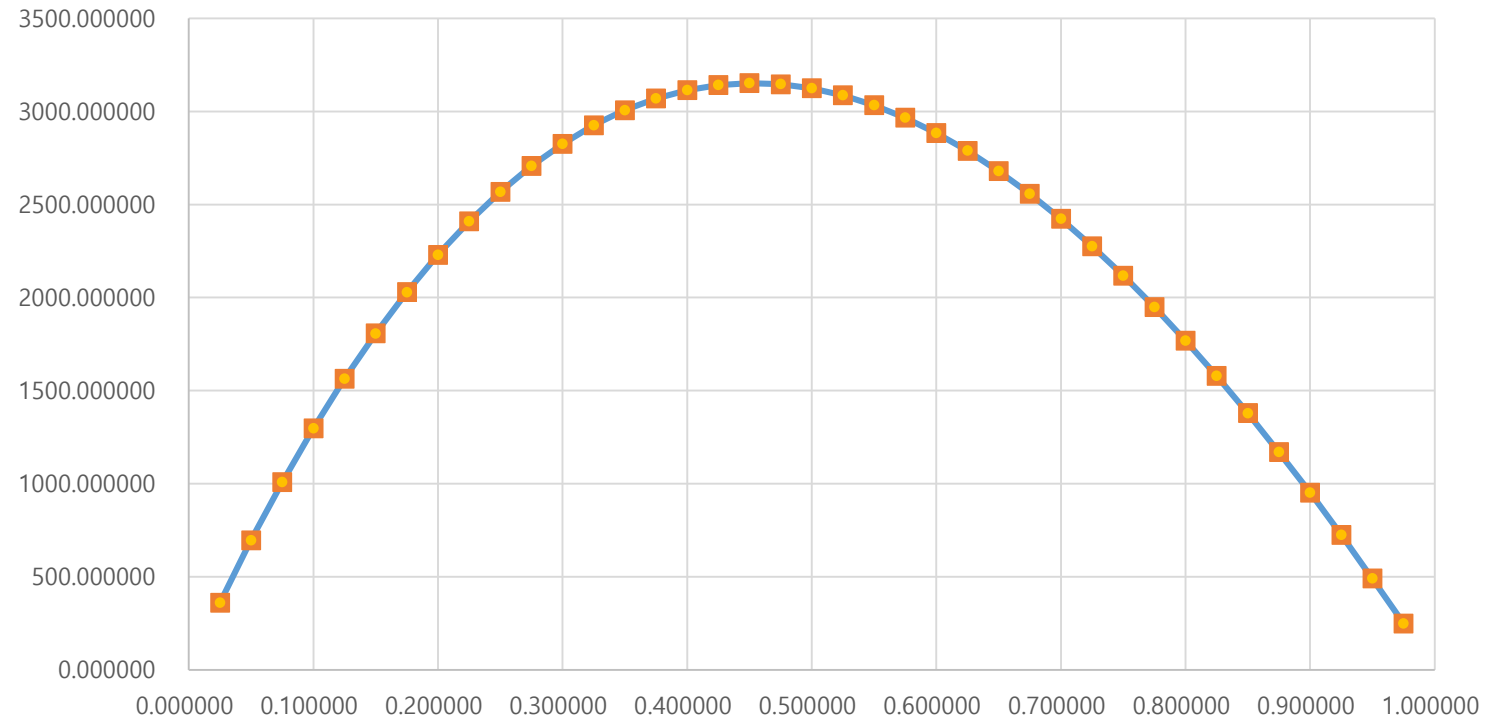
Sub-regular Regular

$$\Delta H_{mix} = X_A(1 - X_A)(L_0^0 - (2X_A - 1)L_1^0) \\ = X_A(1 - X_A)(-4794.9255X_A + 14894.2306)$$

Sum of Square : 5.648705

Value of R : 0.999932

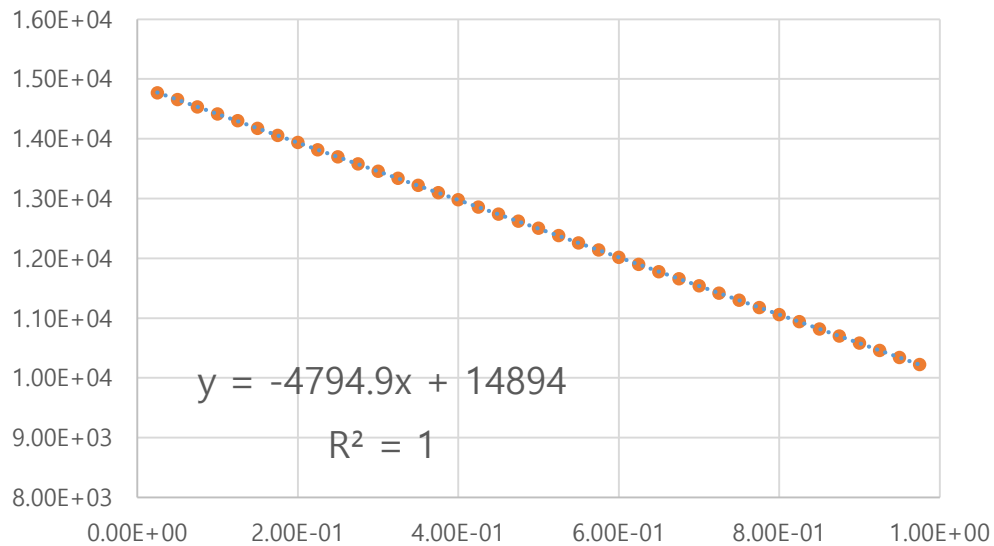
Enthalpy of Mixing



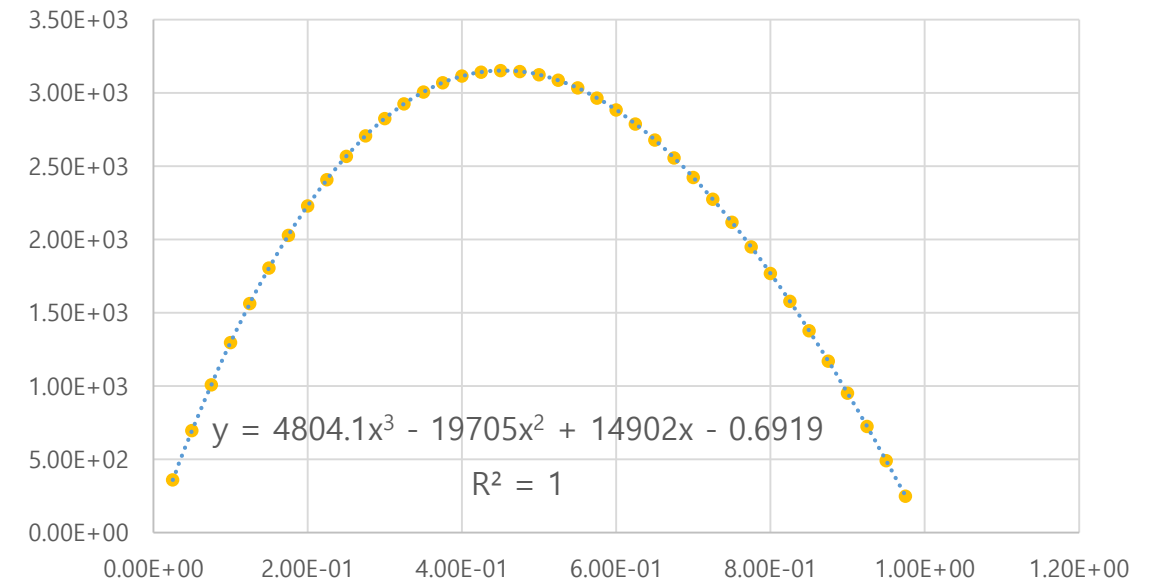
Homework #6

Excel -> Function of Adding Trend Line

Data



Data

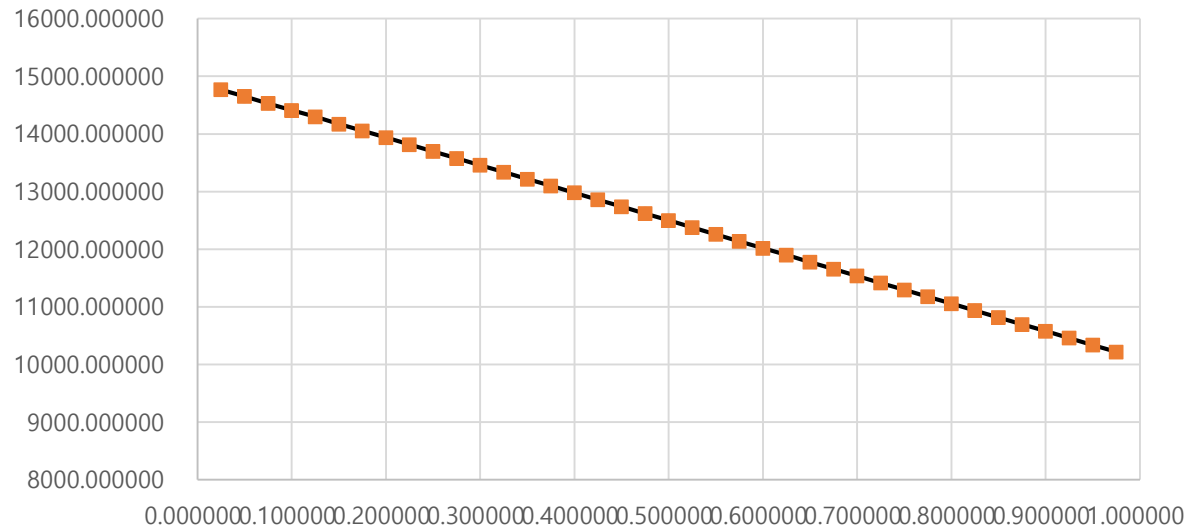


$$= -4794.9255X_A + 14894.2306$$

$$\begin{aligned} &X_A(1 - X_A)(-4794.9255X_A + 14894.2306) \\ &= 4795.9X_A^3 - 19689X_A^2 + 14894X_A \end{aligned}$$

Question & Answer

Enthalpy of Mixing / X (1-X)



$$\frac{\Delta H_{mix}}{X_A(1 - X_A)} = L_0^0 - (2X_A - 1)L_1^0$$

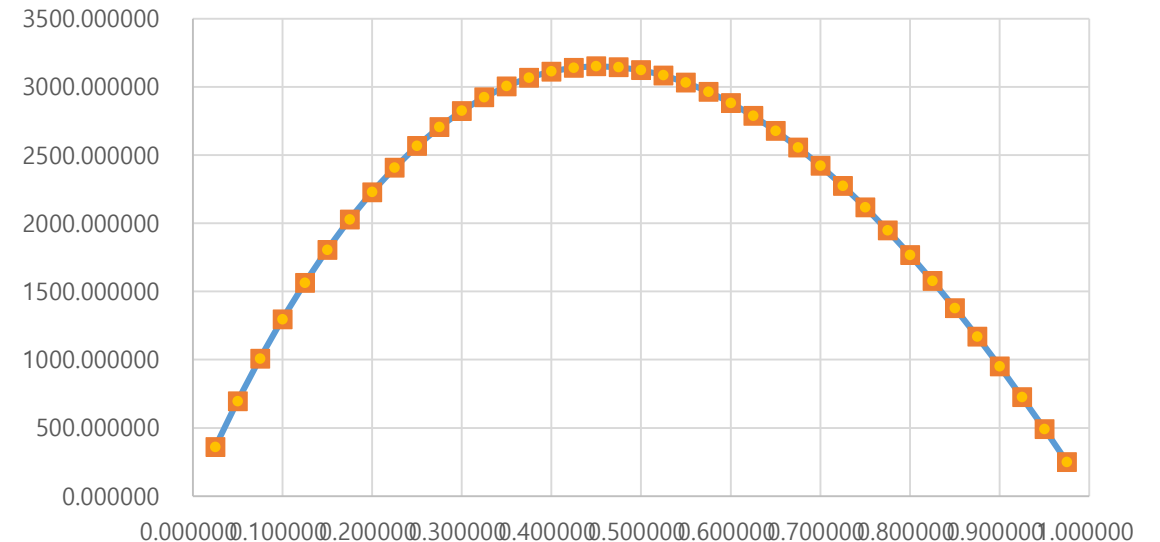
$$= -4794.9255X_A + 14894.2306$$



$$L_1^0 = 2397.4628$$

$$L_0^0 = 12496.768$$

Enthalpy of Mixing



$$\Delta H_{mix} = X_A(1 - X_A)(L_0^0 - (2X_A - 1)L_1^0)$$

$$= X_A(1 - X_A)(-4794.9255X_A + 14894.2306)$$

(Sub-regular Solution Model)