소재수치해석

Final term project

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Problem

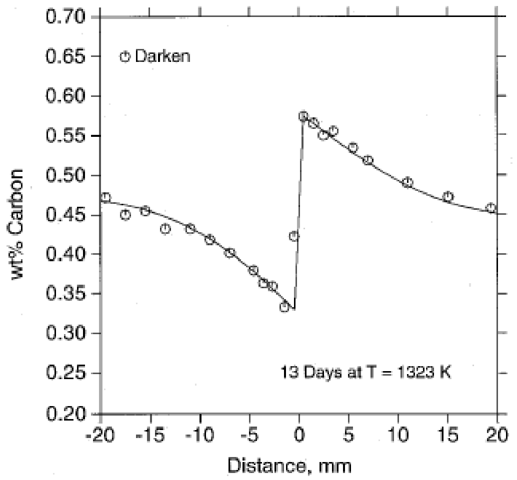
Simulation of Darken's Uphill Diffusion

- 다음의 Mobility 정보와 initial condition 을 이용하여 Darken 의 uphill diffusion 실험을 FDM 으로 simulation 하시오. (SI unit)

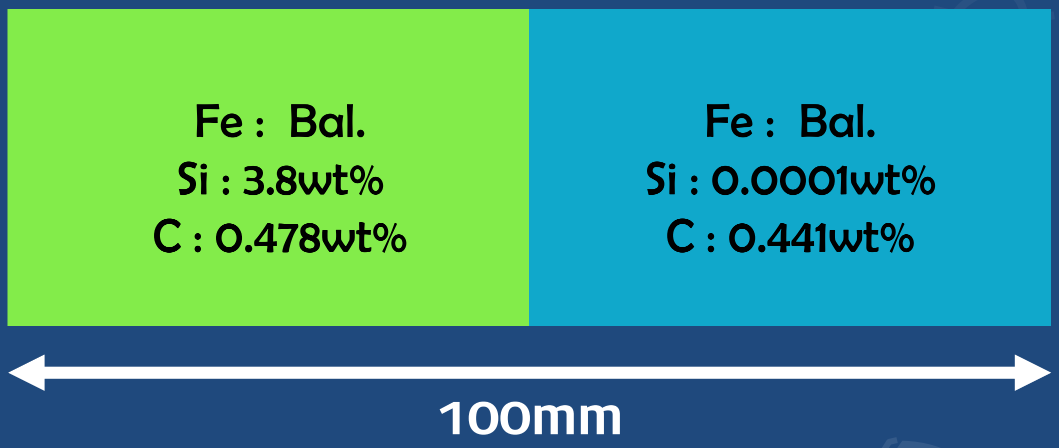
$$\Omega_{Fe}RT = 7.0\times10^{-5}\cdot\exp[-286000/RT]$$

$$\Omega_{Si}RT = 9.05\times10^{-3}\cdot\exp[-322465/RT]$$

$$\Omega_{C}RT = 4.529\times10^{-7}\cdot\exp[-\frac{(1-2.221\cdot10^{-4}T)}{RT}(-72007y_{C}+147723y_{Va})$$



- 각 시편 길이 50mm
- 왼쪽 시편 초기 조성:
  Fe – 3.8wt% Si – 0.478wt% C
- 오른쪽 시편 초기 조성:
  Fe – 0.441 wt% C
- 열처리 온도 1323 K
- 열처리 시간 13 days



Background

$$J_C = -y_C y_{Va} \Omega_C \left(\frac{d\mu_C}{dy_C} \right) \nabla C_C - y_C y_{Va} \Omega_C \left(\frac{d\mu_C}{dy_M} \right) \nabla C_M$$

$$= -\boxed{D_{CC}} \nabla C_C - \boxed{D_{CM}} \nabla C_M$$

$$J_M = -\left(y_{Fe} y_M \Omega_M \frac{d\mu_M}{dy_C} - y_M y_{Fe} \Omega_{Fe} \frac{d\mu_{Fe}}{dy_C} \right) \nabla C_C$$

$$-\left(y_{Fe} y_M \Omega_M \frac{d\mu_M}{dy_M} - y_M y_{Fe} \Omega_{Fe} \frac{d\mu_{Fe}}{dy_M} \right) \nabla C_M$$

$$= -\boxed{D_{MC}} \nabla C_C - \boxed{D_{MM}} \nabla C_M$$

- 확산 유속은 농도 C 의 기울기를 이용하여 표현하지만 실제 simulation 에서는 V 와 C 를 곱한 U-fraction 이 사용된다.

U-fraction

$$u_k = C_k V_S = \frac{x_k}{\sum_{j \in S} x_j}$$

Modeling assumption

$$V_k = V_S \quad \text{for } k \in \mathrm{S}$$

$$V_k = 0 \quad \text{for } k \notin \mathrm{S}$$

y_Fe + y_Si = 1

y_C + y_Va = 1

Background

- Fcc Fe−M−C 침입형 고용상은 $(Fe,M)_1(va,C)_1$ 의 formula unit 을 이용하여 1 mol of formula unit 당 Gibbs free energy 를 다음과 같이 표현한다.

$$G_m = y_{Fe}y_{Va}{}^oG_{Fe:Va} + y_M y_{Va}{}^oG_{M:Va} + y_{Fe}y_C{}^oG_{Fe:C} + y_M y_C{}^oG_{M:C}$$
$$+ RT(y_{Fe}\ln y_{Fe} + y_M \ln y_M) + RT(y_{Va}\ln y_{Va} + y_C \ln y_C)$$
$$+ y_{Fe}y_M y_{Va}L_{Fe,M:Va} + y_{Fe}y_M y_C L_{Fe,M:C}$$
$$+ y_{Fe}y_C y_{Va}L_{Fe:C,Va} + y_M y_C y_{Va}L_{M:C,Va}$$

dl 식을 통해서
chemical potential을 구하고
이를 통해
diffusion coefficien를 구함

$${}^oG_{Fe:Va} = {}^oG_{Fe}^{fcc}$$
$${}^oG_{Si:Va} = {}^oG_{Si}^{Diamond} + 51000 - 21.8\cdot T$$
$${}^oG_{Fe:C} = {}^oG_{Fe}^{fcc} + {}^oG_{C}^{graphite} + 77207 - 15.877\cdot T$$
$${}^oG_{Si:C} = {}^oG_{Si}^{Diamond} + {}^oG_{C}^{graphite} - 20510 + 38.7\cdot T$$

$$L_{Fe,Si:Va} = -125248 + 41.116\cdot T - 142708(y_{Fe} - y_{Si}) + 89907(y_{Fe} - y_{Si})^2$$
$$L_{Fe,Si:C} = +143219.9 + 39.31\cdot T - 216320.5(y_{Fe} - y_{Si})$$
$$L_{Fe:C,Va} = -34671$$

Background

- Gibbs Energy 식으로부터 각 원소의 Chemical Potential 을 얻는 공식은 다음과 같다.

  For substitutional M,

$$\mu_M = G_m + (1 - y_M)\left(\frac{\partial G_m}{\partial y_M} - \frac{\partial G_m}{\partial y_{Fe}}\right) = G_m + (1 - y_M)\frac{dG_m}{dy_M}$$

  For interstitial C

$$\mu_C = \left(\frac{\partial G_m}{\partial y_C} - \frac{\partial G_m}{\partial y_{Va}}\right) = \frac{dG_m}{dy_C}$$

위의 식을 이용하여 $\frac{dG_m}{dy_C}, \frac{dG_m}{dy_{Si}},, \frac{d}{dy_C}\left(\frac{dG_m}{dy_C}\right), \frac{d}{dy_{Si}}\left(\frac{dG_m}{dy_{Si}}\right), \frac{d}{dy_C}\left(\frac{dG_m}{dy_{Si}}\right)$를 각각 계산

$$\frac{dG_m}{dy_C}$$

$$+ (1-y_{Si})\,y_{Si}\,(1-y_c)\,L_{Fe;Si:Va} + (1-y_{Si})\,y_{Si}\,y_c\,L_{Fe,Si:C}$$

$$+ (1-y_{Si})\,y_c(1-y_c)\,L_{Fe:C,Va} + y_{Si}\,y_c(1-y_c)\,L_{Si:C,Va}$$

$$\frac{dG_m}{dy_c} = -\overset{G_1}{(1-y_{Si})\,{}^{\circ}G_{Fe:Va}} - \overset{G_2}{y_{Si}\,{}^{\circ}G_{M:Va}} + \overset{G_3}{(1-y_{Si})\,{}^{\circ}G_{Fe:C}} + \overset{G_4}{y_{Si}\,{}^{\circ}G_{Si:C}}$$

$$+RT\left\{-\ln(1-y_c)-\cancel{1}+\ln y_c+\cancel{1}\right\} = -RT\ln(1-y_c)+RT\ln y_c$$

$$-(1-y_{Si})\,y_{Si}\,\overset{L_1}{L_{Fe:Si:Va}} + (1-y_{Si})\,y_{Si}\,\overset{L_2}{L_{Fe,Si:C}}$$

$$+(1-y_{Si})(1-y_c)\,L_{Fe:C:Va} - (1-y_{Si})\,y_c\,L_{Fe:C:Va} = (1-2y_c)(1-y_{Si})\,\overset{L_3}{L_{Fe:C:Va}}$$

$$+y_{Si}(1-y_c)\,L_{Si:C:Va} - y_{Si}\,y_c\,L_{Si:C:Va} = (1-2y_c)\,y_{Si}\,L_{Si:C:Va}$$

$$\frac{d}{dy_c}\left(\frac{dG_m}{dy_c}\right) = \frac{RT}{1-y_c} + \frac{RT}{y_c} - 2(1-y_{Si})L_{Fe,C:Va} - 2y_{Si}L_{Si:C:Va}$$

$$\frac{d}{dy_C}\left(\frac{dG_m}{dy_C}\right), \frac{dG_m}{dy_{Si}}$$

$$+(1-y_{Si})(1-y_c)L_{Fe:C:Va} - (1-y_{Si})y_c L_{Fe:C:Va} = (1-2y_c)(1-y_{Si})L_{Fe:C:Va}$$

$$+y_{Si}(1-y_c)L_{Si:C:Va} - y_{Si}y_c L_{Si:C:Va} = (1-2y_c)y_{Si}L_{Si:C:Va}$$

$$\frac{d}{dy_c}\left(\frac{dG_m}{dy_c}\right) = \frac{RT}{1-y_c} + \frac{RT}{y_c} - 2(1-y_{Si})L_{Fe,C:Va} - 2y_{Si}L_{Si:C:Va}$$

$$\frac{dG_m}{dy_{Si}} = -(1-y_c)\,{}^{\circ}G_{Fe:Va} + (1-y_c)\,{}^{\circ}G_{Si:Va} - y_c\,{}^{\circ}G_{Fe:C} + y_c\,{}^{\circ}G_{Si:C}$$

$$+RT\{-\ln(1-y_{Si}) - 1 + \ln y_{Si} + 1\} = -RT\ln(1-y_{Si}) + RT\ln y_{Si}$$

$$-y_{Si}(1-y_c)L_{Fe:Si:Va} + (1-y_{Si})(1-y_c)L_{Fe:Si:Va} = (1-2y_{Si})(1-y_c)L_{Fe:Si:Va}$$

$$-y_{Si}y_c L_{Fe:Si:C} + (1-y_{Si})y_c L_{Fe:Si:C} = (1-2y_{Si})y_c L_{Fe:Si:C}$$

$$-y_c(1-y_c)L_{Fe:C:Va} + y_c(1-y_c)L_{Si:C:Va}$$

$$+(1-y_{Si})y_{Si}(1-y_c)\cdot\left(\frac{dL_{Fe:Si:Va}}{dy_{Si}}\right) + (1-y_{Si})y_{Si}y_c\cdot\left(\frac{dL_{Fe:Si:C}}{dy_{Si}}\right)$$

$$\frac{d}{dy_{Si}}\left(\frac{dG_m}{dy_{Si}}\right) = \frac{RT}{1-y_{Si}} + \frac{RT}{y_{Si}} - 2(1-y_c)L_{Fe:Si:Va} - 2y_c L_{Fe:Si:C},$$

$$\left(\frac{dL_{Fe:Si:Va}}{\ldots}\right) \ldots \left(\frac{dL_{Fe:Si:Va}}{\ldots}\right) + (1-y_{Si})y_{Si}(1-y_c)\cdot\left(\frac{d^2L_{\ldots}}{dy_{\ldots}}\right)$$

$$\frac{d}{dy_{Si}}\left(\frac{dG_m}{dy_{Si}}\right)$$

$$-2y_c L_2 + (1-2y_{si})y_c \frac{dL_2}{dy_{si}} + (1-y_{si})y_c \frac{dL_2}{dy_c} - y_{si}y_c \frac{dL_2}{dy_{si}} + y_{si}(1-y_{si}) \ldots$$

$$\frac{d}{ds_i}\left(\frac{dG_m}{ds_i}\right) = \frac{RT}{1-y_{si}} + \frac{RT}{y_{si}} - 2(1-y_c)L_{Fesi:Va} + 2(1-2y_{si})(1-y_c)\frac{dL_{Fesi:Va}}{dy_{si}}$$

$$+ y_{si}(1-y_{si})(1-y_c)\left(\frac{d^2L_{Fesi:Va}}{dy_{si}^2}\right)$$

$$-2y_c L_{Fesi:C} + (1-2y_{si})y_c\frac{dL_{Fesi:C}}{dy_{si}} + (1-2y_{si})y_c\frac{dL_{Fesi:C}}{dy_{si}}$$

$$\frac{d}{dy_C}\left(\frac{dG_m}{dy_{Si}}\right)$$

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$$\frac{d}{dy_C}\left(\frac{dG_m}{dy_{Si}}\right) = {}^{\circ}G_{Fe:Va} - {}^{\circ}G_{Si:Va} - {}^{\circ}G_{Fe:C} + {}^{\circ}G_{Si:C}$$

$$- (1-2y_{Si}) L_{Fe:Si:Va} + (1-2y_{Si}) L_{Fe:Si:C}$$

$$- (1-y_C) L_{Fe:C,Va} + y_C L_{Fe:C:Va} = (2y_C - 1) L_{Fe:C,Va}$$

$$- (1-y_{Si})\, y_{Si} \left(\frac{dL_{Fe:Si:Va}}{dy_{Si}}\right) + (1-y_{Si})\, y_{Si} \left(\frac{dL_{Fe:Si:C}}{dy_{Si}}\right)$$

μ_{Si}

$$
\begin{aligned}
\mu_{Si} = {} & (1-y_{Si})(1-y_c)\,{}^\circ G_{Fe:Va} + y_{Si}(1-y_c)\,{}^\circ G_{Si:Va} + (1-y_{Si})y_c\,{}^\circ G_{Fe:C} + y_{Si}y_c\,{}^\circ G_{Si:C} \\
& + RT\{(1-y_{Si})\ln(1-y_{Si}) + y_{Si}\ln y_{Si}\} + RT\{(1-y_c)\ln(1-y_c) + y_c\ln y_c\} \\
& + (1-y_{Si})y_{Si}(1-y_c)L_{Fe,Si:Va} + (1-y_{Si})y_{Si}y_c L_{Fe:Si:C} \\
& + (1-y_{Si})y_c(1-y_c)L_{Fe:C:Va} + y_{Si}y_c(1-y_c)L_{Si:C:Va} \\
& + (1-y_{Si})\{(1-y_c)\,{}^\circ G_{Si:Va} + y_c\,{}^\circ G_{Si:C} + RT(\ln y_{Si} + 1) + (1-y_{Si})(1-y_c)L_{Fe:Si:Va} \\
& \qquad + (1-y_{Si})y_c L_{Fe:Si:C} + y_c(1-y_c)L_{Si:C:Va}\}
\end{aligned}
$$

Background

$$\frac{d\mu_M}{dy_C} = \mu_C + (1 - y_M)\frac{d}{dy_C}\left(\frac{dG_m}{dy_M}\right)$$

$$\frac{d\mu_M}{dy_M} = (1 - y_M)\frac{d}{dy_M}\left(\frac{dG_m}{dy_M}\right)$$

$$\frac{d\mu_C}{dy_C} = \frac{d}{dy_C}\left(\frac{dG_m}{dy_C}\right)$$

$$\frac{d\mu_C}{dy_M} = \frac{d}{dy_M}\left(\frac{dG_m}{dy_C}\right)$$

$$\frac{d\mu_{Fe}}{dy_C} = \mu_C - y_M\frac{d}{dy_C}\left(\frac{dG_m}{dy_M}\right)$$

$$\frac{d\mu_{Fe}}{dy_M} = -y_M\frac{d}{dy_M}\left(\frac{dG_m}{dy_M}\right)$$

$$D_{CC} = y_c y_{Va}\Omega_C\left(\frac{d\mu_C}{dy_C}\right)$$

$$D_{CM} = y_c y_{Va}\Omega_C\left(\frac{d\mu_C}{dy_M}\right)$$

$$D_{MC} = y_{Fe} y_M \Omega_M\left(\frac{d\mu_M}{dy_C}\right) - y_{Fe} y_M \Omega_{Fe}\left(\frac{d\mu_{Fe}}{dy_C}\right)$$

$$D_{MM} = y_{Fe} y_M \Omega_M\left(\frac{d\mu_M}{dy_M}\right) - y_{Fe} y_M \Omega_{Fe}\left(\frac{d\mu_{Fe}}{dy_M}\right)$$

FDM

Fick's 2nd law

$$\frac{\partial y_C}{\partial t} = -\nabla J_C = \frac{\partial}{\partial x}\left[D_{CC}\frac{\partial y_C}{\partial x} + D_{CSi}\frac{\partial y_{Si}}{\partial x} \right]$$

FDM

$$\frac{y_{C,i}^{j+1} - y_{C,i}^{j}}{\Delta t} = \frac{1}{(\Delta x)^2}\left[\sqrt{D_{CC,i+1}\cdot D_{CC,i}}\,(y_{C,i+1}^{j} - y_{C,i}^{j}) - \sqrt{D_{CC,i-1}\cdot D_{CC,i}}\,(y_{C,i}^{j} - y_{C,i-1}^{j}) \right] + \frac{1}{(\Delta x)^2}\left[\sqrt{D_{CM,i+1}\cdot D_{CM,i}}\,(y_{M,i+1}^{j} - y_{M,i}^{j}) - \sqrt{D_{CM,i-1}\cdot D_{CM,i}}\,(y_{M,i}^{j} - y_{M,i-1}^{j}) \right]$$

(forward difference method, explicit)

$$y_{C,i}^{j+1} = y_{C,i}^{j} + \frac{\Delta t}{(\Delta x)^2}\left[\sqrt{D_{CC,i+1}\cdot D_{CC,i}}\,(y_{C,i+1}^{j} - y_{C,i}^{j}) - \sqrt{D_{CC,i-1}\cdot D_{CC,i}}\,(y_{C,i}^{j} - y_{C,i-1}^{j}) \right] + \frac{\Delta t}{(\Delta x)^2}\left[\sqrt{D_{CM,i+1}\cdot D_{CM,i}}\,(y_{M,i+1}^{j} - y_{M,i}^{j}) - \sqrt{D_{CM,i-1}\cdot D_{CM,i}}\,(y_{M,i}^{j} - y_{M,i-1}^{j}) \right]$$

알고리즘

초기값 입력
Y fraction으로 변환
FDM을 사용하여
D와 y_C, y_Si update
Y fraction을 다시 wt%로 변환
Text 파일에 출력
Time 증가

Key code

```c
#include<stdio.h>
#include<stdlib.h>
#include<math.h>

#define R 8.3144621
#define T 1323
#define Length 0.1
#define M_Fe 55.845
#define M_C 12.0107
#define M_Si 28.0855
```

```c
int  i,j,number;
double G_FeVa,G_SiVa,G_FeC,G_SiC; // free gibbs energy
double*dGm_dycdySi; // G 미분값
double*dGm_dyC;// G 미분값
double*dGm_dySi;// G 미분값
double*dGm_dyC2;// G 미분값
double*dGm_dySi2;
double*dL_FeSiVa_dySi;// L 미분값
double dL_FeSiVa_dySi2;// L 미분값
double dL_FeSiC_dySi;  // L 미분값
double L_FeCVa;// L parameter
double*L_FeSiVa;// L parameter
double*L_FeSiC;// L parameter
double Omega_Fe,Omega_Si;  //Omega
double*Omega_C;
double*Dcc;
double*Dcm;
double*Dmc;
double*Dmm;// D coefficient
double x_Fe,x_Si,x_C; //molar fraction
double*y_C; //y fraction
double*y_Si; //y fraction
double*yc; // FDM y
double*ym;
double lamda,dx,dt,time;
double*xf_C;
double*xf_Si;
double*wtf_C;
double*wtf_Si;
```

```c
FILE*result;

result=fopen("result.txt","w");

printf("Enter dt:");
scanf("%lf",&dt);

printf("Enter dx:");
scanf("%lf",&dx);

number=Length/dx; // 구간 갯수

lamda=dt/(dx*dx); // 람다 지정

time=0; // 초기 시간

L_FeCVa=-34671; // L parameter 지정

G_FeVa=0;
G_SiVa=51000-(21.8*T);
G_FeC=77207-(15.877*T);
G_SiC=-20510+(38.7*T); // G 값 대입

dL_FeSiVa_dySi2=8*89907;
dL_FeSiC_dySi=2*216320.5;// L prameter 미분 계산
Omega_Fe=((0.00007)*exp((-286000)/(R*T)))/(R*T);
Omega_Si=((0.00905)*exp((-322465)/(R*T)))/(R*T);
```

Key code

```
for(i=0;i<(number/2);i++) // 처음 0.05m 부근 y-fraction 대입
{
    x_Fe=(95.722/M_Fe)/((95.722/M_Fe)+(3.8/M_Si)+(0.478/M_C));
    x_Si=(3.8/M_Si)/((95.722/M_Fe)+(3.8/M_Si)+(0.478/M_C));
    x_C=(0.478/M_C)/((95.722/M_Fe)+(3.8/M_Si)+(0.478/M_C));
    y_C[i]=x_C/(x_Fe+x_Si);
    y_Si[i]=x_Si/(x_Fe+x_Si);
}
for(i=(number/2);i<number;i++) // 나중 0.05m 부근 y-fraction 대입
{
    x_Fe=(99.558/M_Fe)/((99.558/M_Fe)+(0.001/M_Si)+(0.441/M_C));
    x_Si=(0.001/M_Si)/((99.558/M_Fe)+(0.001/M_Si)+(0.441/M_C));
    x_C=(0.441/M_C)/((99.558/M_Fe)+(0.001/M_Si)+(0.441/M_C));
    y_C[i]=x_C/(x_Fe+x_Si);
    y_Si[i]=x_Si/(x_Fe+x_Si);
}
```

Ket code

```
while(1)
{
    time=time+dt;



    for(i=0;i<number;i++)
    {
        L_FeSiVa[i]=-125248+(41.116*T)-(142708*(1-2*y_Si[i]))+(89907*((1-2*y_Si[i])*(1-2*y_Si[i])));
        L_FeSiC[i]=143219.9+(39.31*T)-(216320.5*(1-2*y_Si[i]));

        dL_FeSiVa_dySi[i]=(2*142708)-(4*89907*(1-2*y_Si[i]));
        /* ... */
        dGm_dyC[i]=(-(1-y_Si[i])*G_FeVa)-(y_Si[i]*G_SiVa)+((1-y_Si[i])*G_FeC)+(y_Si[i]*G_SiC)-((R*T)*log(1-y_C[i]))
            +((R*T)*log(y_C[i]))-((1-y_Si[i])*y_Si[i]*L_FeSiVa[i])+((1-y_Si[i])*y_Si[i]*L_FeSiC[i])+((1-2*y_C[i])*(1-y_Si[i])*L_FeCVa); // 이상함
        dGm_dySi[i]=-((1-y_C[i])*G_FeVa)+((1-y_C[i])*G_SiVa)-(y_C[i]*G_FeC)+(y_C[i]*G_SiC)-((R*T)*log(1-y_Si[i]))
            +((R*T)*log(y_Si[i]))+((1-2*y_Si[i])*(1-y_C[i])*L_FeSiVa[i])+((1-2*y_Si[i])*y_C[i]*L_FeSiC[i])
            -(y_C[i]*(1-y_C[i])*L_FeCVa)+((1-y_Si[i])*y_Si[i]*(1-y_C[i])*dL_FeSiVa_dySi[i])+((1-y_Si[i])*y_Si[i]*y_C[i]*dL_FeSiC_dySi);
        dGm_dyC2[i]=((R*T)/(1-y_C[i]))+((R*T)/y_C[i])-(2*(1-y_Si[i])*L_FeCVa);
        dGm_dySi2[i]=((R*T)/(1-y_Si[i]))+((R*T)/y_Si[i])-(2*(1-y_C[i])*L_FeSiVa[i])+(2*(1-2*y_Si[i])*(1-y_C[i])*dL_FeSiVa_dySi[i])
            +(y_Si[i]*(1-y_Si[i])*(1-y_C[i])*dL_FeSiVa_dySi2)-(2*y_C[i]*L_FeSiC[i])+((1-2*y_Si[i])*y_C[i]*dL_FeSiC_dySi)+((1-2*y_Si[i])*y_C[i]*dL_FeSiC_dySi); // 계산 실수
        dGm_dycdySi[i]=G_FeVa-G_SiVa-G_FeC+G_SiC-((1-2*y_Si[i])*L_FeSiVa[i])
            +((1-2*y_Si[i])*L_FeSiC[i])+((2*y_C[i]-1)*L_FeCVa)-((1-y_Si[i])*y_Si[i]*dL_FeSiVa_dySi[i])+((1-y_Si[i])*y_Si[i]*dL_FeSiC_dySi); //((2*y_C[i])*L_FeCVa) term ?

        // 여기서 부터 시작
        Omega_C[i]=(0.0000004529*exp(-((1-0.0002221*T)*((147723*(1-y_C[i]))-(72007*y_C[i])))/(R*T)))/(R*T);
        Dcc[i]=y_C[i]*(1-y_C[i])*Omega_C[i]*dGm_dyC2[i];
        Dcm[i]=y_C[i]*(1-y_C[i])*Omega_C[i]*dGm_dycdySi[i];
        Dmc[i]=((1-y_Si[i])*y_Si[i]*Omega_Si*(dGm_dyC[i]*((1-y_Si[i])*dGm_dycdySi[i])))-(y_Si[i]*(1-y_Si[i])*Omega_Fe*(dGm_dyC[i]-((y_Si[i])*dGm_dycdySi[i]))); //
        Dmm[i]=((1-y_Si[i])*y_Si[i]*Omega_Si*((1-y_Si[i])*dGm_dySi2[i]))-(y_Si[i]*(1-y_Si[i])*Omega_Fe*((-y_Si[i])*dGm_dySi2[i]));
}
```

Key code

```
for(i=0;i<number;i++)
{
    if(i==0)
    {
        yc[i]=y_C[i];
        ym[i]=y_Si[i];
    }
    else if(i==number-1)
    {
        yc[i]=y_C[i];
        ym[i]=y_Si[i];
    }
    else
    {
        yc[i]=dt/dx/dx*(sqrt(Dcc[i+1]*Dcc[i])*(y_C[i+1]-y_C[i])-sqrt(Dcc[i]*Dcc[i-1])*(y_C[i]-y_C[i-1])
            +sqrt(Dcm[i+1]*Dcm[i])*(y_Si[i+1]-y_Si[i])-sqrt(Dcm[i]*Dcm[i-1])*(y_Si[i]-y_Si[i-1]))+y_C[i];
        ym[i]=dt/dx/dx*(sqrt(Dmc[i+1]*Dmc[i])*(y_C[i+1]-y_C[i])-sqrt(Dmc[i]*Dmc[i-1])*(y_C[i]-y_C[i-1])
            +sqrt(Dmm[i+1]*Dmm[i])*(y_Si[i+1]-y_Si[i])-sqrt(Dmm[i]*Dmm[i-1])*(y_Si[i]-y_Si[i-1]))+y_Si[i];
    }
}
for(i=0;i<number;i++)
{
    y_C[i]=yc[i];
    y_Si[i]=ym[i];
}
```

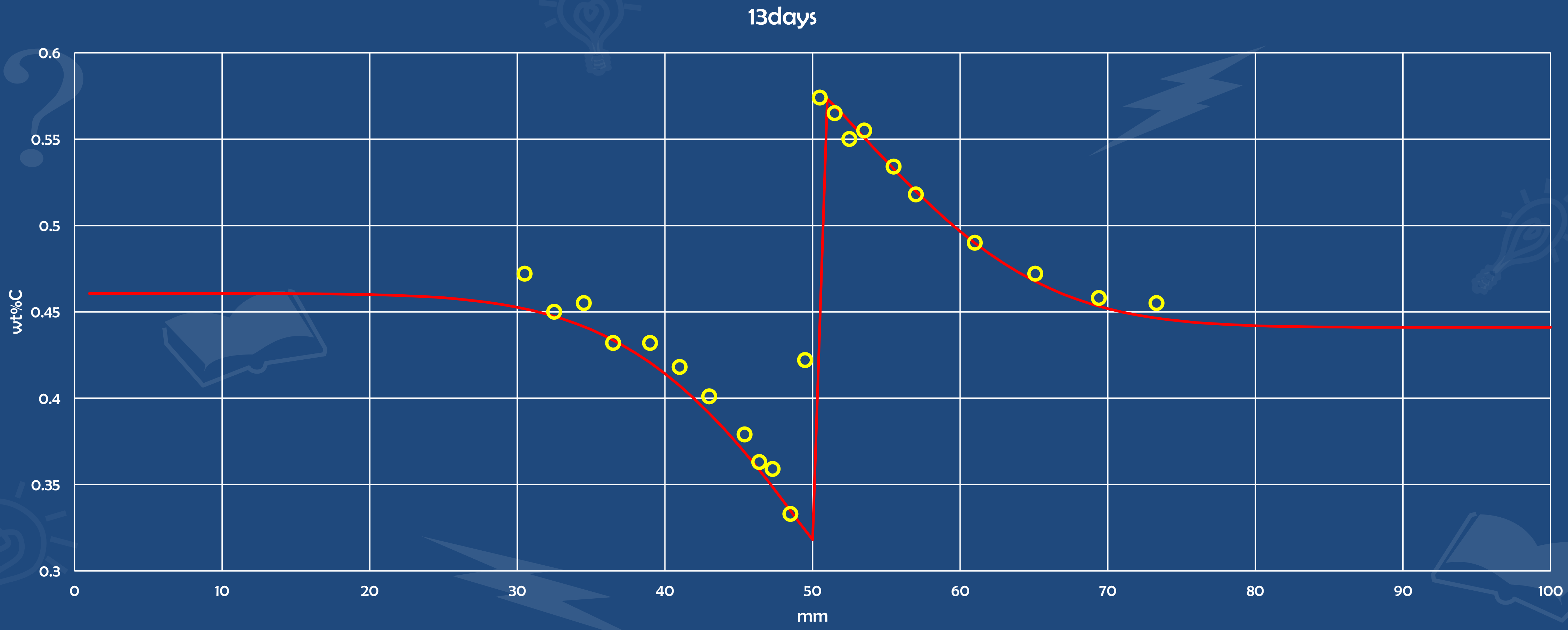
Key code

```
if(time==3600)
{

    for(i=0;i<number;i++)
    {
        xf_C[i]=(yc[i]/(1+yc[i]));
        xf_Si[i]=ym[i]*(1-xf_C[i]);
        wtf_C[i]=((xf_C[i]/M_Fe)/((1/M_C)-((1/M_C)-(1/M_Fe))*xf_C[i]))*100;
        wtf_Si[i]=M_Si*xf_Si[i]*((wtf_C[i]/M_C)+((100-wtf_C[i])/M_Fe));
    }

    for(i=0;i<number;i++)
    {
        fprintf(result,"%d  %.10lf  %.10lf₩n",i+1,wtf_C[i],wtf_Si[i]);
    }
    fprintf(result,"₩n");
    break;
}
```

result

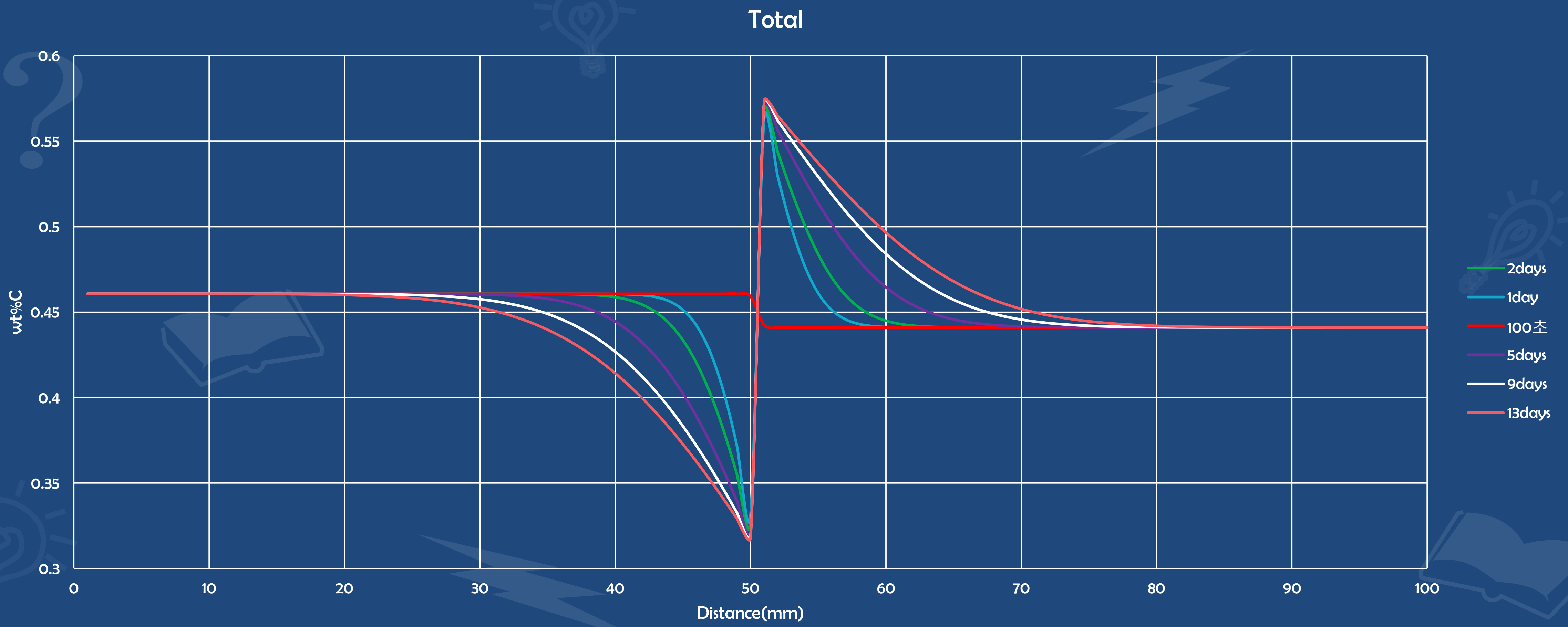
하루		172800	2days		432000	5days		777600	9days		1123200	13days	
wt%C	wt%Si		wt%C	wt%Si		wt%C	wt%Si		wt%C	wt%Si		wt%C	wt%Si
0.4607	3.66244	1	0.4607	3.66244	1	0.4607	3.66244	1	0.4607	3.66244	1	0.4607	3.66244
0.4607	3.66244	2	0.4607	3.66244	2	0.4607	3.66244	2	0.4607	3.66244	2	0.4607	3.66244
0.4607	3.66244	3	0.4607	3.66244	3	0.4607	3.66244	3	0.4607	3.66244	3	0.4607	3.66244
0.4607	3.66244	4	0.4607	3.66244	4	0.4607	3.66244	4	0.4607	3.66244	4	0.46069	3.66244
0.4607	3.66244	5	0.4607	3.66244	5	0.4607	3.66244	5	0.4607	3.66244	5	0.46069	3.66244
0.4607	3.66244	6	0.4607	3.66244	6	0.4607	3.66244	6	0.4607	3.66244	6	0.46069	3.66244
0.4607	3.66244	7	0.4607	3.66244	7	0.4607	3.66244	7	0.4607	3.66244	7	0.46069	3.66244
0.4607	3.66244	8	0.4607	3.66244	8	0.4607	3.66244	8	0.4607	3.66244	8	0.46068	3.66244
0.4607	3.66244	9	0.4607	3.66244	9	0.4607	3.66244	9	0.4607	3.66244	9	0.46068	3.66244
0.4607	3.66244	10	0.4607	3.66244	10	0.4607	3.66244	10	0.4607	3.66244	10	0.46067	3.66244
0.4607	3.66244	11	0.4607	3.66244	11	0.4607	3.66244	11	0.46069	3.66244	11	0.46066	3.66244
0.4607	3.66244	12	0.4607	3.66244	12	0.4607	3.66244	12	0.46069	3.66244	12	0.46064	3.66244
0.4607	3.66244	13	0.4607	3.66244	13	0.4607	3.66244	13	0.46069	3.66244	13	0.46062	3.66245
0.4607	3.66244	14	0.4607	3.66244	14	0.4607	3.66244	14	0.46069	3.66244	14	0.46059	3.66245
0.4607	3.66244	15	0.4607	3.66244	15	0.4607	3.66244	15	0.46068	3.66244	15	0.46055	3.66245
0.4607	3.66244	16	0.4607	3.66244	16	0.4607	3.66244	16	0.46068	3.66244	16	0.46049	3.66245
0.4607	3.66244	17	0.4607	3.66244	17	0.4607	3.66244	17	0.46067	3.66244	17	0.46042	3.66245
0.4607	3.66244	18	0.4607	3.66244	18	0.4607	3.66244	18	0.46065	3.66244	18	0.46032	3.66246
0.4607	3.66244	19	0.4607	3.66244	19	0.4607	3.66244	19	0.46063	3.66245	19	0.46019	3.66246
0.4607	3.66244	20	0.4607	3.66244	20	0.4607	3.66244	20	0.46059	3.66245	20	0.46002	3.66247
0.4607	3.66244	21	0.4607	3.66244	21	0.46069	3.66244	21	0.46054	3.66245	21	0.4598	3.66248
0.4607	3.66244	22	0.4607	3.66244	22	0.46069	3.66244	22	0.46047	3.66245	22	0.45952	3.66249
0.4607	3.66244	23	0.4607	3.66244	23	0.46069	3.66244	23	0.46037	3.66245	23	0.45916	3.6625
0.4607	3.66244	24	0.4607	3.66244	24	0.46068	3.66244	24	0.46023	3.66246	24	0.4587	3.66252
0.4607	3.66244	25	0.4607	3.66244	25	0.46067	3.66244	25	0.46004	3.66247	25	0.45814	3.66254
0.4607	3.66244	26	0.4607	3.66244	26	0.46065	3.66244	26	0.45978	3.66248	26	0.45744	3.66256
0.4607	3.66244	27	0.4607	3.66244	27	0.46062	3.66245	27	0.45942	3.66249	27	0.45657	3.66259
0.4607	3.66244	28	0.4607	3.66244	28	0.46057	3.66245	28	0.45895	3.66251	28	0.45551	3.66263
0.4607	3.66244	29	0.4607	3.66244	29	0.46049	3.66245	29	0.45833	3.66253	29	0.45423	3.66268
0.4607	3.66244	30	0.4607	3.66244	30	0.46036	3.66245	30	0.45753	3.66256	30	0.45269	3.66274
0.4607	3.66244	31	0.4607	3.66244	31	0.46016	3.66246	31	0.4565	3.6626	31	0.45085	3.6628
0.4607	3.66244	32	0.46069	3.66244	32	0.45986	3.66247	32	0.45518	3.66265	32	0.44868	3.66288
0.4607	3.66244	33	0.46069	3.66244	33	0.4594	3.66249	33	0.45353	3.66271	33	0.44613	3.66298
0.4607	3.66244	34	0.46068	3.66244	34	0.45873	3.66252	34	0.45148	3.66278	34	0.44315	3.66309
0.4607	3.66244	35	0.46065	3.66244	35	0.45777	3.66255	35	0.44896	3.66287	35	0.43972	3.66321
0.4607	3.66244	36	0.46059	3.66245	36	0.45641	3.6626	36	0.44591	3.66299	36	0.43578	3.66336
0.46069	3.66244	37	0.46045	3.66245	37	0.45456	3.66267	37	0.44224	3.66312	37	0.43129	3.66352
0.46069	3.66244	38	0.46019	3.66246	38	0.45205	3.66276	38	0.43788	3.66328	38	0.42622	3.66371

result



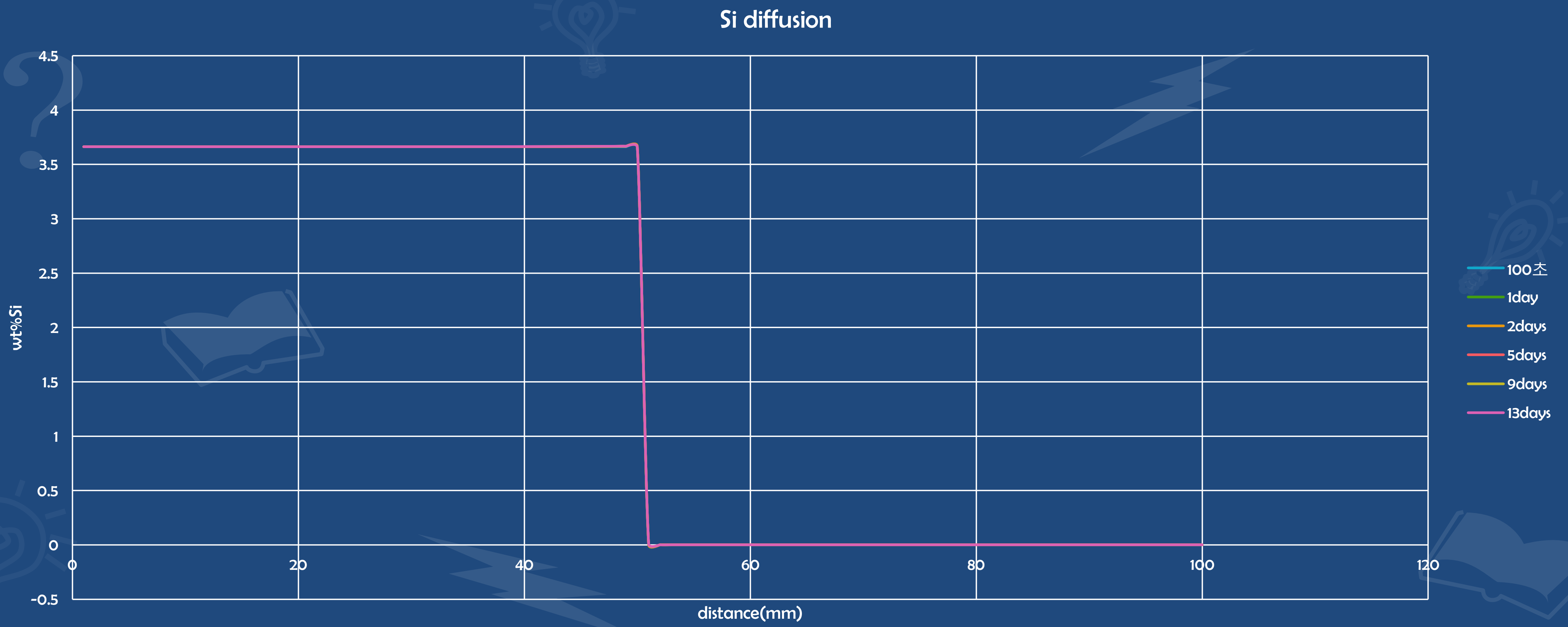
13days
wt%C
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0
10
20
30
40
50
60
70
80
90
100
mm

result



Total
0.6
0.55
0.5
0.45
0.4
0.35
0.3
wt%C
0
10
20
30
40
50
60
70
80
90
100
Distance(mm)
2days
1day
100초
5days
9days
13days

result



실리콘은 탄소에 비해 확산이 매우 안된다!

Conclusion

- FDM을 이용해서 fcc Fe-Si-C 3원계 고용상에서, carbon의 Darken’s uphill diffusion을 simulation 할 수 있다.

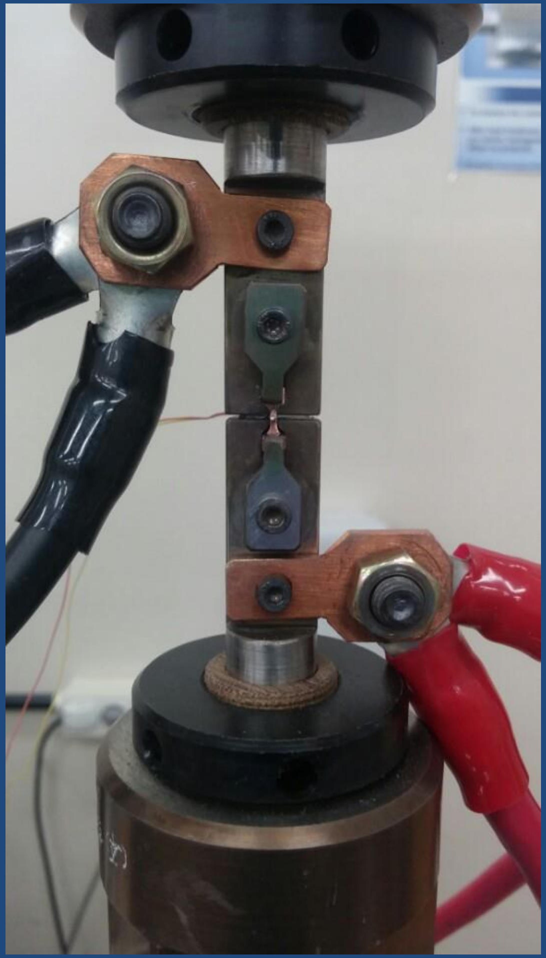
- 왼쪽 시편은 Si 농도가 더 높은데 그로 인해 C의 chemical potential은 왼쪽이 더 높다. 따라서 chemical potential이 같아 질때 까지 확산이 일어난다. (농도 기울기를 거스름 → up hill diffusion)

- 따라서 diffusion은 chemical potential 차이에 dominant한 영향.

- interstitial diffusion을 하는 C와는 달리 Si는 substitutional diffusion 을 하기 때문에 확산이 매우 느리다.

자유 주제
Resistance heating

Resistance heating

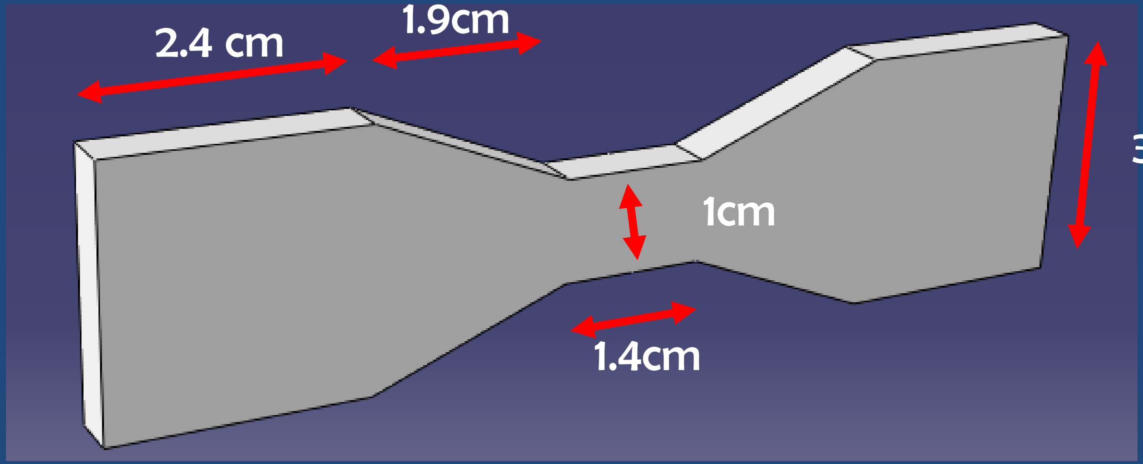


- 사용 시편 **Al 2024**

- 한쪽 면에서 전류 흘려 시편의 전체적인 **resistance heating** 구현
  - 시편의 동시 다발적 전체적인 가열
  - 시간에 따른 시편의 각 부분의 온도 경향성 파악
- **Resistance heating** 후 **tensile test**
  - **Strain**에 따른 **gauge** 부분의 온도 및 **energy** 경향성 파악

전제 조건

두께: 0.5cm



3.5cm

- 설정 값 : 50V, 120A
- **Q= I*V*t=P*t, Q= c*m*ΔT,**
- **Density = 2780kg/m3**
- **Specific heat = 795.0j/kg*˚C**
- Strain rate = 10^-2 고정
- 열전달 계수 α=8.418*10^-5
- Poisson's ratio : 0.32
- 목표온도: 400 ˚C

FDM 이용!

알고자 하는 것!

- 실제로 아주 빠른 가열을 경향을 보이는데, 대략적으로 몇 초 만에 목표 온도에 도달할까?

- **Tensile test**가 일어나면서, **necking**으로 인한 단면적 감소가 일어나는데, 단면적 감소 비율과 열에너지 감소 비율 중 어느 요소가 더욱 **dominant** 할까?

알고리즘

초기값 입력
(P,want_T,dx,dt)

↓

각 부분의 넓이, 미소 부피, 미소질량, 온도 변화량 초기화

↓

시편의 각 부분 온도 초기화

↓

FDM을 통한 각 시편의 온도 update

↓

목표 온도 도달 시 온도 초기화 stop! → FDM 을 통한 guage 부분의 넓이, 미소 잘량, 온도 , 열 에너지 update

0.001 초 증가 및 txt 파일 출력

Key code

```c
#define Length 0.1
#define D 0.00008418
#define Density 2780
#define specific_Heat 795.0
#define strain_rate 0.01
#define ratio 0.32
```

```c
for(i=0;i<24;i++)
    Area[i]=0.035*0.005;
for(i=24;i<43;i++)
    Area[i]=Area[i-1]-(((0.035*0.005)-(0.01*0.005))/19);
for(i=43;i<57;i++)
    Area[i]=Area[i-1];
for(i=57;i<76;i++)
    Area[i]=Area[i-1]+(((0.035*0.005)-(0.01*0.005))/19);
for(i=76;i<n;i++)
    Area[i]=Area[i-1];

for(i=0;i<n;i++)
{
    dV[i]=0.001*Area[i];
}

for(i=0;i<n;i++)
{
    dm[i]=(dV[i]*Density);
}

for(i=0;i<n;i++)
{
    del_T[i]=((P*0.001)/(specific_Heat*dm[i]));
}
```

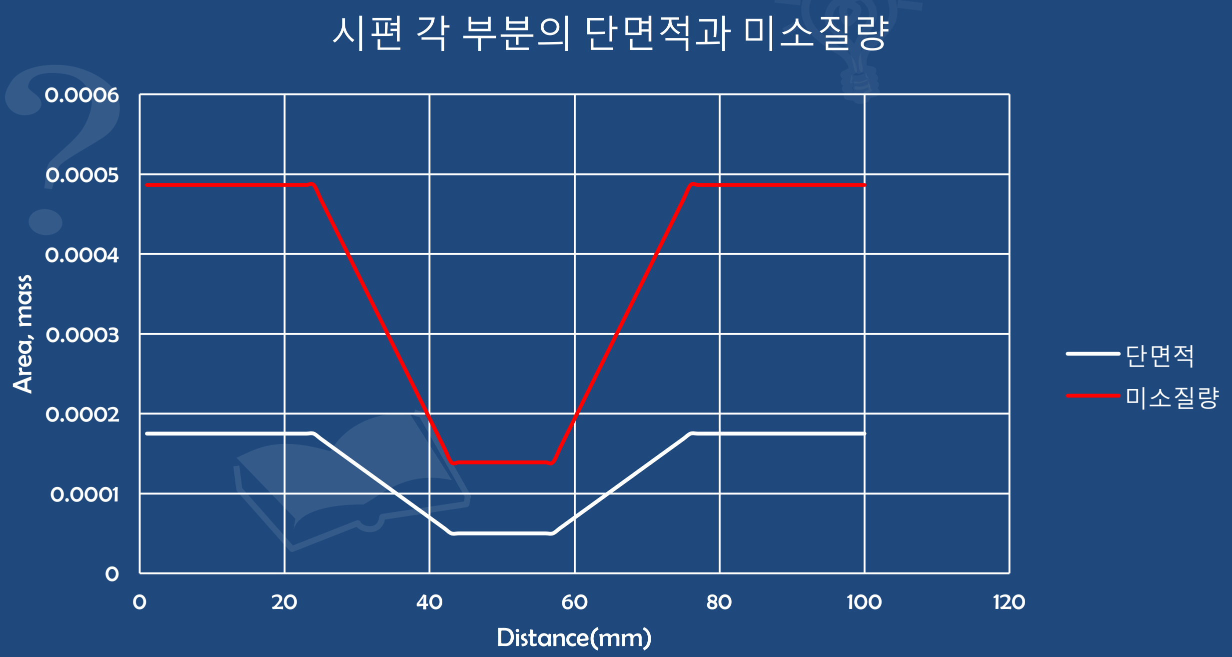
```c
for(i=0;i<n;i++) //Q와 T를 연결 시켜 주어야 한다.
{
    if(i==49 || i==50)
        T[i]=((P*0.001)/(specific_Heat*dm[i]))+300.15;
    else
        T[i]=300.15;
}
```

```c
for(i=0;i<n;i++)
{
    if(i==0)
    {
        Tfinal[i]=T[i];
    }
    else if(i==n-1)
    {
        Tfinal[i]=T[i];
    }
    else
    {
        Tfinal[i]=(1-(2*lamda))*T[i]+(lamda*(T[i+1]+T[i-1]));
    }
}
```

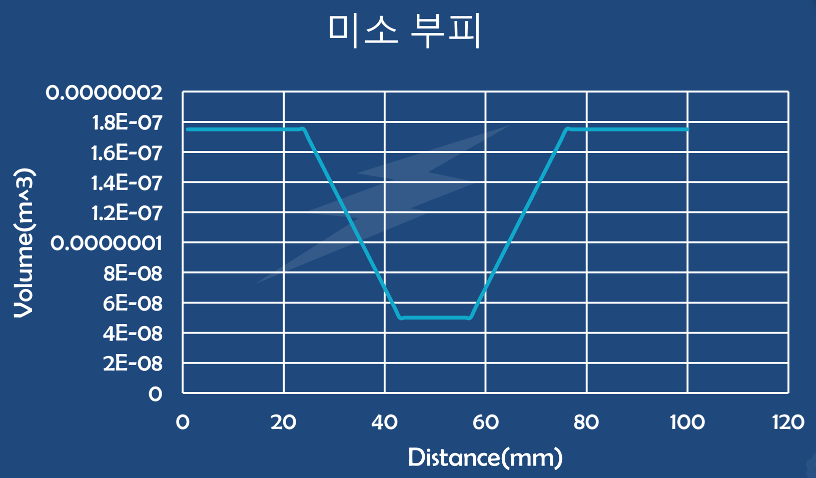
```c
for(i=0;i<n;i++)
{
    if(i==49 || i==50)
    {
        if(T[i]<want_T)
        {
            T[i]=T[i]+del_T[i];
        }
        else
        {
            T[i]=want_T;
        }
    }
    else
    {
        if(T[49]==want_T)
        {
            T[i]=Tfinal[i];
        }
        else
        {
            T[i]=Tfinal[i]+del_T[i];
        }
    }
}
```

Key code

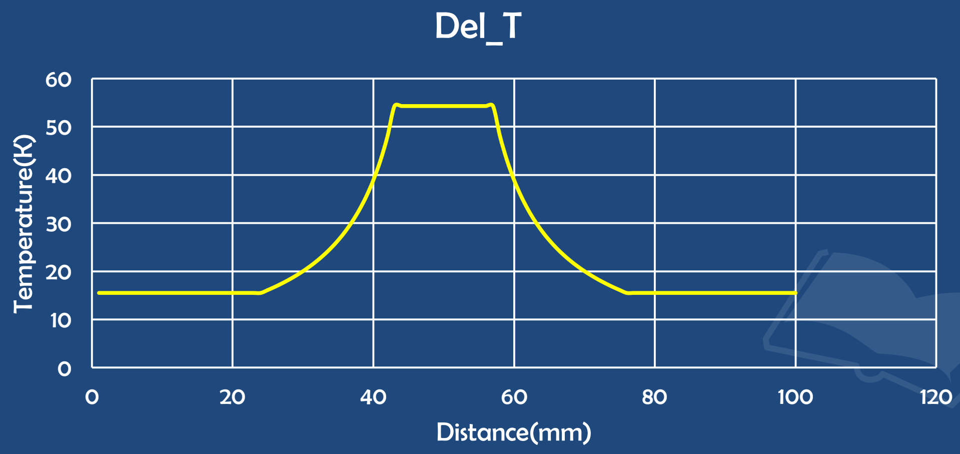
```
if(T[49]>want_T)
{
    T[49]=want_T;
    T[50]=want_T;
}

gauge_Q=(T[49]-300.15)*specific_Heat*dm[49];

if(strain==0)
    fprintf(result,"%.10lf  %.10lf  %.10lf₩n",strain,T[49],gauge_Q);
else
{
    gauge_area=(0.01-((strain/ratio)*0.01))*(0.005-((strain/ratio)*0.005));
    gauge_mass=gauge_area*0.001*Density;
    gauge_T=((T[49]-300.15)*(dm[49]/gauge_mass))+300.15;

    if(gauge_T<=want_T)
    {
        gauge_Q=(gauge_T-300.15)*specific_Heat*gauge_mass;
    }
    else
        gauge_Q=(want_T-300.15)*specific_Heat*gauge_mass;

    fprintf(result,"%.10lf  %.10lf  %.10lf₩n",strain,gauge_T,gauge_Q);
}

time=time+dt;
```



시편 각 부분의 단면적과 미소질량
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0
Area, mass
0
20
40
60
80
100
120
Distance(mm)
단면적
미소질량

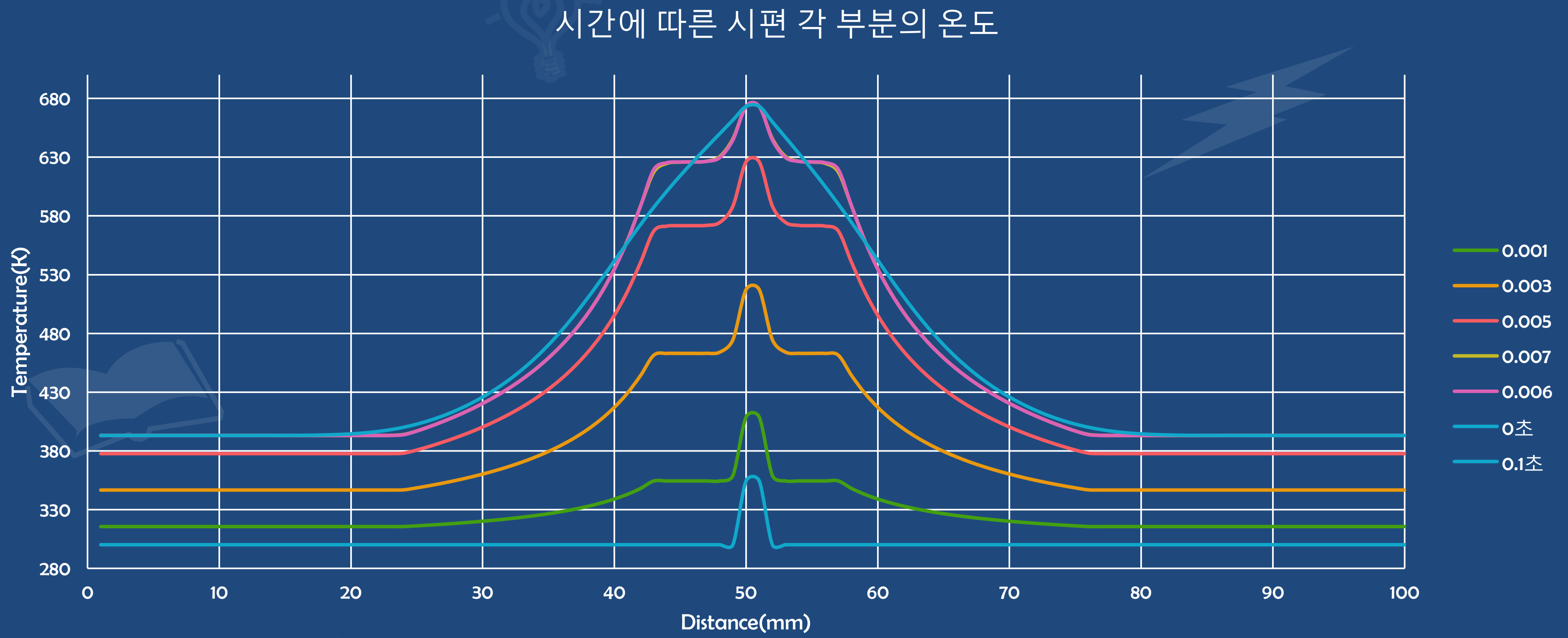


미소 부피
0.0000002
1.8E-07
1.6E-07
1.4E-07
1.2E-07
0.0000001
8E-08
6E-08
4E-08
2E-08
0
Volume(m^3)
0
20
40
60
80
100
120
Distance(mm)

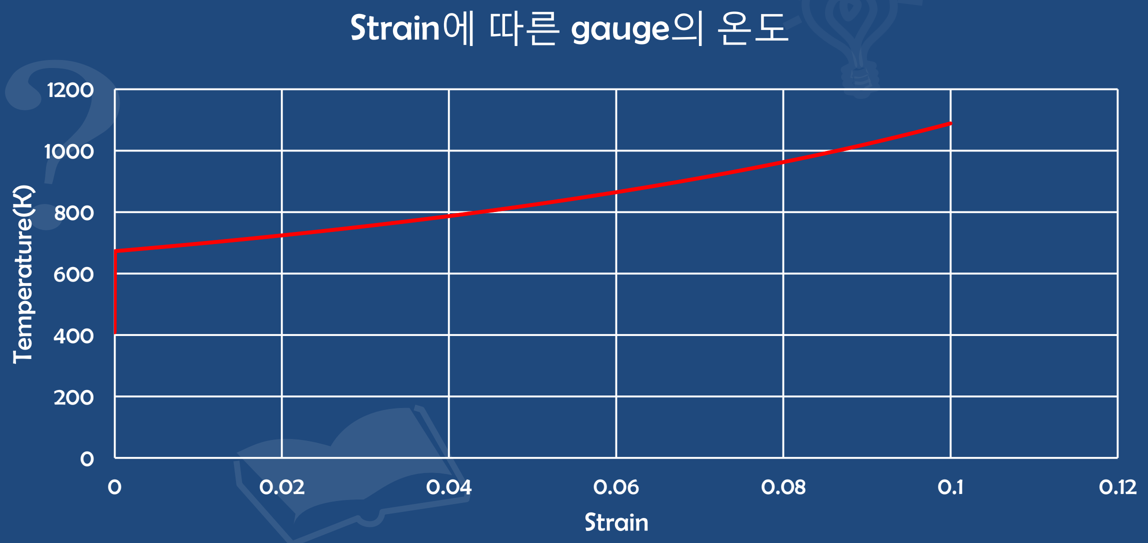


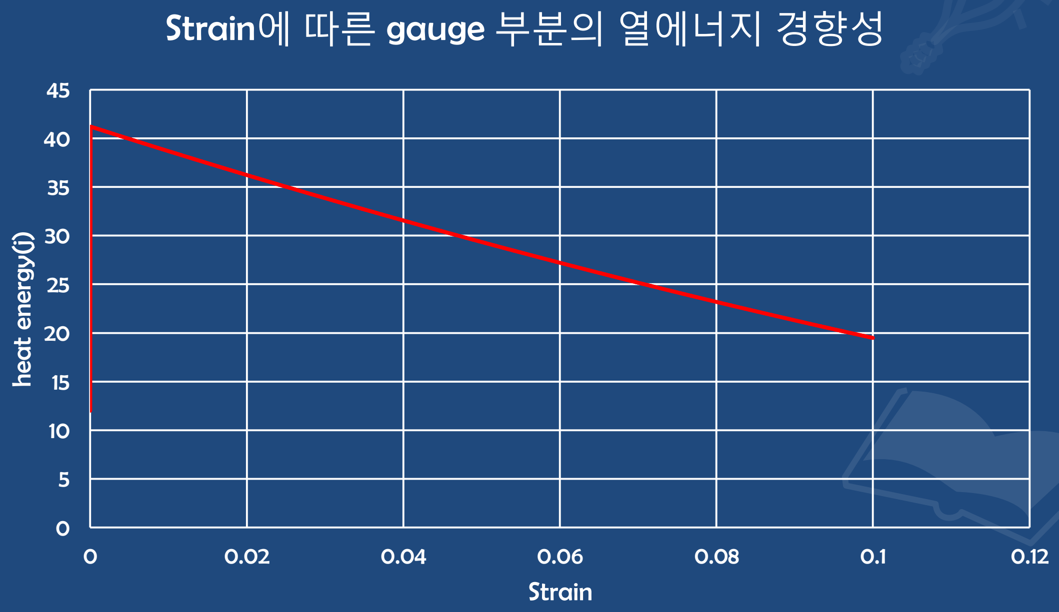
Del_T
60
50
40
30
20
10
0
Temperature(K)
0
20
40
60
80
100
120
Distance(mm)

Result



Cubic spline 결과: 목표 온도 까지 걸리는 시간 =0.00599675초

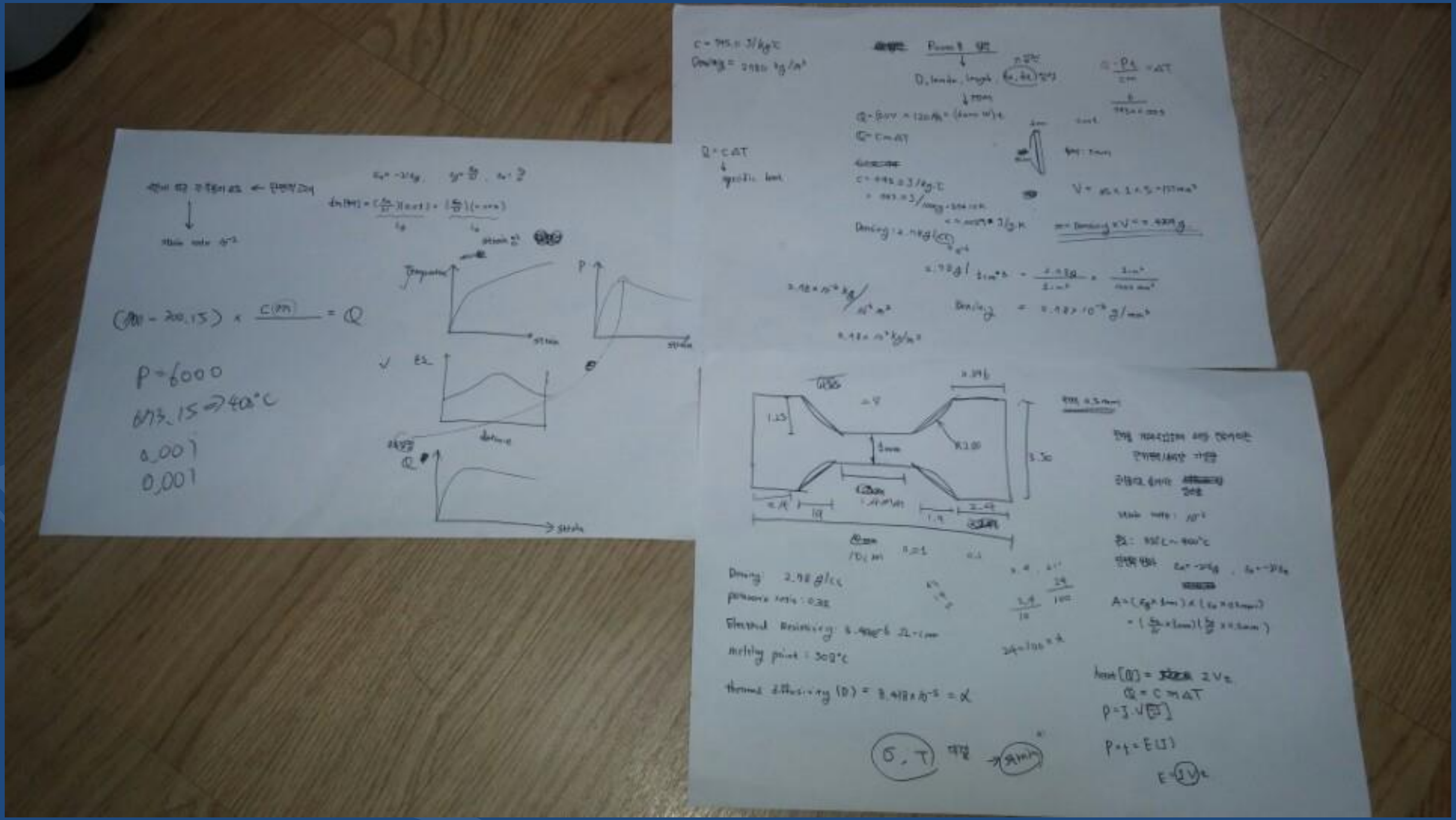




Poisson's ratio에 의한 단면적 감소의 효과가 더욱 dominant

Conclusion

- FDM 내부 알고리즘에 추가적 코딩을 더해 원하는 데이터를 뽑을 수 있다.
- 온도 도달 시간이 대략적으로 0.00599 초 임을 파악!
- Resistance heating tensile 시, 단면적 감소 비율이 열 에너지 손실 비율보다 gauge 온도 경향에 dominan한 경향을 가짐을 파악!
  - 실제 실험 시 strain rate를 더욱 낮게 잡을 필요가 있다!



직접 문제를 design, 설계 해보고 제 생각을 구현할 수 있다는 게 정말 재미 있었습니다!
한 학기 동안 정말 감사했습니다 교수님~!