소재수치해석 Final

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1. Problem

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

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

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

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

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

- 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

$${}^oG_{Fe:Va} = {}^oG^{fcc}_{Fe}$$

$${}^oG_{Si:Va} = {}^oG^{Diamond}_{Si} + 51000 - 21.8\cdot T$$

$${}^oG_{Fe:C} = {}^oG^{fcc}_{Fe} + {}^oG^{graphite}_{C} + 77207 - 15.877\cdot T$$

$${}^oG_{Si:C} = {}^oG^{Diamond}_{Si} + {}^oG^{graphite}_{C} - 20510 + 38.7\cdot T$$

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

$$L_{Fe,Si:C} = +143219.9 + 39.31\cdot T - 216320.5(y_{Fe} - y_{Si})$$

$$L_{Fe:C,Va} = -34671$$

$$L_{Si:C,Va} = 0$$

2. Theory

$$\mu_{Fe} = G_m + (1 - y_{Fe})\frac{dG_m}{dy_{Fe}} = G_m - y_{Si}\frac{dG_m}{dy_{Si}}$$

$$\mu_{Si} = G_m + (1 - y_{Si})\frac{dG_m}{dy_{Si}}$$

$$\mu_C = \frac{dG_m}{dy_C}$$

$$D_{CC} = y_C y_{va}\Omega_C\frac{d\mu_C}{dy_C} = y_C(1 - y_C)\Omega_C\frac{d^2G_m}{dy_C^2}$$

$$D_{CSi} = y_C y_{va}\Omega_C\frac{d\mu_C}{dy_{Si}} = y_C(1 - y_C)\Omega_C\frac{d^2G_m}{dy_C dy_{Si}}$$

$$D_{SiC} = y_{Si}(1 - y_{Si})[\Omega_{Si}\left(\frac{dG_m}{dy_C} + (1 - y_{Si})\frac{d^2G_m}{dy_C dy_{Si}}\right) + \Omega_{Fe}\left(\frac{dG_m}{dy_C} - y_{Si}\frac{d^2G_m}{dy_C dy_{Si}}\right)]$$

$$D_{SiSi} = y_{Si}(1 - y_{Si})[\Omega_{Si}(1 - y_{Si})\frac{d^2G_m}{dy_{Si}^2} - \Omega_{Fe} y_{Si}\frac{d^2G_m}{dy_{Si}^2}]$$

$$\boxed{\begin{aligned} J_C &= -y_C y_{Va}\Omega_C\left(\frac{d\mu_C}{dy_C}\right)\nabla C_C - y_C y_{Va}\Omega_C\left(\frac{d\mu_C}{dy_M}\right)\nabla C_M \\ &= -D_{CC}\nabla C_C - D_{CM}\nabla C_M \\ J_M &= -\left(y_{Fe}y_M\Omega_M\frac{d\mu_M}{dy_C} - y_M y_{Fe}\Omega_{Fe}\frac{d\mu_{Fe}}{dy_C}\right)\nabla C_C \\ &\quad -\left(y_{Fe}y_M\Omega_M\frac{d\mu_M}{dy_M} - y_M y_{Fe}\Omega_{Fe}\frac{d\mu_{Fe}}{dy_M}\right)\nabla C_M \\ &= -D_{MC}\nabla C_C - D_{MM}\nabla C_M \end{aligned}}$$

2. Theory

$$\mu_{Fe} = G_m + (1 - y_{Fe})\frac{dG_m}{dy_{Fe}} = G_m - y_{Si}\frac{dG_m}{dy_{Si}}$$

$$\mu_{Si} = G_m + (1 - y_{Si})\frac{dG_m}{dy_{Si}}$$

$$\mu_C = \frac{dG_m}{dy_C}$$

$$D_{CC} = y_C y_{va}\Omega_C\frac{d\mu_C}{dy_C} = y_C(1 - y_C)\Omega_C\boxed{\frac{d^2G_m}{dy_C^2}}$$

$$D_{CSi} = y_C y_{va}\Omega_C\frac{d\mu_C}{dy_{Si}} = y_C(1 - y_C)\Omega_C\boxed{\frac{d^2G_m}{dy_C dy_{Si}}}$$

$$D_{SiC} = y_{Si}(1 - y_{Si})\left[\Omega_{Si}\left(\boxed{\frac{dG_m}{dy_C}} + (1 - y_{Si})\boxed{\frac{d^2G_m}{dy_C dy_{Si}}}\right) + \Omega_{Fe}\left(\boxed{\frac{dG_m}{dy_C}} - y_{Si}\boxed{\frac{d^2G_m}{dy_C dy_{Si}}}\right)\right]$$

$$D_{SiSi} = y_{Si}(1 - y_{Si})\left[\Omega_{Si}(1 - y_{Si})\boxed{\frac{d^2G_m}{dy_{Si}^2}} - \Omega_{Fe} y_{Si}\boxed{\frac{d^2G_m}{dy_{Si}^2}}\right]$$

$$\boxed{\begin{aligned}
J_C &= -y_C y_{Va}\Omega_C\left(\frac{d\mu_C}{dy_C}\right)\nabla C_C - y_C y_{Va}\Omega_C\left(\frac{d\mu_C}{dy_M}\right)\nabla C_M \\
&= -D_{CC}\nabla C_C - D_{CM}\nabla C_M \\
J_M &= -\left(y_{Fe}y_M\Omega_M\frac{d\mu_M}{dy_C} - y_M y_{Fe}\Omega_{Fe}\frac{d\mu_{Fe}}{dy_C}\right)\nabla C_C \\
&\quad -\left(y_{Fe}y_M\Omega_M\frac{d\mu_M}{dy_M} - y_M y_{Fe}\Omega_{Fe}\frac{d\mu_{Fe}}{dy_M}\right)\nabla C_M \\
&= -D_{MC}\nabla C_C - D_{MM}\nabla C_M
\end{aligned}}$$

2. Theory

$$\frac{dG_m}{dy_{Si}} = (1-y_C)\cdot\left(-G^0_{Fe:Va} + G^0_{Si:Va}\right) + y_C\cdot\left(-G^0_{Fe:C} + G^0_{Si:C}\right) + RT\left(-\ln(1-y_{Si}) + \ln y_{Si}\right)$$

$$+ (1-2y_{Si})(1-y_C)\cdot L_1 + (1-y_{Si})\cdot y_{Si}(1-y_C)\cdot\frac{dL_1}{dy_{Si}}$$

$$+ (1-2y_{Si})\cdot y_C\, L_2 + (1-y_{Si})\, y_{Si}\cdot y_C\,\frac{dL_2}{dy_{Si}} + (1-y_C)\, y_C\cdot(-L_3 + L_4)$$

$$\frac{d^2G_m}{dy_{Si}^2} = \frac{RT}{1-y_{Si}} + \frac{RT}{y_{Si}} - 2(1-y_C)\cdot L_1 + 2\cdot(1-2y_{Si})(1-y_C)\cdot\frac{dL_1}{dy_{Si}}$$

$$+ (1-y_{Si})\, y_{Si}\,(1-y_C)\cdot\frac{d^2L_1}{dy_{Si}^2} - 2\times y_C\times L_2 + 2\cdot(1-2y_{Si})\cdot y_C\,\frac{dL_2}{dy_{Si}}$$

2. Theory

$$\frac{d^2G_m}{dy_{si}dy_c} = G^0_{Fe:Va} - G^0_{Si:Va} - G^0_{Fe:C} + G^0_{Si:C} + (1-2y_{Si})\cdot(-L_1+L_2) + (1-2y_c)(-L_3+L_4) + y_{Si}(1-y_{Si})\left(-\frac{dL_1}{dy_{Si}} + \frac{dL_2}{dy_{Si}}\right)$$

$$\frac{dG_m}{dy_c} = (1-y_{Si})(-G^0_{Fe:Va} + G^0_{Fe:C}) + y_{Si}(-G^0_{Si:Va} + G^0_{Si:C}) + RT(-\ln(1-y_c) + \ln y_c) + (1-y_{Si})\cdot y_{Si}(-L_1+L_2) + (1-y_{Si})(1-2y_c)(L_3+L_4)$$

$$\frac{d^2G_m}{dy_c^2} = \frac{RT}{1-y_c} + \frac{RT}{y_c} - 2(1-y_{Si})L_3 - 2\cdot y_{Si}L_4.$$

2. Theory

$$\frac{\partial C_C}{\partial t} = \frac{\partial}{\partial x}\left[D_{CC}\frac{\partial C_C}{\partial x} + D_{CSi}\frac{\partial C_{Si}}{\partial x}\right]$$

$$\frac{\partial C_{Si}}{\partial t} = \frac{\partial}{\partial x}\left[D_{SiC}\frac{\partial C_C}{\partial x} + D_{SiSi}\frac{\partial C_{Si}}{\partial x}\right]$$

$$\frac{\partial C_i}{\partial t} = \frac{C_i^{j+1} - C_i^j}{\Delta t}$$

$$\frac{\partial}{\partial x}\left[D_i\frac{\partial C_i}{\partial x}\right] = \frac{1}{\Delta x}\left[\sqrt{D_{i+1}D_i}\,\frac{C_{i+1}^j - C_i^j}{\Delta x} - \sqrt{D_i D_{i-1}}\,\frac{C_i^j - C_{i-1}^j}{\Delta x}\right]$$

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for (i = 1; i < section-1; i++)
{
    yc_f[i] = yc_i[i];
    yc_f[i] += dtdx*sqrt(D_CC(ysi_i[i + 1], yc_i[i + 1], T)*D_CC(ysi_i[i], yc_i[i], T))*(yc_i[i + 1] - yc_i[i]);
    yc_f[i] += dtdx*-sqrt(D_CC(ysi_i[i], yc_i[i], T)*D_CC(ysi_i[i - 1], yc_i[i - 1], T))*(yc_i[i] - yc_i[i - 1]);
    yc_f[i] += dtdx*sqrt(D_CSi(ysi_i[i + 1], yc_i[i + 1], T)*D_CSi(ysi_i[i], yc_i[i], T))*(ysi_i[i + 1] - ysi_i[i]);
    yc_f[i] += dtdx*-sqrt(D_CSi(ysi_i[i], yc_i[i], T)*D_CSi(ysi_i[i - 1], yc_i[i - 1], T))*(ysi_i[i] - ysi_i[i - 1]);
    ysi_f[i] = ysi_i[i];
    ysi_f[i] += dtdx*sqrt(D_SiC(ysi_i[i + 1], yc_i[i + 1], T)*D_SiC(ysi_i[i], yc_i[i], T))*(yc_i[i + 1] - yc_i[i]);
    ysi_f[i] += dtdx*-sqrt(D_SiC(ysi_i[i], yc_i[i], T)*D_SiC(ysi_i[i - 1], yc_i[i - 1], T))*(yc_i[i] - yc_i[i - 1]);
    ysi_f[i] += dtdx*sqrt(D_SiSi(ysi_i[i + 1], yc_i[i + 1], T)*D_SiSi(ysi_i[i], yc_i[i], T))*(ysi_i[i + 1] - ysi_i[i]);
    ysi_f[i] += dtdx*-sqrt(D_SiSi(ysi_i[i], yc_i[i], T)*D_SiSi(ysi_i[i - 1], yc_i[i - 1], T))*(ysi_i[i] - ysi_i[i - 1]);
}
```

3. Algorithm

dt, dx 설정, Initial condition 입력

각 시편 길이 = 50mm, dx = 0.1mm, dt = 60s, total time step = 18720

왼쪽 시편 초기 조성: Fe – 3.8wt% Si – 0.478wt% C

오른쪽 시편 초기 조성: Fe – 0.01wt% Si – 0.441wt% C

↓

Weight percent를 y fraction으로 변환

$$x_i = \frac{w_i}{M_i} / \left(\sum_i \frac{w_i}{M_i}\right) \qquad y_{si} = \frac{x_{si}}{x_{si} + x_{Fe}} \qquad y_C = \frac{x_C}{x_C + x_{Va}} = \frac{x_C}{x_{si} + x_{Fe}}$$

↓

FDM 계산

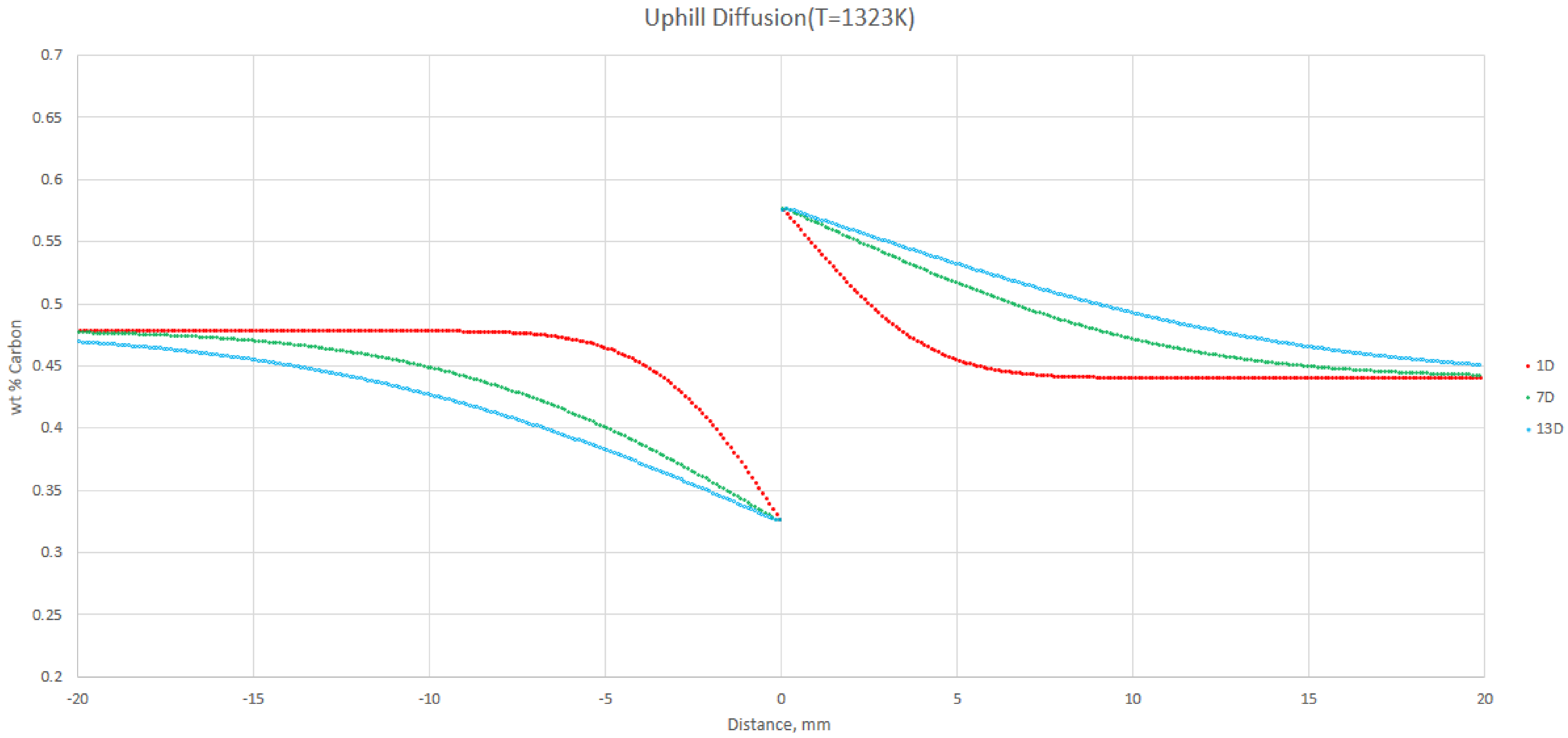
$$y_{i,j+1}^{C} = y_{i,j}^{C} + \frac{\Delta t}{(\Delta x)^2}\Big[\sqrt{D_{i+1}^{CC} D_i^{CC}}\left(y_{i+1,j}^{C} - y_{i,j}^{C}\right) - \sqrt{D_i^{CC} D_{i-1}^{CC}}\left(y_{i,j}^{C} - y_{i-1,j}^{C}\right)$$
$$+ \sqrt{D_{i+1}^{CSi} D_i^{CSi}}\left(y_{i+1,j}^{Si} - y_{i,j}^{Si}\right) - \sqrt{D_i^{CSi}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

↓

y fraction을 weight percent로 변환 후 출력

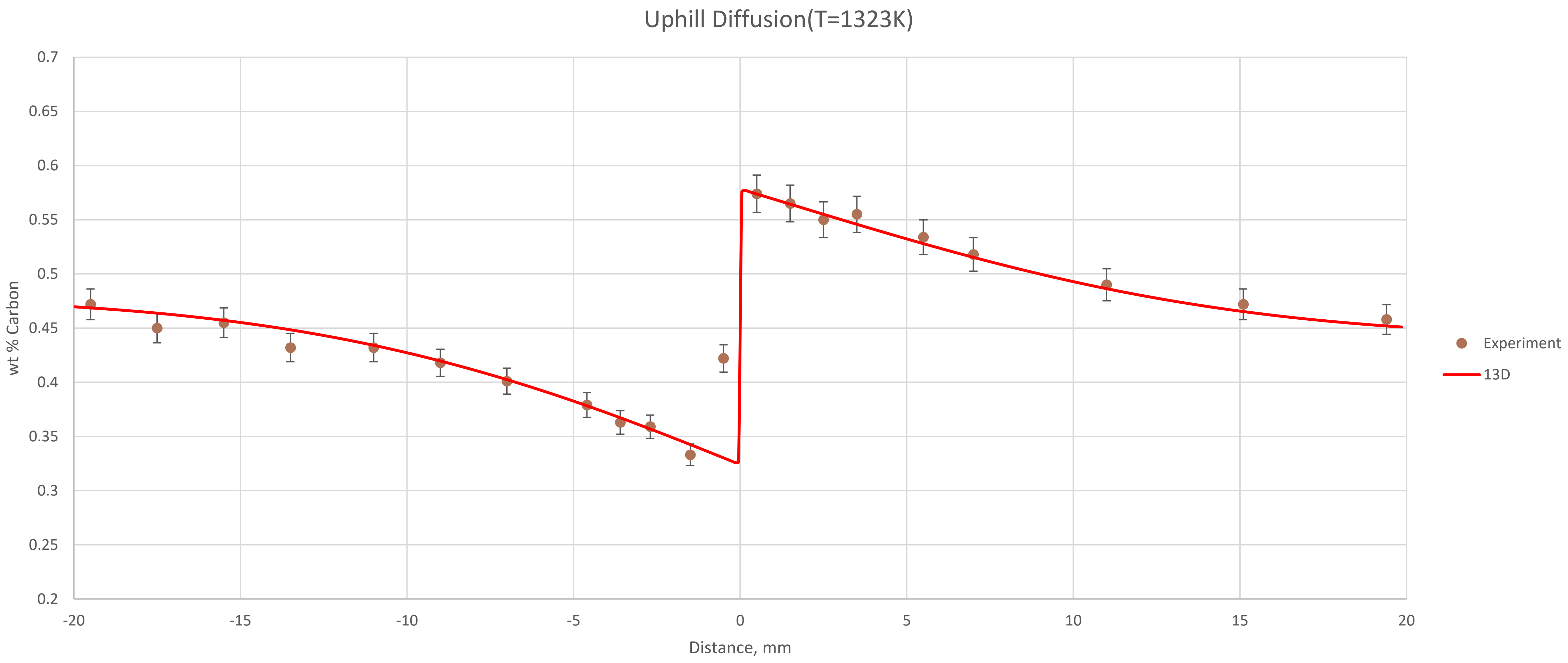
$$x_C = \frac{y_c}{1 + y_c} \qquad x_{si} = y_{Si}(1 - x_c) \qquad w_i = x_i M_i / \left(\sum_i x_i M_i\right)$$

4. Result



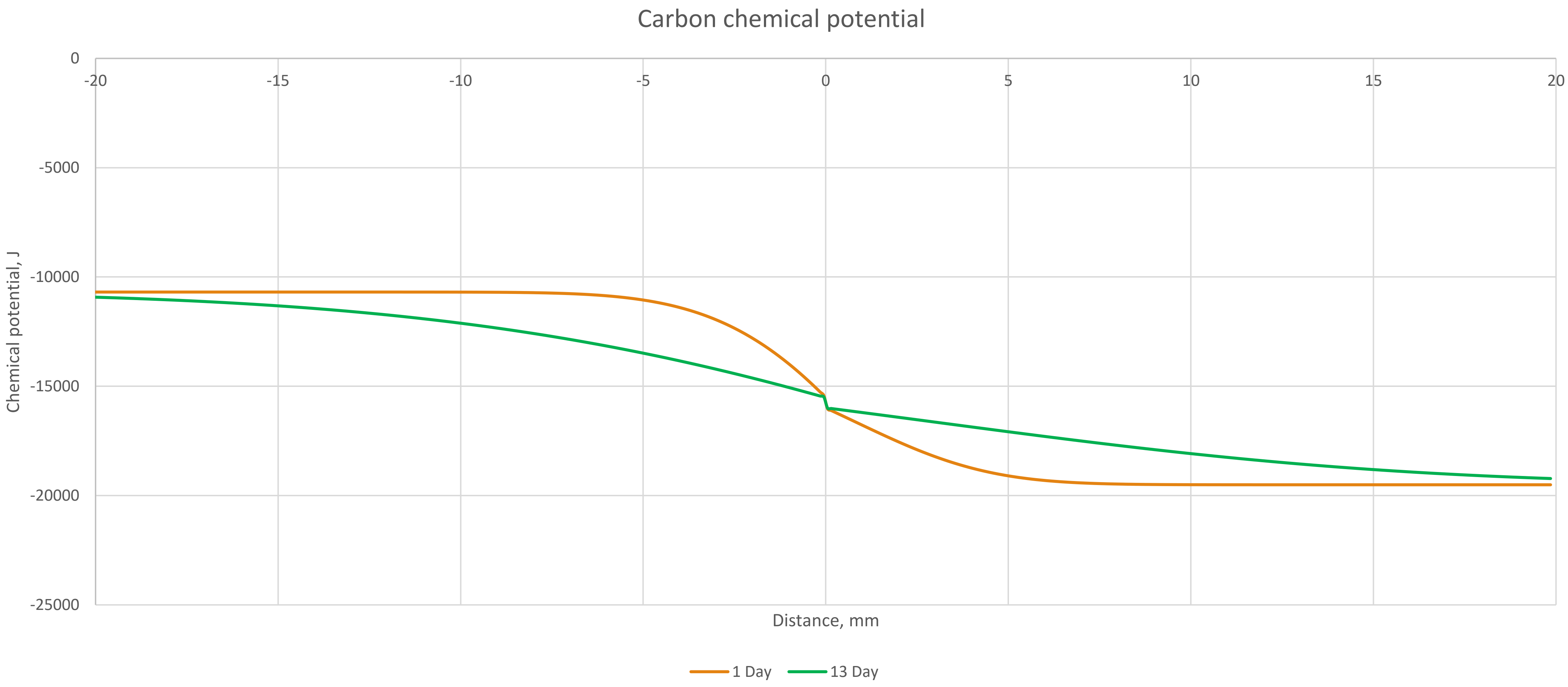
Uphill Diffusion(T=1323K)
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
wt % Carbon
-20
-15
-10
-5
0
5
10
15
20
Distance, mm
1D
7D
13D

4. Result



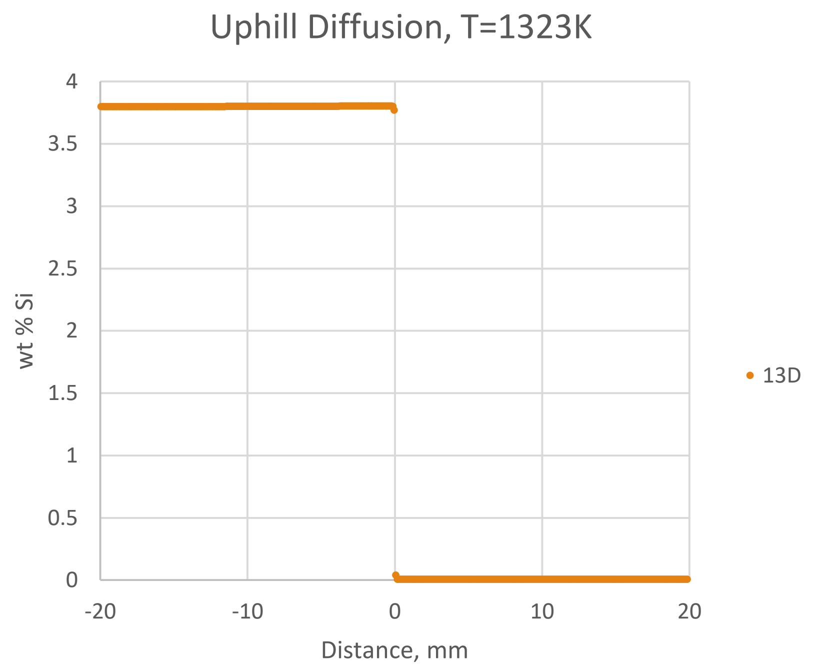
실험 데이터에 3% 오차막대를 넣어서 비교해본 결과 실험 데이터와 시뮬레이션 데이터가 거의 비슷하다.

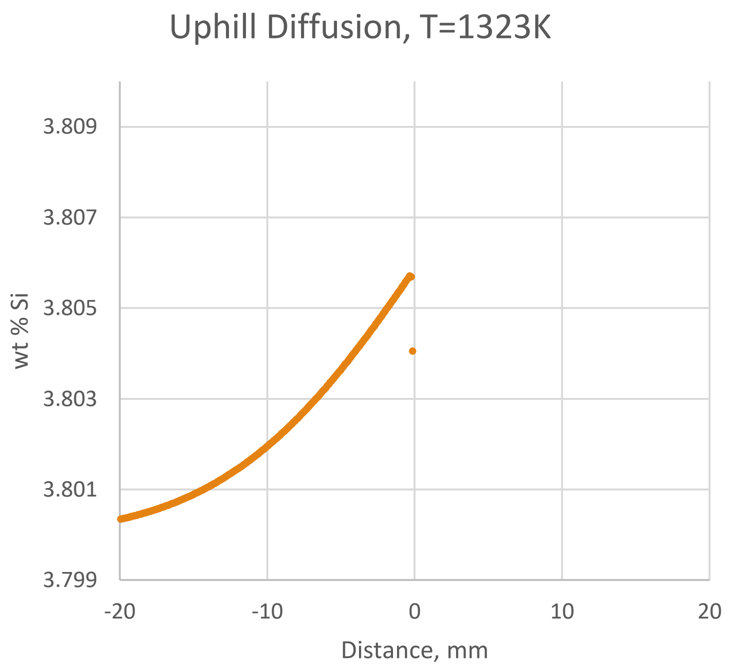
4. Result

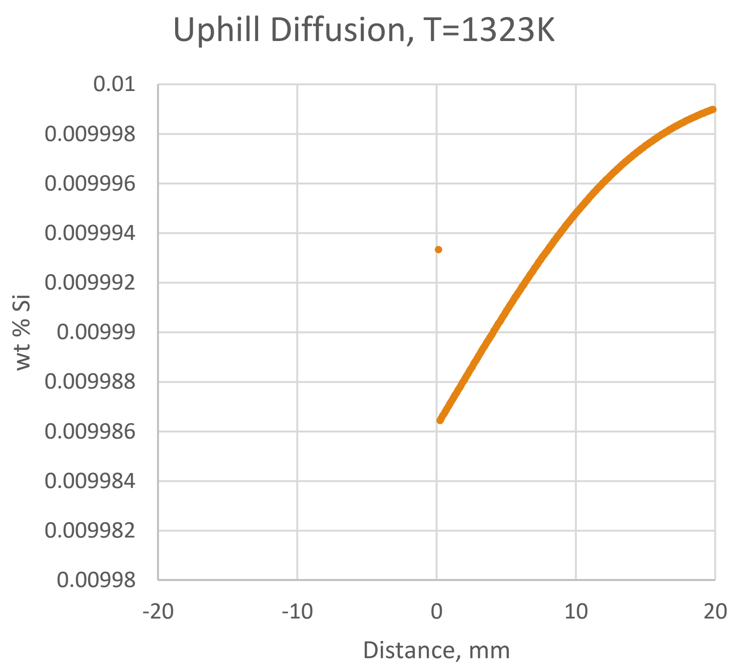


Carbon chemical potential
0
-5000
-10000
-15000
-20000
-25000
-20
-15
-10
-5
0
5
10
15
20
Chemical potential, J
Distance, mm
1 Day
13 Day

4. Result







Si 역시 uphill diffusion 현상을 보임.

5. Conclusion

1. 코딩을 통해서 Darken’s uphill diffusion을 직접 시뮬레이션해 볼 수 있었다.

2. 시간 계산 step을 크게 하였더니, 프로그램이 결과를 내는데 5분 정도로 시간이 오래 걸렸다.

3. Diffusion이 단순히 농도 gradient에 비례하지 않는 것을 확인할 수 있었다.

4. Si는 substitutional diffusion 이므로 C에 비해 diffusion이 잘 일어나지 않는다.