8. 편미분 방정식 (Partial Differential Equation)

1. 서론

편미분 방정식의 종류

자연과학에서 가장 널리 취급되는 편미분방정식: 2 차원 2 계 방정식

$$a\frac{\partial^2 u}{\partial x^2}+b\frac{\partial^2 u}{\partial x\partial y}+c\frac{\partial^2 u}{\partial y^2}+d\frac{\partial u}{\partial x}+e\frac{\partial u}{\partial y}+fu+g=0$$

- $b^2-4ac > 0$ 일 때: Hyperbolic Partial Differential Equation
  1 차원 파동 방정식

$$\frac{\partial^2 u}{\partial x^2}-\frac{\partial^2 u}{\partial y^2}=0$$

- $b^2-4ac = 0$ 일 때: Parabolic Partial Differential Equation
  1 차원 확산 방정식

$$\frac{\partial u}{\partial t}-\frac{\partial^2 u}{\partial x^2}=0$$

- $b^2-4ac < 0$ 일 때: Elliptic Partial Differential Equation
  2 차원 Laplace 방정식 (우변이 0 이 아니면 Poisson 방정식)

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$$

편미분 방정식은 초기조건과 경계조건을 이용하여 해석한다.

초기/경계 조건의 일반식

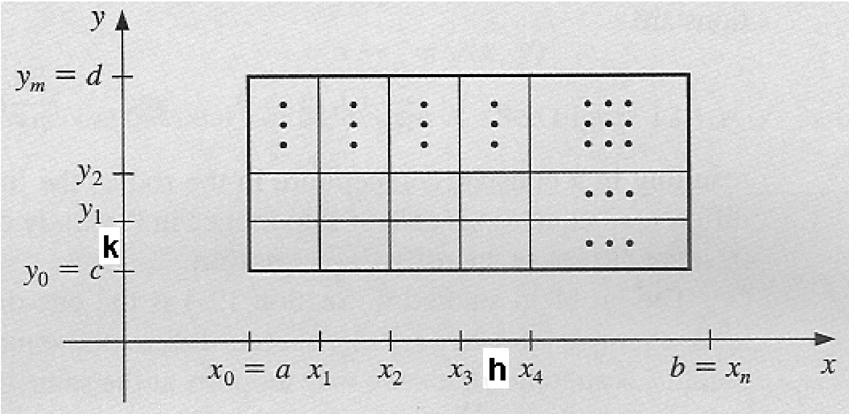
$$\alpha\frac{\partial u}{\partial n}+\beta u=\phi(x,y)$$ (n 은 경계면의 법선)

- $\alpha=0,\ \beta\neq 0$: Dirichlet 조건 (경계면에서 u 가 주어짐)
- $\alpha\neq 0,\ \beta=0$: Neumann 조건 (경계면에서 u 의 편미분이 주어짐)
- $\alpha\neq 0,\ \beta\neq 0$: Cauchy 조건

2. Finite Difference Methods for Elliptic Problems

$$\nabla^2 u(x,y) = \frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) = f(x,y)$$ on R={(x,y)| a<x<b, c<y<d}

with $u(x,y) = g(x,y)$ for (x,y) ∈ S where S denotes the boundary pf R.



$$x_i = a + ih \qquad \text{and} \qquad y_j = c + jk$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j) = \frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{h^2} - \frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(\xi_i, y_j)$$

$$\frac{\partial^2 u}{\partial y^2}(x_i, y_j) = \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1})}{k^2} - \frac{k^2}{12}\frac{\partial^4 u}{\partial y^4}(x_i, \eta_j)$$

$$\frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{h^2} + \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1})}{k^2} = f(x_i, y_j) + \frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(\xi_i, y_j) + \frac{k^2}{12}\frac{\partial^4 u}{\partial y^4}(x_i, \eta_j),$$

$$2\left[\left(\frac{h}{k}\right)^2 + 1\right] w_{ij} - (w_{i+1,j} + w_{i-1,j}) - \left(\frac{h}{k}\right)^2 (w_{i,j+1} + w_{i,j-1}) = -h^2 f(x_i, y_j)$$

for each $i = 1, 2, \ldots, n-1$ and $j = 1, 2, \ldots, m-1$, and

$$w_{0j} = g(x_0, y_j), \quad w_{nj} = g(x_n, y_j), \quad w_{i0} = g(x_i, y_0), \quad \text{and} \quad w_{im} = g(x_i, y_m)$$

for each $i = 1, 2, \ldots, n-1$ and $j = 0, 1, \ldots, m$, where w_{ij} approximates $u(x_i, y_j)$.

⇨ (n-1) x (m-1) by (n-1) x (m-1) linear equation system

Example)

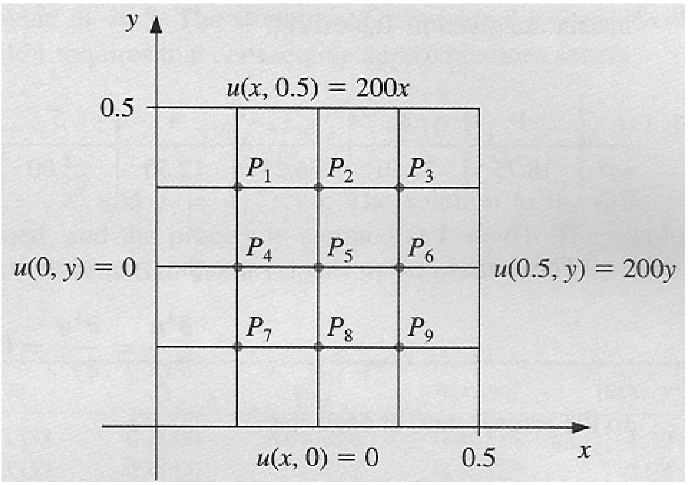
Consider the problem of determining the steady-state heat distribution in a thin square metal plate 0.5 meters on a side. Two adjacent boundaries are held at 0°C, and the heat on the other boundaries increases linearly from 0°C at one corner to 100°C where the sides meet. If we place the sides with the zero boundary conditions along the x- and y-axes, the problem is expressed as

$$\frac{\partial^2 u}{\partial x^2}(x, y) + \frac{\partial^2 u}{\partial y^2}(x, y) = 0,$$

for (x, y) in the set $R = \{(x, y) \mid 0 < x < 0.5;\ 0 < y < 0.5\}$, with the boundary conditions

$$u(0, y) = 0, \quad u(x, 0) = 0, \quad u(x, 0.5) = 200x, \quad u(0.5, y) = 200y.$$

$$4w_{i,j} - w_{i+1,j} - w_{i-1,j} - w_{i,j-1} - w_{i,j+1} = 0,$$



$$\begin{aligned}
P_1:&\quad 4w_1 - w_2 - w_4 = w_{0,3} + w_{1,4},\\
P_2:&\quad 4w_2 - w_3 - w_1 - w_5 = w_{2,4},\\
P_3:&\quad 4w_3 - w_2 - w_6 = w_{4,3} + w_{3,4},\\
P_4:&\quad 4w_4 - w_5 - w_1 - w_7 = w_{0,2},\\
P_5:&\quad 4w_5 - w_6 - w_4 - w_2 - w_8 = 0,\\
P_6:&\quad 4w_6 - w_5 - w_3 - w_9 = w_{4,2},\\
P_7:&\quad 4w_7 - w_8 - w_4 = w_{0,1} + w_{1,0},\\
P_8:&\quad 4w_8 - w_9 - w_7 - w_5 = w_{2,0},\\
P_9:&\quad 4w_9 - w_8 - w_6 = w_{3,0} + w_{4,1},
\end{aligned}$$

w_i = {18.75, 37.50, 56.25, 12.50, 25.00, 37.50, 6.25, 12.50, 18.75}

3. Finite Difference Methods for Parabolic Problems

- Heat or diffusion equation

$$\frac{\partial u}{\partial t}(x,t) = \alpha \ \frac{\partial^2 u}{\partial x^2}(x,t) \qquad \text{for} \quad 0 < x < l \quad \text{and} \quad t > 0$$

subject to the condition

$u(0,t) = u(l,t) = 0$ for $t > 0$

$u(x,0) = f(x)$ for $0 \le x \le l$

set $x_i = i\Delta x$ for i = 0, 1, 2, ⋯, m

$t_j = j\Delta t$ for j = 0, 1, 2, ⋯

$$\frac{\partial u}{\partial t}(x_i,t_j) = \frac{u(x_i,t_j+\Delta t)-u(x_i,t_j)}{\Delta t} - \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_i,\mu_j)$$

$$\frac{\partial^2 u}{\partial x^2}(x_i,t_j) = \frac{u(x_i+\Delta x,t_j)-2u(x_i,t_j)+u(x_i-\Delta x,t_j)}{\Delta x^2} - \frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4}(\xi_i,t_j)$$

$$\frac{w_{i,j+1}-w_{i,j}}{\Delta t} = \alpha \ \frac{w_{i+1,j}-2w_{i,j}+w_{i-1,j}}{\Delta x^2}$$

$$w_{i,j+1} = w_{i,j} + \frac{\alpha\Delta t}{\Delta x^2}(w_{i+1,j}-2w_{i,j}+w_{i-1,j}) = \left(1-2\frac{\alpha\ \Delta t}{\Delta x^2}\right) w_{i,j} + \frac{\alpha\ \Delta t}{\Delta x^2}(w_{i+1,j}+w_{i-1,j})$$

$$A = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \cdots & 0 \\ \lambda & (1-2\lambda) & \lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda \\ 0 & \cdots & 0 & \lambda & (1-2\lambda) \end{bmatrix} \qquad \lambda = \frac{\alpha\Delta t}{\Delta x^2}$$

$$\mathbf{w}^{(0)} = (f(x_1), f(x_2), \ldots, f(x_{m-1}))^t$$

$$\mathbf{w}^{(j)} = (w_{1j}, w_{2j}, \ldots, w_{m-1,j})^t, \quad \text{for each } j = 1, 2, \ldots,$$

$$\mathbf{w}^{(j)} = A\mathbf{w}^{(j-1)}, \quad \text{for each } j = 1, 2, \ldots .$$

⇒ Forward Difference Method (Explicit Method)

Example 1) Consider the heat equation

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) \qquad \text{for} \quad 0 < x < 1 \quad \text{and} \quad t > 0$$

With boundary and initial conditions

$u(0,t) = u(l,t) = 0$ for $t > 0$

$u(x,0) = \sin(\pi x)$ for $0 \le x \le 1$

Exact solution is $u(x,t) = e^{-\pi^2 t} \sin \pi x$

Using FDM 1) with Δx = 0.1 and Δt = 0.0005 (λ = 0.05)

2) with Δx = 0.1 and Δt = 0.01 (λ = 1)

x_i	$u(x_i, 0.5)$	$w_{i,1000}$ $k = 0.0005$	$\lvert u(x_i, 0.5) - w_{i,1000}\rvert$	$w_{i,50}$ $k = 0.01$	$\lvert u(x_i, 0.5) - w_{i,50}\rvert$
0.0	0	0		0	
0.1	0.00222241	0.00228652	6.411×10^{-5}	8.19876×10^{7}	8.199×10^{7}
0.2	0.00422728	0.00434922	1.219×10^{-4}	-1.55719×10^{8}	1.557×10^{8}
0.3	0.00581836	0.00598619	1.678×10^{-4}	2.13833×10^{8}	2.138×10^{8}
0.4	0.00683989	0.00703719	1.973×10^{-4}	-2.50642×10^{8}	2.506×10^{8}
0.5	0.00719188	0.00739934	2.075×10^{-4}	2.62685×10^{8}	2.627×10^{8}
0.6	0.00683989	0.00703719	1.973×10^{-4}	-2.49015×10^{8}	2.490×10^{8}
0.7	0.00581836	0.00598619	1.678×10^{-4}	2.11200×10^{8}	2.112×10^{8}
0.8	0.00422728	0.00434922	1.219×10^{-4}	-1.53086×10^{8}	1.531×10^{8}
0.9	0.00222241	0.00228652	6.511×10^{-5}	8.03604×10^{7}	8.036×10^{7}
1.0	0	0		0	

∴ Stability condition of explicit method: $\dfrac{\alpha \Delta t}{\Delta x^2} \le \dfrac{1}{2}$

● To obtain a more stable method, an implicit method is used.

$$\frac{\partial u}{\partial t}(x_i, t_j) = \frac{u(x_i, t_j) - u(x_i, t_j - \Delta t)}{\Delta t} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_i, \mu_j)$$

$$\frac{w_{i,j} - w_{i,j-1}}{\Delta t} = \alpha \ \frac{w_{i+1,j} - 2w_{i,j} + w_{i-1,j}}{\Delta x^2}$$

$$\left(1 + 2\frac{\alpha \Delta t}{\Delta x^2}\right) w_{i,j} - \frac{\alpha \Delta t}{\Delta x^2}(w_{i+1,j} + w_{i-1,j}) = w_{i,j-1}$$

set $\lambda = \dfrac{\alpha \Delta t}{\Delta x^2}$

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \cdots & 0 \\ -\lambda & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\lambda \\ 0 & \cdots & 0 & -\lambda & (1+2\lambda) \end{bmatrix} \begin{bmatrix} w_{1j} \\ w_{2j} \\ \vdots \\ w_{m-1,j} \end{bmatrix} = \begin{bmatrix} w_{1,j-1} \\ w_{2,j-1} \\ \vdots \\ w_{m-1,j-1} \end{bmatrix}$$

$$\mathbf{A}\mathbf{w}^{(j)} = \mathbf{w}^{(j-1)}$$

Example 2) Solve the same equation as in Example 1 using an implicit method with Δx = 0.1 and Δt = 0.01 (λ = 1)

x_i	$w_{i,50}$	$u(x_i, 0.5)$	$\lvert w_{i,50} - u(x_i, 0.5)\rvert$
0.0	0	0	
0.1	0.00289802	0.00222241	6.756×10^{-4}
0.2	0.00551236	0.00422728	1.285×10^{-3}
0.3	0.00758711	0.00581836	1.769×10^{-3}
0.4	0.00891918	0.00683989	2.079×10^{-3}
0.5	0.00937818	0.00719188	2.186×10^{-3}
0.6	0.00891918	0.00683989	2.079×10^{-3}
0.7	0.00758711	0.00581836	1.769×10^{-3}
0.8	0.00551236	0.00422728	1.285×10^{-3}
0.9	0.00289802	0.00222241	6.756×10^{-4}
1.0	0	0	

● To make the error of order $O(\Delta t^2 + \Delta x^2)$, by averaging the Forward- and Backward-Difference Methods.

$$\frac{w_{i,j+1} - w_{i,j}}{\Delta t} = \alpha \frac{w_{i+1,j} - 2w_{i,j} + w_{i-1,j}}{\Delta x^2}$$

$$\frac{w_{i,j+1} - w_{i,j}}{\Delta t} = \alpha \frac{w_{i+1,j+1} - 2w_{i,j+1} + w_{i-1,j+1}}{\Delta x^2}$$

$$\frac{w_{i,j+1} - w_{i,j}}{\Delta t} = \frac{\alpha}{2}\left[\frac{w_{i+1,j+1} - 2w_{i,j+1} + w_{i-1,j+1}}{\Delta x^2} + \frac{w_{i+1,j} - 2w_{i,j} + w_{i-1,j}}{\Delta x^2}\right]$$

$$A\mathbf{w}^{(j+1)} = B\mathbf{w}^{(j)}$$

Crank-Nicolson Method

$$A = \begin{bmatrix} (1+\lambda) & -\frac{\lambda}{2} & 0 & \cdots & \cdots & 0 \\ -\frac{\lambda}{2} & \ddots & \ddots & \ddots & & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & -\frac{\lambda}{2} \\ 0 & \cdots & \cdots & 0 & -\frac{\lambda}{2} & (1+\lambda) \end{bmatrix} \qquad B = \begin{bmatrix} (1-\lambda) & \frac{\lambda}{2} & 0 & \cdots & \cdots & 0 \\ \frac{\lambda}{2} & \ddots & \ddots & \ddots & & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \frac{\lambda}{2} \\ 0 & \cdots & \cdots & 0 & \frac{\lambda}{2} & (1-\lambda) \end{bmatrix}$$

Example 3) Solve the same equation as in Example 1 using a Crank-Nicolson method with $\Delta x = 0.1$ and $\Delta t = 0.01$ ($\lambda = 1$)

x_i	$w_{i,50}$	$u(x_i, 0.5)$	$\lvert w_{i,50} - u(x_i, 0.5)\rvert$
0.0	0	0	
0.1	0.00230512	0.00222241	8.271×10^{-5}
0.2	0.00438461	0.00422728	1.573×10^{-4}
0.3	0.00603489	0.00581836	2.165×10^{-4}
0.4	0.00709444	0.00683989	2.546×10^{-4}
0.5	0.00745954	0.00719188	2.677×10^{-4}
0.6	0.00709444	0.00683989	2.546×10^{-4}
0.7	0.00603489	0.00581836	2.165×10^{-4}
0.8	0.00438461	0.00422728	1.573×10^{-4}
0.9	0.00230512	0.00222241	8.271×10^{-5}
1.0	0	0	

4. Finite Difference Methods for Hyperbolic Problems

- Wave equation

$$\frac{\partial^2 u}{\partial t^2}(x,t) = c^2 \frac{\partial^2 u}{\partial x^2}(x,t) \qquad \text{for} \quad 0 < x < l \quad \text{and} \quad t > 0$$

subject to the conditions

u(0,t) = u(l,t) = 0 for $t > 0$

u(x,0) = f(x) and ∂u(x,0)/∂t = g(x) for $0 \le x \le l$

set $x_i = i\Delta x$ for i = 0, 1, 2, ⋯, m

$t_j = j\Delta t$ for j = 0, 1, 2, ⋯

$$\frac{\partial^2 u}{\partial t^2}(x_i,t_j) = \frac{u(x_i,t_j+\Delta t) - 2u(x_i,t_j) + u(x_i,t_j-\Delta t)}{\Delta t^2} - \frac{\Delta t^2}{12}\frac{\partial^4 u}{\partial t^4}(x_i,\mu_j)$$

$$\frac{\partial^2 u}{\partial x^2}(x_i,t_j) = \frac{u(x_i+\Delta x,t_j) - 2u(x_i,t_j) + u(x_i-\Delta x,t_j)}{\Delta x^2} - \frac{\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4}(\xi_i,t_j)$$

$$\frac{w_{i,j+1} - 2w_{i,j} + w_{i,j-1}}{\Delta t^2} = c^2 \frac{w_{i+1,j} - 2w_{i,j} + w_{i-1,j}}{\Delta x^2}$$

$$w_{i,j+1} = 2(1-\lambda^2)w_{i,j} + \lambda^2(w_{i+1,j} + w_{i-1,j}) - w_{i,j-1}, \qquad \lambda^2 = \frac{c^2\Delta t^2}{\Delta x^2}$$

This equation holds for each $i = 1, 2, \ldots, (m-1)$ and $j = 1, 2, \ldots$. The boundary conditions give

$$w_{0j} = w_{mj} = 0, \quad \text{for each } j = 1, 2, 3, \ldots,$$

and the initial condition implies that

$$w_{i0} = f(x_i), \quad \text{for each } i = 1, 2, \ldots, m-1.$$

$$\begin{bmatrix} w_{1,j+1} \\ w_{2,j+1} \\ \vdots \\ w_{m-1,j+1} \end{bmatrix} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 & \cdots & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda^2 \\ 0 & \cdots & 0 & \lambda^2 & 2(1-\lambda^2) \end{bmatrix} \begin{bmatrix} w_{1,j} \\ w_{2,j} \\ \vdots \\ w_{m-1,j} \end{bmatrix} - \begin{bmatrix} w_{1,j-1} \\ w_{2,j-1} \\ \vdots \\ w_{m-1,j-1} \end{bmatrix}$$

- A small problem arises when computing values for j=1 because information at j=−1 is necessary.

$$w_{i,j+1} = 2(1-\lambda^2)w_{i,j} + \lambda^2(w_{i+1,j} + w_{i-1,j}) - w_{i,j-1}$$

u values at j=−1 (t=−Δt) can be estimated without losing accuracy as follows:

$$\frac{\partial u}{\partial t}(x_i,0) = \frac{u(x_i,t_1)-u(x_i,t_{-1})}{2\Delta t} - \frac{\Delta t^2}{6}\frac{\partial^3 u}{\partial t^3}(x_i,\mu_0) = g(x_i)$$

$$w_{i,-1} = w_{i,1} - 2\Delta t \cdot g(x_i)$$

$$w_{i,1} = 2(1-\lambda^2)f(x_i) + \lambda^2(f(x_{i+1}) + f(x_{i-1})) - (w_{i,1} - 2\Delta t \cdot g(x_i))$$

$$w_{i,1} = (1-\lambda^2)f(x_i) + \frac{\lambda^2}{2}f(x_{i+1}) + \frac{\lambda^2}{2}f(x_{i-1}) + \Delta t \cdot g(x_i)$$

j = 1 일 때 값들을 별도로 먼저 계산하고, j = 2 부터 iteration.
Perform the calculation separately when j = 1, then do the iteration from j = 2.

Example 4)

Consider the hyperbolic problem

$$\frac{\partial^2 u}{\partial t^2}(x,t) - 4\frac{\partial^2 u}{\partial x^2}(x,t) = 0, \quad \text{for } 0 < x < 1 \quad \text{and} \quad 0 < t,$$

with boundary conditions

$$u(0,t) = u(1,t) = 0, \quad \text{for } 0 < t,$$

and initial conditions

$$u(x,0) = 2\sin(3\pi x), \quad 0 \le x \le 1, \quad \text{and} \quad \frac{\partial u}{\partial t}(x,0) = -12\sin(2\pi x), \quad \text{for } 0 \le x \le 1.$$

Find the solution at t = 1

Exact solution:

$$u(x,t) = 2\cos(6\pi t)\sin(3\pi x) - \frac{3}{\pi}\sin(4\pi t)\sin(2\pi x).$$

Using FDM with Δx = 0.1 and Δt = 0.05 (λ = 1)

x_i	$w_{i,20}$
0.0	0.0000000000
0.1	1.618033989
0.2	1.902113033
0.3	0.618033989
0.4	−1.175570505
0.5	−2.0000000000
0.6	−1.175570505
0.7	0.618033989
0.8	1.902113033
0.9	1.618033989
1.0	0.0000000000

Problem) Consider injection of an alloying element B in a metallic matrix A. The initial composition of B in A is 0.01. Injection is carried out by maintaining the surface composition of B to be 0.05. The diffusion coefficient of B in A is 4.529×10^{-7} exp[-147723(J)/RT] (m^2/s). The injection temperature is between 1173K and 1473K. Injection distance is defined to be the distance from the surface of a point where the composition of B is half of the target value (0.03). Perform the followings:

(a) How does the injection distance depend on injection time?
(b) How does the injection distance depend on temperature?
(c) How can you determine the activation energy for the reaction, and what is it?

Hint:

from $f = K\cdot t^n$ or $f = 1 - \exp(-K\cdot t^n)$

$$\because\ Q^{reac} = R\cdot\frac{\partial(\ln t_f)}{\partial(1/T)}$$

ex) for a diffusion controlled reaction, $t_f \propto 1/D$

$$D = D_o\cdot exp\ (-Q^{diff}/RT)$$

$$Q^{reac} = R\cdot\frac{\partial(\ln 1/D)}{\partial(1/T)} = -R\frac{\partial(-Q^{diff}/RT)}{\partial(1/T)} = Q^{diff}$$