

Equations

Karolis Petrauskas

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Abstract

Mathematical part of the solvers.

1 Implicit 2D solver in the cartesian and cylindrical coordinate systems

1.1 Mathematical model

Lets define the following symbols. S is the substance concentration in time and two-dimensional space and R is a speed of the reaction. Generic equation, that governs processes inside of area is:

$$\frac{\partial S}{\partial t} = D\Delta S + R. \quad (1)$$

Here Δ is the Laplace operator. It has different forms in the different coordinate system.

1.1.1 Diffusion

In the cartesian coordinate system $S = S(x, y, t)$ and $R = R(x, y, t)$.

$$\Delta S = \frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2}. \quad (2)$$

In the cylindrical (r,z plane) coordinate system $S = S(r, z, t)$ and $R = R(r, z, t)$.

$$\Delta S = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{\partial^2 f}{\partial z^2}. \quad (3)$$

1.1.2 Reactions

Michaelis-menten reaction:

$$R_{mm} = \langle V_{max}, K_M, S, P \rangle \quad (4)$$

$$R = \begin{cases} -\frac{V_{max}S}{K_M+S} & \text{in equation for substrate } S, \\ +\frac{V_{max}S}{K_M+S} & \text{in equation for product } P. \end{cases} \quad (5)$$

ReductionOxidation reaction:

$$R_{ro} = \langle k, S_{s_1}, S_{s_2}, S_{p_1}, S_{p_2} \rangle \quad (6)$$

$$R = - \sum_{R_{ro}: S \in \{S_{s_1}, S_{s_2}\}} k S_{s_1} S_{s_2} + \sum_{R_{ro}: S \in \{S_{p_1}, S_{p_2}\}} k S_{s_1} S_{s_2} \quad (7)$$

1.1.3 Bounds

Constant condition:

$$S(x, y, t) = C, \quad (x, y) \in \Gamma. \quad (8)$$

Non-leakage (wall) condition:

$$\left. \frac{\partial S}{\partial n} \right|_{\Gamma} = 0. \quad (9)$$

Merge condition:

$$D_A \left. \frac{\partial S_A}{\partial n} \right|_{\Gamma} = D_B \left. \frac{\partial S_B}{\partial n} \right|_{\Gamma}. \quad (10)$$

1.2 Finite differences

The partial derivate from (1) by time is aproximated as follows:

$$\frac{\partial S}{\partial t} \approx \frac{S_{i,j,k} - S_{i,j,k-1}}{\tau} \quad (11)$$

The Laplace operator, formulated in the cartesian coordinate system (2) is aproximated as follows:

$$\begin{aligned} \frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2} &\approx \\ &\approx \frac{S_{i+1,j,k} - 2S_{i,j,k} + S_{i-1,j,k}}{g^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\ &= -2 \frac{g^2 + h^2}{g^2 h^2} S_{i,j,k} + \frac{1}{g^2} S_{i+1,j,k} + \frac{1}{g^2} S_{i-1,j,k} + \frac{1}{h^2} S_{i,j+1,k} + \frac{1}{h^2} S_{i,j-1,k} \end{aligned} \quad (12)$$

Cylindrical coordinate system, (r, z) plane. $S = S(r, z, t)$. Case one – non simetrical by inner r . Note that $r_{i+1} = r_i + g$.

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial S}{\partial r} \right) + \frac{\partial^2 S}{\partial z^2} &\approx \\ &\approx \frac{1}{r} \frac{\partial}{\partial r} \left(r_i \frac{S_{i,j,k} - S_{i-1,j,k}}{g} \right) + \frac{\partial^2 S}{\partial z^2} \approx \\ &\approx \frac{r_{i+1} \frac{S_{i+1,j,k} - S_{i,j,k}}{g} - r_i \frac{S_{i,j,k} - S_{i-1,j,k}}{g}}{r_i g} + \frac{\partial^2 S}{\partial z^2} \approx \\ &\approx \frac{r_{i+1} S_{i+1,j,k} - (r_{i+1} + r_i) S_{i,j,k} + r_i S_{i-1,j,k}}{r_i g^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\ &= \frac{(r_i + g) S_{i+1,j,k} - (2r_i + g) S_{i,j,k} + r_i S_{i-1,j,k}}{r_i g^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\ &= -\frac{2(h^2 + g^2) r_i + g h^2}{r_i g^2 h^2} S_{i,j,k} + \frac{r_i + g}{r_i g^2} S_{i+1,j,k} + \frac{1}{g^2} S_{i-1,j,k} + \frac{1}{h^2} S_{i,j+1,k} + \frac{1}{h^2} S_{i,j-1,k} \end{aligned} \quad (13)$$

Case two – symmetrical by inner r . Note that $r_{i+1/2} = r_i + \frac{g}{2}$ and $r_{i-1/2} = r_i - \frac{g}{2}$. The difference from the previous case is in the second equation, here we replaced r with $r_{i-1/2}$ instead of r_i .

$$\begin{aligned}
& \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial S}{\partial r} \right) + \frac{\partial^2 S}{\partial z^2} \approx \\
& \approx \frac{1}{r} \frac{\partial}{\partial r} \left(r_{i-1/2} \frac{S_{i,j,k} - S_{i-1,j,k}}{g} \right) + \frac{\partial^2 S}{\partial z^2} \approx \\
& \approx \frac{r_{i+1/2} \frac{S_{i+1,j,k} - S_{i,j,k}}{g} - r_{i-1/2} \frac{S_{i,j,k} - S_{i-1,j,k}}{g}}{r_i g} + \frac{\partial^2 S}{\partial z^2} \approx \\
& \approx \frac{r_{i+1/2} S_{i+1,j,k} - (r_{i+1/2} + r_{i-1/2}) S_{i,j,k} + r_{i-1/2} S_{i-1,j,k}}{r_i g^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
& = \frac{(r_i + \frac{g}{2}) S_{i+1,j,k} - 2r_i S_{i,j,k} + (r_i - \frac{g}{2}) S_{i-1,j,k}}{r_i g^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
& = -2 \frac{g^2 + h^2}{g^2 h^2} S_{i,j,k} + \frac{r_i + \frac{g}{2}}{r_i g^2} S_{i+1,j,k} + \frac{r_i - \frac{g}{2}}{r_i g^2} S_{i-1,j,k} + \frac{1}{h^2} S_{i,j+1,k} + \frac{1}{h^2} S_{i,j-1,k}
\end{aligned} \tag{14}$$

Constant bound condition:

$$S(x, y, t) = C \approx S_{i,j,k} = C, \quad S(r, z, t) = C \approx S_{i,j,k} = C. \tag{15}$$

Wall bound condition:

$$\left. \frac{\partial S}{\partial n} \right|_{\Gamma} = 0 \approx \begin{cases} \frac{S_{i,j,k} - S_{i+1,j,k}}{h} = 0 & \text{for vertical bounds} \\ \frac{S_{i,j,k} - S_{i,j+1,k}}{g} = 0 & \text{for horizontal bounds} \end{cases} \tag{16}$$

Merge condition:

$$\begin{aligned}
& D_A \left. \frac{\partial S_A}{\partial n} \right|_{\Gamma} = D_B \left. \frac{\partial S_B}{\partial n} \right|_{\Gamma} \approx \\
& \approx \begin{cases} D_A \frac{S_{A,i-1,j,k} - S_{A,i,j,k}}{h} = D_B \frac{S_{B,i,j,k} - S_{B,i+1,j,k}}{h} & \text{for vertical bounds} \\ D_A \frac{S_{A,i,j-1,k} - S_{A,i,j,k}}{g} = D_B \frac{S_{B,i,j,k} - S_{B,i,j+1,k}}{g} & \text{for horizontal bounds} \end{cases} \tag{17}
\end{aligned}$$

1.2.1 Alternating directions and tridiagonal matrixes

The main equation system for one area is:

$$\begin{aligned}
& b_0 S_0 + c_0 S_1 = f_0 \\
& a_l S_{l-1} + b_l S_l + c_l S_{l+1} = f_l, \quad l = 1..N-1 \\
& a_N S_{N-1} + b_N S_N = f_N
\end{aligned} \tag{18}$$

here:

$$a = a_D, \quad b = b_T + b_D, \quad c = c_D, \quad f = f_T + f_D + f_R. \tag{19}$$

Functions $a_D, b_T, b_D, c_D, f_T, f_D$ and f_R are defined below. Coefficients for Δ are taken from (12) and (14).

From (11) we get:

$$b_T = -\frac{2}{\tau}, \quad f_T = \begin{cases} -\frac{2S_{i,j,k-1}}{\tau} & \text{for first direction;} \\ -\frac{2S_{i,j,k-0.5}}{\tau} & \text{for second direction.} \end{cases} \tag{20}$$

In the cylindrical coordinate system, by the coordinate r (to find $S_{i,j,k-0.5}$):

$$\begin{aligned} a_D &= D \frac{r_i - \frac{g}{2}}{r_i g^2}, \quad b_D = -\frac{2D}{g^2}, \quad c_D = D \frac{r_i + \frac{g}{2}}{r_i g^2}, \\ f_D &= -D \frac{S_{i,j+1,k-1} - 2S_{i,j,k-1} + S_{i,j-1,k-1}}{h^2}. \end{aligned} \quad (21)$$

In the cylindrical coordinate system, by the coordinate z (to find $S_{i,j,k}$):

$$\begin{aligned} a_D &= \frac{D}{h^2}, \quad b_D = -\frac{2D}{h^2}, \quad c_D = \frac{D}{h^2}, \\ f_D &= -D \frac{(r_i + \frac{g}{2})S_{i+1,j,k-0.5} - 2r_i S_{i,j,k-0.5} + (r_i - \frac{g}{2})S_{i-1,j,k-0.5}}{r_i g^2}. \end{aligned} \quad (22)$$

In the cartesian coordinate system, by coordinate x (to find $S_{i,j,k-0.5}$):

$$\begin{aligned} a_D &= \frac{D}{g^2}, \quad b_D = -\frac{2D}{g^2}, \quad c_D = \frac{D}{g^2}, \\ f_D &= -D \frac{S_{i,j+1,k-1} - 2S_{i,j,k-1} + S_{i,j-1,k-1}}{h^2}. \end{aligned} \quad (23)$$

In the cartesian coordinate system, by coordinate y (to find $S_{i,j,k}$):

$$\begin{aligned} a_D &= \frac{D}{h^2}, \quad b_D = -\frac{2D}{h^2}, \quad c_D = \frac{D}{h^2}, \\ f_D &= -D \frac{S_{i+1,j,k-0.5} - 2S_{i,j,k-0.5} + S_{i-1,j,k-0.5}}{g^2}. \end{aligned} \quad (24)$$

For Michaelis-Menten¹ reaction (for both directions is the same):

$$f_R = \begin{cases} +\frac{V_{max} S_{i,j,k-1}}{K_M + S_{i,j,k-1}} & \text{for a substrate;} \\ -\frac{V_{max} S_{i,j,k-1}}{K_M + S_{i,j,k-1}} & \text{for a product.} \end{cases} \quad (25)$$

For ReductionOxidation² reaction (for both directions is the same):

$$f_R = \sum_{R_{ro}: S \in \{S_{s_1}, S_{s_2}\}} k S_{s_1,i,j,k-1} S_{s_2,i,j,k-1} - \sum_{R_{ro}: S \in \{S_{p_1}, S_{p_2}\}} k S_{s_1,i,j,k-1} S_{s_2,i,j,k-1} \quad (26)$$

The tri-diagonal matrix can be solved easily by the following algorithm. It has four main steps:

1. Find p_0 and q_0 :

$$p_0 = -\frac{c_0}{b_0}, \quad q_0 = \frac{f_0}{b_0} \quad (27)$$

For the *constant* bound condition:

$$b_0 = 1, \quad c_0 = 0, \quad f_0 = C \quad \Rightarrow \quad p_0 = -\frac{0}{1} = 0, \quad q_0 = \frac{C}{1} = C. \quad (28)$$

¹Expression in the same for the both directions, so results can be reused

²Expression in the same for the both directions, so results can be reused

For the *wall condition*:

$$b_0 = 1, c_0 = -1, f_0 = 0 \Rightarrow p_0 = -\frac{-1}{1} = 1, q_0 = \frac{0}{1} = 0. \quad (29)$$

Values for p_0 and q_0 for the merge condition is calculated by the formula, defined in the second step.

$$D_A \frac{S_{A,l-1} - S_{A,l}}{h_A} = D_B \frac{S_{B,l} - S_{B,l+1}}{h_B} \quad (30)$$

$$\frac{D_A}{h_A} S_{A,l-1} - \left(\frac{D_A}{h_A} + \frac{D_B}{h_B} \right) S_{0,l} + \frac{D_B}{h_B} S_{B,l+1} = 0 \quad (31)$$

The following coefficients should be used in (33) in order to find p_0 and q_0 for the *merge condition*:

$$a_0 = \frac{D_A}{h_A}, b_0 = -\left(\frac{D_A}{h_A} + \frac{D_B}{h_B} \right), c_0 = \frac{D_B}{h_B}, f_0 = 0 \quad (32)$$

2. Recurrently find p_i and q_i .

$$p_l = -\frac{c_l}{a_l p_{l-1} + b_l}, \quad q_l = \frac{f_l - a_l q_{l-1}}{a_l p_{l-1} + b_l} \quad (33)$$

3. Find y_N .

$$y_N = \frac{f_N - a_N q_{N-1}}{a_N p_{N-1} + b_N} \quad (34)$$

For the *constant bound condition*:

$$a_N = 0, b_N = 1, f_0 = C \Rightarrow y_N = \frac{C - 0 q_{N-1}}{0 p_{N-1} + 1} = C \quad (35)$$

For the *wall condition*:

$$a_N = 1, b_N = -1, f_0 = 0 \Rightarrow y_N = \frac{0 - 1 q_{N-1}}{1 p_{N-1} - 1} = -\frac{q_{N-1}}{p_{N-1} - 1} \quad (36)$$

For the *merge condition* (37) should be used.

4. Recurrently find y_i .

$$y_l = p_l y_{l+1} + q_l. \quad (37)$$

The end³.

³Bound conditions are solved using explicit scheme, when solving along the bound.