Equations

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Abstract

Mathematical part of the solvers.

1 Implicid 2D solver in the cartesian and cylindrical coordinate sstems

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:

$$\frac{\partial S}{\partial t} = D\Delta S + R. \tag{1}$$

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

1.1.1 Diffusion

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

$$\Delta S = \frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2}. \tag{2}$$

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

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

1.1.2 Reactions

Michaelis-menten reaction:

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

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

ReductionOxidation reaction:

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

$$R = -\sum_{R_{ro}:S\in\{S_{s_1},S_{s_2}\}} kS_{s_1}S_{s_2} + \sum_{R_{ro}:S\in\{S_{p_1},S_{p_2}\}} kS_{s_1}S_{s_2} \tag{7}$$

1.1.3 Bounds

Constant condition:

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

Non-leakage (wall) condition:

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

Merge condition:

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

1.2 Finite differences

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

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

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

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

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

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

Case two – symetrical 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 tme previous case is in the second equation, here we replaced r with $r_{i-1/2}$ instead of r_i.

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

Constant bound condition:

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

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:

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

1.2.1 Alternating directions and tridiagonal matrixes

The main equation system for one area is:

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

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 bellow. Coefficients for Δ are taken from (12) and (14).
From (11) we get:

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

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

$$
a_D=D\frac{r_i-\frac{g}{2}}{r_i g^2}, \quad b_D=-\frac{2D}{g^2}, \quad c_D=D\frac{r_i+\frac{g}{2}}{r_i g^2},
$$
$$
f_D=-D\frac{S_{i,j+1,k-1}-2S_{i,j,k-1}+S_{i,j-1,k-1}}{h^2}. \tag{21}
$$

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

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

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

$$
a_D=\frac{D}{g^2}, \quad b_D=-\frac{2D}{g^2}, \quad c_D=\frac{D}{g^2},
$$
$$
f_D=-D\frac{S_{i,j+1,k-1}-2S_{i,j,k-1}+S_{i,j-1,k-1}}{h^2}. \tag{23}
$$

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

$$
a_D=\frac{D}{h^2}, \quad b_D=-\frac{2D}{h^2}, \quad c_D=\frac{D}{h^2},
$$
$$
f_D=-D\frac{S_{i+1,j,k-0.5}-2S_{i,j,k-0.5}+S_{i-1,j,k-0.5}}{g^2}. \tag{24}
$$

For Michaelis-Menten[1] reaction (for both directions is the same):

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

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

For ReductionOxidation[2] reaction (for both directions is the same):

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

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

1. Find p_0 and q_0:

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

For the *constant* bound condition:

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

For the *wall condition*:

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

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

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

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

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

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

2. Recurrently find p_i and q_i.

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

3. Find y_N.

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

For the *constant* bound condition:

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

For the *wall condition*:

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

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

4. Recurrently find y_i.

$$y_l = p_l y_{l+1} + q_l. \tag{37}$$

The end[3].

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

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