Equations

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December 15, 2008

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:

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

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

“Simple” reaction:

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

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

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:

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

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.

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

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 boundCondition:

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

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:

$$aS+bS+cS=f\tag{18}$$

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 $S_{i,j,k-0.5}$):

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

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

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

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

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

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

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

For Michaelis-Menten 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 “Simple” reaction:

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