Equations

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Abstract

Mathematical part of the solvers.

1 Implicid 2D solver in the cartesian coordinates

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 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 $R = R(r, z, t)$.

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

1.2 Reactions

Michaelis-menten reaction:

$$R = \begin{cases} -\frac{V_{max}S}{K_M+S} & \text{in equation for substrate } S, \\ +\frac{V_{max}S}{K_M+S} & \text{in equation for product } P. \end{cases} \tag{4}$$

"Simple" reaction:

$$R = \sum_i k_{R_i} S_{R_{i,a}} S_{R_{i,b}} - \sum_j k_{R_j} P_{R_{j,a}} P_{R_{j,b}} \tag{5}$$

1.3 Finite differences

$$\frac{\partial S}{\partial t} \approx \frac{S_{i,j,k} - S_{i,j,k-1}}{\tau} \tag{6}$$

$$\begin{aligned}
&\frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2} \approx \\
&\approx \frac{S_{i+1,j,k} - 2S_{i,j,k} + S_{i-1,j,k}}{g^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
&= -2\frac{g^2+h^2}{g^2h^2}S_{i,j,k} + \frac{1}{g^2}S_{i+1,j,k} + \frac{1}{g^2}S_{i-1,j,k} + \frac{1}{h^2}S_{i,j+1,k} + \frac{1}{h^2}S_{i,j-1,k}
\end{aligned} \tag{7}$$

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

$$\begin{aligned}
&\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial S}{\partial r}\right) + \frac{\partial^2 S}{\partial z^2} \approx \\
&\approx \frac{1}{r}\frac{\partial}{\partial r}\left(r_i\frac{S_{i,j,k} - S_{i-1,j,k}}{g}\right) + \frac{\partial^2 S}{\partial z^2} \approx \\
&\approx \frac{r_{i+1}\frac{S_{i+1,j,k}-S_{i,j,k}}{g} - r_i\frac{S_{i,j,k}-S_{i-1,j,k}}{g}}{r_i g} + \frac{\partial^2 S}{\partial z^2} \approx \\
&\approx \frac{r_{i+1}S_{i+1,j,k} - (r_{i+1}+r_i)S_{i,j,k} + r_iS_{i-1,j,k}}{r_ig^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
&= \frac{(r_i+g)S_{i+1,j,k} - (2r_i+g)S_{i,j,k} + r_iS_{i-1,j,k}}{r_ig^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
&= -\frac{2(h^2+g^2)r_i + gh^2}{r_ig^2h^2}S_{i,j,k} + \frac{r_i+g}{r_ig^2}S_{i+1,j,k} + \frac{1}{g^2}S_{i-1,j,k} + \frac{1}{h^2}S_{i,j+1,k} + \frac{1}{h^2}S_{i,j-1,k}
\end{aligned} \tag{8}$$

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.

$$\begin{aligned}
&\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial S}{\partial r}\right) + \frac{\partial^2 S}{\partial z^2} \approx \\
&\approx \frac{1}{r}\frac{\partial}{\partial r}\left(r_{i-1/2}\frac{S_{i,j,k} - S_{i-1,j,k}}{g}\right) + \frac{\partial^2 S}{\partial z^2} \approx \\
&\approx \frac{r_{i+1/2}\frac{S_{i+1,j,k}-S_{i,j,k}}{g} - r_{i-1/2}\frac{S_{i,j,k}-S_{i-1,j,k}}{g}}{r_i g} + \frac{\partial^2 S}{\partial z^2} \approx \\
&\approx \frac{r_{i+1/2}S_{i+1,j,k} - (r_{i+1/2}+r_{i-1/2})S_{i,j,k} + r_{i-1/2}S_{i-1,j,k}}{r_ig^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
&= \frac{(r_i+\frac{g}{2})S_{i+1,j,k} - 2r_iS_{i,j,k} + (r_i-\frac{g}{2})S_{i-1,j,k}}{r_ig^2} + \frac{S_{i,j+1,k} - 2S_{i,j,k} + S_{i,j-1,k}}{h^2} = \\
&= -2\frac{g^2+h^2}{g^2h^2}S_{i,j,k} + \frac{r_i+\frac{g}{2}}{r_ig^2}S_{i+1,j,k} + \frac{r_i-\frac{g}{2}}{r_ig^2}S_{i-1,j,k} + \frac{1}{h^2}S_{i,j+1,k} + \frac{1}{h^2}S_{i,j-1,k}
\end{aligned} \tag{9}$$

Var	cyl^1	cyl^2	dec^1	dec^2
a_D	$\frac{r_i - \frac{g}{2}}{r_i g^2}$	$\frac{1}{h^2}$		
b_D	$-\frac{2}{g^2}$	$-\frac{2}{h^2}$		
c_D	$\frac{r_i + \frac{g}{2}}{r_i g^2}$	$\frac{1}{h^2}$		

So:

$$a_D = \frac{r_i - \frac{g}{2}}{r_i g^2} \tag{10}$$

$$b_D = \frac{2}{g^2} \tag{11}$$

$$c_D = \frac{r_i + \frac{g}{2}}{r_i g^2} \tag{12}$$