Vignoles single pore model

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1 Problem statement

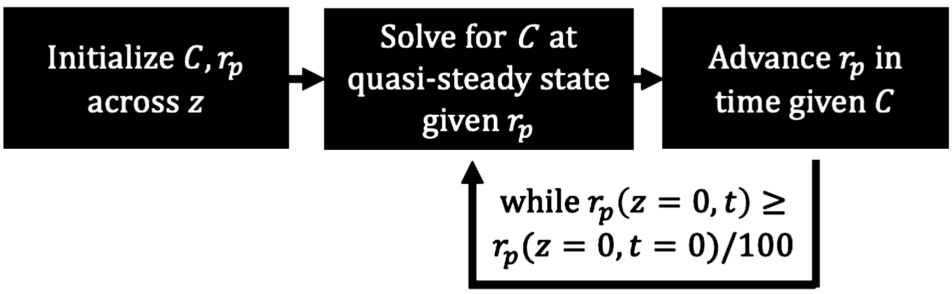
Couple

$$\frac{\partial}{\partial z}\left(r_p^2(z)\frac{\partial c}{\partial z}\right)=\frac{2k_{het}}{D_g}r_p(z)c(z), \quad c(0)=\frac{1}{1+\alpha}\frac{P}{RT}, \quad c(L)=c(L-\Delta z) \tag{1}$$

with

$$\frac{\partial}{\partial t}r_p=-r_pk_{het}cV_s, \quad r_p'(z,0)=0. \tag{2}$$

2 High level algorithm structure



It is assumed that at initially before penetration, the gas concentration is zero everywhere except at the interface, at which $c(z,t)=c(0,0)=\frac{1}{1+\alpha}\frac{P}{RT}$. Otherwise, $c(z\neq 0, t=0)=0$.

3 Discretizaton

3.1 Gas concentration

The goal is to develop a finite difference scheme for Eq. 1 which takes the shape of the general differential equation

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u=f(x), \quad a<x<b, \tag{3}$$

$$0<p_{min}\leq p\leq p_{max}, \quad q_{min}=0\leq q(x)\leq q_{max}. \tag{4}$$

Existence and uniqueness of a solution u requires that f, q are continuous on $[a, b]$ and that p has a continuous first derivative there. If

$$z = x,$$

$$r_p^2(z) \leftrightarrow p(x) \Longrightarrow 2r_p(z)\frac{dr_p}{dz} \leftrightarrow p'(x),$$

$$c(z) \leftrightarrow u(x) \Longrightarrow \frac{dc}{dz} \leftrightarrow \frac{du}{dx},$$

$$\frac{2k_{het}}{D_g}r_p(z) \leftrightarrow q(x),$$

$$f(x) = 0,$$

the governing equation for gas concentration evolution over space is derived. Specifically

$$\frac{\partial}{\partial z}\left(r_p^2(z)\frac{\partial c}{\partial z}\right) = \frac{2k_{het}}{D_g}r_p(z)c(z). \tag{5}$$

Using the product rule,

$$2r_p(z)\frac{dr_p}{dz}\frac{dc}{dz} + r_p^2(z)\frac{d^2c}{dz^2} = \frac{2k_{het}}{D_g}r_p(z)c(z). \tag{6}$$

The general Taylor series expansion of $F(y)$ around a is

$$F(y) = F(a) + \frac{F'(a)}{1!}(y-a)^1 + \frac{F''(a)}{2!}(y-a)^2 + \frac{F'''(a)}{3!}(y-a)^3 + \dots .$$

If $F(y) \leftrightarrow c(z+h)$, $a \leftrightarrow z$, then

$$c(z+h) = c(z) + hc'(z) + \frac{h^2}{2!}c''(z) + \frac{h^3}{3!}c'''(z) + \mathcal{O}(h^4). \tag{7}$$

If instead $F(y) \leftrightarrow c(z-h)$, $a \leftrightarrow z$, then

$$c(z-h) = c(z) - hc'(z) + \frac{h^2}{2!}c''(z) - \frac{h^3}{3!}c'''(z) + \mathcal{O}(h^4). \tag{8}$$

Adding these two expressions together,

$$c(z+h)+c(z-h) = 2c(z)\cancel{+hc'(z)}+\frac{h^2}{2!}c''(z)+\cancel{\frac{h^3}{3!}c'''(z)}\cancel{-hc'(z)}+\frac{h^2}{2!}c''(z)\cancel{-\frac{h^3}{3!}c'''(z)}+\dots \tag{9}$$

implies

$$c''(z) = \frac{c(z+h) - 2c(z) + c(z-h)}{h^2} + \mathcal{O}(h^2). \tag{10}$$

If one is to subtract the two expressions instead of adding them,

$$c(z+h) - c(z-h)$$

$$= \cancel{c(z)} + hc'(z) + \cancel{\frac{h^2}{2!}c''(z)} + \frac{h^3}{3!}c'''(z) - \left(\cancel{c(z)} - hc'(z) + \cancel{\frac{h^2}{2!}c''(z)} - \frac{h^3}{3!}c'''(z)\right) \tag{11}$$

implies

$$c(z+h) - c(z-h) = 2hc'(z) + \mathcal{O}(h^3) \tag{12}$$

which implies

$$c'(z) = \frac{c(z+h) - c(z-h)}{2h} + \mathcal{O}(h^2). \tag{13}$$

Now we subdivide the domain $[0, L]$ into $n+1$ subintervals using $n+2$ uniformly spaced points z_i, where $i = \{0, 1, 2, \ldots, n+1\}$ with

$$z_0 = 0, \quad z_1 = z_0 + h, \ \ldots \ z_i = z_{i-1} + h, \ \ldots \ z_{n+1} = z_n + h = L \tag{14}$$

where $h = L/(n+1)$ is the grid spacing. z_i are called grid points or nodes. $z_1, z_2, \ldots z_n$ are interior nodes, and z_0, z_{n+1} are boundary nodes. Letting $C_i \approx c(z_i)$, then the finite difference approximation at the node z_i is, based on Eq. 6,

$$\begin{gathered} r_p^2(z)\frac{d^2c}{dz^2} + 2r_p(z)\frac{dr_p}{dz}\frac{dc}{dz} = \frac{2k_{het}}{D_g}r_p(z)c(z) \\ \longrightarrow r_p^2(z)\left(-\frac{d^2c}{dz^2}\right) - \left(2r_p(z)\frac{dr_p}{dz}\right)\left(\frac{dc}{dz}\right) + \frac{2k_{het}}{D_g}r_p(z)c(z) = 0 \\ \longrightarrow r_p^2(z)\left(\frac{-C_{i+1} + 2C_i - C_{i-1}}{h^2}\right) - \left(2r_p(z)\frac{dr_p}{dz}\right)\left(\frac{C_{i+1} - C_{i-1}}{2h}\right) + \frac{2k_{het}}{D_g}r_p(z)C_i = 0. \end{gathered} \tag{15}$$

Because of the boundary conditions

$$c(0) = C_0 = \frac{1}{1+\alpha}\frac{P}{RT}, \quad c(L) = C_{n+1} = C_n, \tag{16}$$

there exist n unknowns $C_i = \{C_1, C_2, \ldots C_n\}$ and an equation of the form Eq. 15 at each of the n interior grid points $z_1, z_2, \ldots, z_n$. For example at z_1,

$$r_p^2(z_1)\left(\frac{-C_2 + 2C_1 - C_0}{h^2}\right) - \left(2r_p(z_1)r_p'(z_1)\right)\left(\frac{C_2 - C_0}{2h}\right) + \frac{2k_{het}}{D_g}r_p(z_1)C_1 = 0.$$

$$\longrightarrow r_p^2(z_1)\left(\frac{-C_2 + 2C_1 - \frac{1}{1+\alpha}\frac{P}{RT}}{h^2}\right) - \left(2r_p(z_1)r_p'(z_1)\right)\left(\frac{C_2 - \frac{1}{1+\alpha}\frac{P}{RT}}{2h}\right) + \frac{2k_{het}}{D_g}r_p(z_1)C_1 = 0.$$

There are still two unknowns and they are C_1 and C_2. At the next point z_2, it contains the three unknowns C_1, C_2, C_3, in that

$$\longrightarrow r_p^2(z_2)\left(\frac{-C_3 + 2C_2 - C_1}{h^2}\right) - \left(2r_p(z_2)r_p'(z_2)\right)\left(\frac{C_3 - C_1}{2h}\right) + \frac{2k_{het}}{D_g}r_p(z_2)C_2 = 0.$$

There will always be the three unknowns C_{i-1}, C_i, C_{i+1} except at boundary-adjacent nodes. Therefore we must solve for all unknowns at one time by writing the n difference equations as a linear system. Isolating the three unknowns in the general difference equation Eq. 15,

$$\frac{r_p^2(z_i)}{h^2}(-C_{i+1}+2C_i-C_{i-1})-\left(\frac{r_p(z_i)r_p'(z_i)}{h}\right)(C_{i+1}-C_{i-1})+\left(\frac{2k_{het}}{D_g}r_p(z_i)\right)C_i=0$$

implies

$$\frac{r_p^2(z_i)}{h}(-C_{i+1}+2C_i-C_{i-1})-\left(r_p(z_i)r_p'(z_i)\right)(C_{i+1}-C_{i-1})+\left(\frac{2k_{het}h}{D_g}r_p(z_i)\right)C_i=0$$

which implies

$$C_{i+1}\underbrace{\left(-\frac{r_p^2(z_i)}{h}-r_p(z_i)r_p'(z_i)\right)}_{\mathscr{A}_3(z_i)}+C_i\underbrace{\left(2\frac{r_p^2(z_i)}{h}+2\frac{k_{het}h}{D_g}r_p(z_i)\right)}_{\mathscr{A}_2(z_i)}+C_{i-1}\underbrace{\left(-\frac{r_p^2(z_i)}{h}+r_p(z_i)r_p'(z_i)\right)}_{\mathscr{A}_1(z_i)}=0$$

$$\Leftrightarrow \mathscr{A}_3(z_i)C_{i+1}+\mathscr{A}_2(z_i)C_i+\mathscr{A}_1(z_i)C_{i-1}=0. \tag{17}$$

The corresponding matrix form is $\mathbf{AC}=\mathbf{f}$ where $\mathbf{C}=\{C_1,C_2,\dots,C_n\}^T$ and

$$[\mathbf{A}]= \tag{18}$$

$$\begin{bmatrix}
\mathscr{A}_2(z_1) & \mathscr{A}_3(z_1) & 0 & 0 & \dots & 0 & 0 & 0 & 0\\
\mathscr{A}_1(z_2) & \mathscr{A}_2(z_2) & \mathscr{A}_3(z_2) & 0 & \dots & 0 & 0 & 0 & 0\\
0 & \mathscr{A}_1(z_3) & \mathscr{A}_2(z_3) & \mathscr{A}_3(z_3) & \dots & 0 & 0 & 0 & 0\\
\dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots\\
0 & 0 & 0 & 0 & \dots & \mathscr{A}_1(z_{n-2}) & \mathscr{A}_2(z_{n-2}) & \mathscr{A}_3(z_{n-2}) & 0\\
0 & 0 & 0 & 0 & \dots & 0 & \mathscr{A}_1(z_{n-1}) & \mathscr{A}_2(z_{n-1}) & \mathscr{A}_3(z_{n-1})\\
0 & 0 & 0 & 0 & \dots & 0 & 0 & \mathscr{A}_1(z_n) & \mathscr{A}_2(z_n)+\mathscr{A}_3(z_n)
\end{bmatrix}$$

and $\mathbf{f}=\{-\mathscr{A}_1(z_1)\frac{1}{1+\alpha}\frac{P}{RT},\quad 0,\quad 0,\quad \dots,\quad 0\}^T$ because of the boundary condition $C_0=\frac{1}{1+\alpha}\frac{P}{RT}$. The bottom right term includes $\mathscr{A}_3(z_n)$ because of the boundary condition $c(L)=c(L-\Delta z)\to C_{n+1}=C_n$. Since $\mathbf{A}$ is symmetric and tridiagonal and positive definite, the Cholesky factorization $\mathbf{A}$=$\mathbf{LL}^T$ can be used, and this only requires $\mathcal{O}(n)$ operations to solve.

Since r_p and r_p' are initialized across z, all $\mathscr{A}_n(z_m)$ can be solved for, meaning the entire system of equations can be solved for, and the vector $\mathbf{C}$, which represents discrete values for c separated by h, can be solved for.

3.2 Pore radius

Recall Eq. 2, which is

$$\frac{\partial}{\partial t}r_p=-r_pk_{het}cV_s.$$

Because c is now known across all z, it is possible to solve for r_p at the next time step using

$$\frac{\partial}{\partial t} r_p \approx \frac{r_p(t + \Delta t) - r_p(t)}{\Delta t}.$$

Substituting,

$$r_p(t + \Delta t) - r_p(t) = -r_p(t) k_{het} c V_s \Delta t$$

implies

$$r_p(t + \Delta t) = r_p(t)(1 - 2\Delta t k_{het} c V_s).$$

Once the pore radius across the depth at the new time step is revealed, this data can be fed back into the matrices **A** and **f**, as in Eq. 18.