Biosorption model

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1 Kinetic equation

Table 1: Naming convention

x , r, t	axial coordinate
H, M, N	radial coordinate
i, j, k	time coordinate
m, p	upper-inner loop variables
s, Ed	coefficients
τ	timestep t_{k+1} - t_k

Kinetic equation

$$\frac{\partial q(x,r,t)}{\partial t} = \frac{E_d}{r^s} \cdot \frac{\partial}{\partial r}\left(r^s \frac{\partial q(x,r,t)}{\partial r}\right) \tag{1}$$

$$\frac{\partial q(x,r,t)}{\partial t} = E_d \frac{s}{r}\frac{\partial q(x,r,t)}{\partial r} + E_d \frac{\partial^2 q(x,r,t)}{\partial r^2} \tag{2}$$

Initial and boundary conditions

$$q(x_i, r_j, t_1) = 0 \qquad \left.\frac{\partial q(x,r,t)}{\partial r}\right|^{(i,1,k)} = 0 \qquad q(x_i, r_M, t_k) = S_s(x_i, t_k)^n \tag{3}$$

Simplify and make expansion in (i, j, k) point

$$\left.\frac{\partial q(x,r,t)}{\partial t}\right|^{(i,j,k)} = E_d \frac{s}{r} \cdot \left.\frac{\partial q(x,r,t)}{\partial r}\right|^{(i,j,k)} + E_d \left.\frac{\partial^2 q(x,r,t)}{\partial r^2}\right|^{(i,j,k)} \tag{4}$$

Lagrange polynomial approximation

$$q(x,r,t) = \sum_{m=1}^{M} \prod_{p=1}^{M} \frac{r - r_p}{r_m - r_p} \cdot q(x, r_m, t) = \sum_{m=1}^{M} l_m(r) \cdot q(x, r_m, t) \tag{5}$$

$$\left.\frac{\partial q(x,r,t)}{\partial r}\right|^{(i,j,k)} = \left.\sum_{m=1}^{M} l'_m(r) \cdot q(x, r_m, t)\right|^{(i,j,k)} = \sum_{m=1}^{M} A_{jm} \cdot q(x_i, r_m, t_k) \tag{6}$$

$$\left.\frac{\partial^2 q(x,r,t)}{\partial r^2}\right|^{(i,j,k)} = \left.\sum_{m=1}^{M} l''_m(r) \cdot q(x, r_m, t)\right|^{(i,j,k)} = \sum_{m=1}^{M} B_{jm} \cdot q(x_i, r_m, t_k) \tag{7}$$

$$\left.\frac{\partial q(x,r,t)}{\partial t}\right|^{(i,j,k)} = \frac{q(x_i,r_j,t_k) - q(x_i,r_j,t_{k-1})}{\tau} \tag{8}$$

Insert (6), (7), (8) into (4)

$$\frac{q(x_i,r_j,t_k) - q(x_i,r_j,t_{k-1})}{\tau} = E_d \frac{s}{r_j} \cdot \sum_{m=1}^{M} A_{jm} \cdot q(x_i,r_m,t_k) + E_d \sum_{m=1}^{M} B_{jm} \cdot q(x_i,r_m,t_k) \tag{9}$$

$$\tau E_d \sum_{m=1}^{M} \left(\frac{s}{r_j} A_{jm} + B_{jm}\right) q(x_i,r_m,t_k) - q(x_i,r_j,t_k) + q(x_i,r_j,t_{k-1}) = 0 \tag{10}$$

Upper boundary equation

$$q(x_i,r_M,t_k) = S_s(x_i,t_k)^n, \qquad r_M = 1 \tag{11}$$

Inserting equation (11) into (10) we will get

$$\tau E_d \sum_{m=1}^{M-1} \left(\frac{s}{r_j} \cdot A_{jm} + B_{jm}\right) q(x_i,r_m,t_k) + \tau E_d \left(s A_{jM} + B_{jM}\right) S_s(x_i,t_k)^n - q(x_i,r_j,t_k) + q(x_i,r_j,t_{k-1}) = 0 \tag{12}$$

for each slice of column $x_i \in [x_1, x_2..., x_i, ..., x_{H-1}]$ (roots of Legendre polynomial of $H-1$ degree)
for each time layer $t_i \in [t_2, t_3, ..., t_k, ..., t_N]$, where $t_k = \tau * (k-1)$
for each radial layer $r_j \in [r_2..., r_j, ..., r_{M-1}]$ (roots of Legendre polynomial of $M-2$ degree) we use (12)
for t_1 we have already known q from initial conditions $q(x_i, r_j, t_1) = 0$
The last equation are added from lower boundary condition

$$\left.\frac{\partial q(x,r,t)}{\partial r}\right|^{(i,1,k)} = \frac{q(x_i,r_2,t_k) - q(x_i,r_1,t_k)}{r_2 - r_1} = 0 \qquad \Rightarrow \qquad q(x_i,r_2,t_k) - q(x_i,r_1,t_k) = 0 \tag{13}$$

Depends on $S_s(x,t)$.

2 Adsorbent phase material balance

$$\frac{\partial}{\partial t} \cdot \int_0^1 q(x,r,t) r^2 dr = St(1 + B_0 L_{fmax})^2 \left(S(x,t) - \frac{D_g L_f(x,t) S_{f,av}(x,t)}{B_1 + S_{f,av}(x,t)}\right) \tag{14}$$

, where

$$D_1 = St(1 + B_0 L_{fmax})^2 \qquad S_{f,av}(x,t) = \frac{1}{M} \sum_{j=1}^{M} S_f(x,r_j,t) \tag{15}$$

Let's introduce new function

$$S_{av}(x,t) = \frac{S_{f,av}(x,t)}{B_1 + S_{f,av}(x,t)} = \frac{\frac{1}{M}\sum_{j=1}^{M} S_f(x,f_j,t)}{B_1 + \frac{1}{M}\sum_{j=1}^{M} S_f(x,f_j,t)} = \frac{S_s(x,t) + \sum_{j=2}^{M-1} S_f(x,f_j,t) + S_{fs}(x,t)}{MB_1 + S_s(x,t) + \sum_{j=2}^{M-1} S_f(x,f_j,t) + S_{fs}(x,t)} \tag{16}$$

Substitute and get

$$\frac{\partial}{\partial t} \cdot \int_0^1 q(x,r,t) r^2 dr = D_1(S(x,t) - D_g L_f(x,t) S_{av}(x,t)) \tag{17}$$

Depends on L_f, S_f, S

As we use Legandre polynomials with weight function $W(x) = r^\alpha(1-r)^\beta$, with $\alpha = 0$ and $\beta = 2$ we get $W(x) = r^2$, that is why in (i,j,k) we get

$$\frac{\partial}{\partial t}\cdot\int_0^1 q(x_i,r,t)r^2dr = \frac{\partial}{\partial t}\cdot\sum_{m=1}^{M} W_m\cdot q(x_i,r_m,t) = \sum_{m=1}^{M} W_m\cdot\frac{\partial q(x_i,r_m,t)}{\partial t} = \sum_{m=1}^{M} W_m\cdot\frac{q(x_i,r_m,t_k)-q(x_i,r_m,t_{k-1})}{\tau} \tag{18}$$

All together in (i,j,k) we get

$$\sum_{m=1}^{M} W_m\cdot\frac{q(x_i,r_m,t_k)-q(x_i,r_m,t_{k-1})}{\tau} = D_1(S(x_i,t_k) - D_1S(x_i,t_k) - D_1D_gL_f(x_i,t_k)S_{av}(x_i,t_k) \tag{19}$$

$$\sum_{m=1}^{M} W_m\cdot q(x_i,r_m,t_k) - \tau D_1S(x_i,t_k) - \tau D_1D_gL_f(x_i,t_k)S_{av}(x_i,t_k) = \sum_{m=1}^{M} W_m\cdot q(x_i,r_m,t_{k-1}) \tag{20}$$

3 Liquid phase material balance

$$\frac{\partial S(x,t)}{\partial t} = D\cdot\frac{\partial^2 S(x,t)}{\partial x^2} - D_gSt(1+B_0L_{max})^2(S(x,t)-S_{fs}(x,t)) \tag{21}$$

Initial and boundary conditions

$$S(x,t_1) = 0 \qquad S(x_1,t) = 1 \qquad \frac{\partial S(x_H,t)}{\partial x} = 0 \tag{22}$$

Depends on $S_{fs}(x,t)$

Let $D_1 = D_gSt(1+B_0L_{max})^2$ and use extension in (i,k)

$$\left.\frac{\partial S(x,t)}{\partial t}\right|^{(i,k)} = D\cdot\left.\frac{\partial^2 S(x,t)}{\partial x^2}\right|^{(i,k)} - D_1(S(x_i,t_k)-S_{fs}(x_i,t_k)) \tag{23}$$

Using for (23) the same Lagrange polynomial expansion (7) and finite difference scheme (8) as for kinetic equation (4) we get:

$$\frac{S(x_i,t_k)-S(x_i,t_{k-1})}{\tau} = D\sum_{m=1}^{N} B_{im}\cdot S(x_i,t_k) - D_1(S(x_i,t_k)-S_{fs}(x_i,t_k)) \tag{24}$$

$$S(x_i,t_k)-S(x_i,t_{k-1}) = \tau D\sum_{m=2}^{N} B_{im}\cdot S(x_i,t_k) + \tau DB_{i1}S(x_1,t_k) - \tau D_1(S(x_i,t_k)-S_{fs}(x_i,t_k)) \tag{25}$$

With lower boundary condtions (22) we get

$$(1+\tau D_1)S(x_i,t_k) - \tau D\sum_{m=2}^{N} B_{im}S(x_i,t_k) - S_{fs}(x_i,t_k) = \tau DB_{i1} + S(x_i,t_{k-1}) \tag{26}$$

for each time layer $t_i \in [t_2,t_3,...,t_k,...,t_N]$, where $t_k = \tau * (k-1)$

for each slice of column $x_i \in [x_2,x_3...,x_i,...,x_{H-1}]$ (roots of Legendre polynomial of $H-2$ degree) we use (26), for t_1 we have already known $S(t_1,x)$ from initial conditions $S(t_1,x) = 0$

The last equation are added from upper boundary condition (22)

$$\left.\frac{\partial S(x,t)}{\partial x}\right|^{(i,k)} = \frac{S(x_i,t_k)-S(x_{i+1},t_k)}{x_2-x_1} = 0 \qquad \Rightarrow \qquad S(x_i,t_k)-S(x_{i+1},t_k) = 0 \tag{27}$$

4 Biofilm equations: diffusion and biodegradation, grows and decay

diffusion and biodegradation

$$\frac{\partial^2 S_f(x,r,t)}{\partial r^2} = A_2 \frac{L_f^2(x,t) S_f(x,r,t)}{B_1 + S_f(x,r,t)} \tag{28}$$

Boundary condition for S_f

$$S_f(x, r=1, t) = S_s(x,t) \qquad S_f(x, r = 1 + L_f/R, t) = S_{fs}(x,t) \tag{29}$$

S_f defines only on interval $(1, 1 + L_f/R)$ and q only on the interval $(0,1)$. For me it is seems more logical totally separate this variables, introducing a new variable on the interval $(0,1)$. That will make possible to use orthogonal collocation and normalize result. The linear transformation $f = (r-1)\cdot R/L_f$ maps the interval $(1, 1+L_f/R)$ to the interval $(0,1)$, replace r with f using $r = 1 + f L_f/R$ we get

$$\left(\frac{R}{L_f}\right)^2 \frac{\partial^2 S_f(x,f,t)}{\partial f^2} = A_2 \frac{L_f^2(x,t) S_f(x,f,t)}{B_1 + S_f(x,f,t)} \tag{30}$$

But what is more important the boundary conditions are

$$S_f(x, f=0, t) = S_s(x,t) \qquad S_f(x, f=1, t) = S_{fs}(x,t) \tag{31}$$

The grows and decay looks like that

$$\frac{\partial L_f(x,t)}{\partial t} = D_g A_3 \frac{S_{f,av}(x,t)}{B_1 + S_{f,av}(x,t)} - D_g A_3 L_f(x,t) \tag{32}$$

Initial and boundary conditions

$$L_f(x,t_1) = L_{f0} \qquad L_f(x,t_N) = 1 \tag{33}$$

Depends on $S_s(x,t)$ and $S_{fs}(x,t)$

Let's for f the collocation discretization be the same as for r, and we will use the same notation just for convenience. Using (7) and expansion in (i,j,k) we get

$$\sum_{m=1}^{M} B_{jm}\cdot S_f(x_i,f_m,t_k) \equiv B_{j1} S_s(x_i,t) + \sum_{m=2}^{M-1} B_{jm} S_f(x_i,f_m,t_k) + S_{fs}(x_i,t_k) = A_2 \frac{L_f^2(x_i,t_j) S_f(x_i,f_j,t_k)}{B_1 + S_f(x_i,f_j,t_k)} \tag{34}$$

substitute (16) to (32) and make expansion in (i,k) we get

$$\frac{L_f(x_i,t_k) - L_f(x_i,t_{k-1})}{\tau} = D_g A_3 S_{av}(x_i,t_k) - D_g A_3 L_f(x_i,t_k) \tag{35}$$

$$L_f(x_i,t_k) - \tau D_g A_3 S_{av}(x_i,t_k) + \tau D_g A_3 L_f(x_i,t_k) = L_f(x_i,t_{k-1}) \tag{36}$$

5 all together

Unknown function $L_f(x,t)$, $q(x,r,t)$, $S_s(x,t)$, $S_f(x,r,t)$, $S_{fs}(x,t)$, $S(x,t)$

Initial conditions

$$\begin{gathered} L_f(x,t_1) = L_{f0} \quad q(x,r,t_1) = 0 \\ S_s(x,t_1) = 0, \qquad S_f(x,r,t_1) = 0, \qquad S_{fs}(x,t_1) = 0, \qquad S(x,t_1) = 0 \end{gathered} \tag{37}$$

Boundary conditions

$$\left.\frac{\partial q(x,r,t)}{\partial r}\right|^{(i,1,k)} = 0 \qquad q(x_i, r_M, t_k) = S_s(x_i, t_k)^n$$
$$S(x_1,t) = 1 \qquad \left.\frac{\partial S(x,t)}{\partial x}\right|^{(H,j,k)} = 0 \tag{38}$$
$$S_f(x, f_1, t) = S_s(x,t) \qquad S_f(x, f_M, t) = S_{fs}(x,t)$$

For each time step $t = [t_2, t_3, ..., t_N]$. Do not forget that on t_N the $L_f(x,t) = L_{fmax}$, so it is already known. for each slice of column $x_i \in [x_1, x_2..., x_i, ..., x_H]$ and for each radial layer $r_j \in [r_2..., r_j, ..., r_{M-1}]$ and for $f_j \in [f_2..., f_j, ..., f_{M-1}]$ we have discretization. So it's big non linear equation and we need to solve it. Just do it, man!

For x_1 due to boundary conditions we get simpler system, so $S(x_1,t) = 1$ and $S_{fs}(x_1,t) = 1$ are already known. We get:

$$\tau E_d \sum_{m=1}^{M-1} \left(\frac{s}{r_j} \cdot A_{jm} + B_{jm}\right) q(x_1, r_m, t_k) + \tau E_d \left(sA_{jM} + B_{jM}\right) S_s(x_i, t_k)^n - q(x_1, r_j, t_k) + q(x_1, r_j, t_{k-1}) = 0 \tag{39}$$

$$\sum_{m=1}^{M} W_m \cdot q(x_1, r_m, t_k) - \tau D_1 D_g L_f(x_1, t_k) S_{av}(x_1, t_k) = \tau D_1 + \sum_{m=1}^{M} W_m \cdot q(x_1, r_m, t_{k-1}) \tag{40}$$

$$L_f(x_1, t_k) - \tau D_g A_3 S_{av}(x_1, t_k) + \tau D_g A_3 L_f(x_1, t_k) = L_f(x_i, t_{k-1}) \tag{41}$$

$$B_{j1} S_s(x_1, t) + \sum_{m=2}^{M-1} B_{jm} S_f(x_1, f_m, t_k) + 1 = A_2 \frac{L_f^2(x_1, t_j) S_f(x_1, f_j, t_k)}{B_1 + S_f(x_1, f_j, t_k)} \tag{42}$$

$$S_{av}(x_1, t_k) = \frac{S_s(x_1, t_k) + \sum_{j=2}^{M-1} S_f(x_1, f_j, t_k) + 1}{MB_1 + S_s(x_1, t) + \sum_{j=2}^{M-1} S_f(x_1, f_j, t_k) + 1} \tag{43}$$

We can found out extra boundary conditions

$$S_{fs}(x_1, t) = 1 \tag{44}$$