SUPPLEMENTAL MATERIAL A

Application of the Perturbation and Matching Technique

Considering the differential equation (11) and the rate expression (21), the mass balance differential equation for the key substrate *A* is:

$$\frac{d}{dx^*} D^*_{fA} \frac{dC^*_A}{dx^*} = \phi^2 \; X^*_f \;\; (\beta_A + 1)(\beta_B + 1) \frac{C^*_A}{(\beta_A + C^*_A)} \frac{[\Gamma_B (C^*_A - 1) + 1]}{[\beta_B + \Gamma_B (C^*_A - 1) + 1]} \qquad \text{(A-1)}$$

Perturbation solutions

When ϕ^2<< *1*, one notices that Eq. (A-1) itself suggests the following series as an approximate solution for C_A:

$$C^*_A = 1 + A(x^*)\, \phi^2 + O(\phi^4) \qquad \text{(A-2)}$$

One can also expand $r^*(C^*_A)$ in a Taylor series to obtain:

$$r^*(C^*_A) = r^*(1) + r^*{}'(1)\; A(x^*)\, \phi^2 + O(\phi^4) \qquad \text{(A-3)}$$

Here $r^*{}'(1)$ is given by Eq. (22) and denotes the first derivative with respect to C^*_A, evaluated at C^*_A =*1*. Also, $r^*(1) = 1$.

By replacing C^*_A and $r^*(C^*_A)$, as given by Eqs. (A-2) and (A-3), in Eq. (A-1) and collecting terms of equal power of ϕ, the following linear ordinary equation is found:

$$\frac{1}{dx*} D^*_{fA}(x^*) \frac{dA}{dx*} = X^*_f(x^*) \qquad \text{(A-4)}$$

which must be solved subject to the following boundary conditions:

$$A = 0 \quad \text{at} \quad x* = 1 \quad \text{and} \quad \frac{dA}{dx*} = 0 \quad \text{at} \quad x* = 0 \qquad \text{(A-5)}$$

In solving Eq. (A-4) with standard analytical methods, and taking into account Eqs. (27) and (28), the following equation is found:

$$A(x^*) = \frac{b\,\Psi^2}{c\,\overline{X}_f\ 0.2218}\left[\frac{1}{0.2218}\left[\left(1+\frac{x^*}{\Psi}\right)^{0.2218} - \left(1+\frac{1}{\Psi}\right)^{0.2218}\right] + \ln\left[\frac{\left(1+\frac{1}{\Psi}\right)}{\left(1+\frac{x^*}{\Psi}\right)}\right]\right] \quad \text{(A-6)}$$

By substituting Eq. (A-6) into Eq. (A-3) and then in Eq. (29), the asymptotic expression for the effectiveness factor for the continuum heterogeneous biofilm model (η), is found:

$$\eta = \int_0^1 X_f^*\ r^*(C_A^*)\ dx^* = \int_0^1 X_f^*\ \left[1 + r^{*\prime}(1)\ A(x^*)\ \phi^2\right] dx^* \qquad \text{(A-7)}$$

Then:

$$\eta = 1 - \sigma\,\phi^2 \qquad \text{(A-8)}$$

Where

$$\sigma = \frac{b\,\Psi^2}{\overline{X}_f^2\ c\ (0.2218)}\ r^{*\prime}(1)\,(F) \qquad \text{(A-9)}$$

and

$$F = -\frac{a\ \Psi}{(0.2218)(1.2218)}\left[\left(1+\frac{1}{\Psi}\right)^{1.2218} - 1\right] + \frac{a\left(1+\frac{1}{\Psi}\right)^{0.2218}}{(0.2218)} -$$

$$- a\int_0^1 \ln\left[\frac{1+\frac{1}{\Psi}}{1+\frac{x^*}{\Psi}}\right] dx^* - \frac{b\,\Psi\left[\left(1+\frac{1}{\Psi}\right)^{0.4436} - 1\right]}{(0.2218)\ (0.4436)} +$$

$$+\ \frac{b\,\Psi\left(1+\dfrac{1}{\Psi}\right)^{0.2218}}{(0.2218)^2}\left[\left(1+\frac{1}{\Psi}\right)^{0.2218}-1\right]-b\int_0^1\left(1+\frac{x^*}{\Psi}\right)^{-0.7782}\ln\left[\frac{1+\dfrac{1}{\Psi}}{1+\dfrac{x^*}{\Psi}}\right]dx^*$$

(A-10)

When $\phi^2 \to \infty$, the reaction rate is very fast and the rate of diffusion low; therefore, the key substrate is completely consumed at the biofilm-fluid interface. The dimensionless biofilm density and the nutrient effective diffusivity have values corresponding to $x^* = 1$:

$$X_f^*(x^*) = X_f^*(1) \qquad \text{and} \qquad D_f^*(x^*) = D_{fA}^*(1) \tag{A-11}$$

Therefore, Eq. (A-1) yields:

$$D_{fA}^*(1)\,\frac{d^2C_A^*}{dx^{*2}} = \phi^2\ X_f^*(1)\ r^*(C_A^*) \tag{A-12}$$

Defining:

$$\frac{dC_A^*}{dx^*} = P \tag{A-13}$$

$$\frac{d^2C_A^*}{dx^{*2}} = \frac{dP}{dC_A^*}\,\frac{dC_A^*}{dx^*} = P\,\frac{dP}{dC_A^*} = \frac{1}{2}\,\frac{dP^2}{dC_A^*} \tag{A-14}$$

Considering boundary conditions defined in Eqs. (17) and (18):

$$P(1) = \frac{dC_A^*}{dx^*}\Big|_{x^*=1} \qquad \text{and} \qquad P(0) = \frac{dC_A^*}{dx^*}\Big|_{x^*=0} = 0$$

Then, Eq. (A-12) yields:

$$\frac{dP^2}{dC_A^*} = \phi^2\ \frac{2\ X_f^*(1)}{D_{fA}^*(1)}\ r^*(C_A^*) \tag{A-15}$$

Solving Eq. (A-15), the first derivative of C_A^* at the biofilm-fluid interphase is obtained:

$$P(1)^2 = \left[\frac{dC_A^*}{dx^*} \Big|_{x^*=1} \right]^2 = \phi^2 \ \frac{2 \ X_f^*(1)}{D_{fA}^*(1)} \ I \qquad \text{(A-16)}$$

With

$$I = (\beta_A + 1)\,(\beta_B + 1) \int_0^1 \frac{C_A^*}{(\beta_A + C_A^*)} \ \frac{[\Gamma_B (C_A^* - 1) + 1]}{[\beta_B + \Gamma_B (C_A^* - 1) + 1]} \, dC_A^* \qquad \text{(A-17)}$$

Thus, with Eqs. (31) and Eqs.(A-16), the asymptotic expression for the effectiveness factor for large values of ϕ is found:

$$\eta = \frac{\left(2 \ D_{fA}^*(1) \ \ X_f^*(1) \ \ I\right)^{1/2}}{\phi} = \frac{\rho}{\phi} = \frac{1}{\phi^*} \qquad \text{(A-18)}$$

Matching expression for the effectiveness factor

The challenge is to find an expression capable of reproducing Eqs. (A-8) and (A-18) when ϕ<<1 and ϕ>>1, respectively.

After several attempts (Churchill, 1977; Wedel and Luss, 1980; Gottifredi et al., 1981), Gonzo and Gottifredi (2007) succeeded in finding a rational expression that overcomes the inconvenience presented by previous expressions. The matching equation proposed here is (see Eq. (32):

$$\eta = \left[\phi^{*2} + \exp(-d \ \phi^{*2})\right]^{-(1/2)} \qquad \text{(A-19)}$$

After expanding Eq. (A-19) for large and small values of ϕ*, yields:

$$\eta = \frac{1}{\phi^*} \qquad \text{(A-20)}$$

And for $\phi^2 << 1$

$$\eta \approx 1 - \frac{1}{2}(1-d)\,\phi^{*2} \qquad \text{(A-21)}$$

By comparing Eqs. (A-20) and (A-21) with Eqs. (A-8) and (A-18), respectively, conditions for the unknown parameter (*d*) of Eq. (A-19), are found:

$$d = 1 - 2\,\sigma^{*} \qquad \text{(A-22)}$$

with

$$\sigma^{*} = \sigma\,\rho^{2} \qquad \text{(A-23)}$$

REFERENCES

Churchill SW. 1977. A generalized expression for the effectiveness factor of porous catalyst pellets. AIChE J 23:208-212.

Gonzo EE, Gottifredi JC. 2007. A simple and accurate method for simulation of hollow fiber biocatalyst membrane reactors. Biochem Eng J 37:80-85.

Gottifredi JC, Gonzo EE, Quiroga OD. 1981. Isothermal effectiveness factor I. Analytical expression for single reaction with arbitrary kinetics. Slab geometry. Chem Eng Sci 36:705-713.

Wedel S, Luss D. 1980. A rational approximation of the effectiveness factor. Chem Eng Commun 7:145-152.