Supplementary Information: Secondary Effectiveness Factors for Catalytic Reactions in Series: Extension to Slab, Cylindrical, and Spherical Geometries

Armin Shayesteh Zadeh and Baron Peters

S.1 Concentration profile of $\boldsymbol{B}$ in cylindrical geometry

Mass balance equation for $\boldsymbol{B}$ in cylindrical geometry is

$$\frac{d^2\bar{C}_B}{d\bar{r}^2} + \frac{1}{\bar{r}}\frac{d\bar{C}_B}{d\bar{r}} - \Phi_B^2\bar{C}_B = -\Phi_A^2\gamma\delta\bar{C}_A \tag{S.1}$$

with boundary conditions

$$\begin{cases} \bar{C}_B(1) = 1 \\ \bar{C}_B(\bar{r}) \text{ bounded as } \bar{r} \to 0. \end{cases}$$

With definitions for dimensionless parameters from the main text, the solution to equation (S.1) will be

$$\bar{C}_B(\bar{r}) = C_1 I_0(\Phi_B\bar{r}) + C_2 K_0(\Phi_B\bar{r}) + \bar{C}_{B_{NH}}. \tag{S.2}$$

Here, $\bar{C}_{B_{NH}}$ is the solution for the non-homogeneous part of the ODE. Substituting for $\bar{C}_A$ from the results in the main text and using the method of undetermined coefficients, we get

$$\bar{C}_{B_{NH}} = \frac{\Phi_A^2\gamma\delta}{\Phi_B^2 - \Phi_A^2}\frac{I_0(\Phi_A\bar{r})}{I_0(\Phi_A)}. \tag{S.3}$$

Substituting $\bar{C}_{B_{NH}}$ back into equation (S.2) and matching the boundary conditions gives

$$\begin{aligned} \bar{C}_B(\bar{r}) &= \left[1 - \frac{\Phi_A^2\gamma\delta}{\Phi_B^2 - \Phi_A^2}\right]\frac{I_0(\Phi_B\bar{r})}{I_0(\Phi_B)} + \frac{\Phi_A^2\gamma\delta}{\Phi_B^2 - \Phi_A^2}\frac{I_0(\Phi_A\bar{r})}{I_0(\Phi_A)} \\ &= \frac{I_0(\Phi_B\bar{r})}{I_0(\Phi_B)} - \gamma\delta\Phi_A^2\frac{\frac{I_0(\Phi_B\bar{r})}{I_0(\Phi_B)} - \frac{I_0(\Phi_A\bar{r})}{I_0(\Phi_A)}}{\Phi_B^2 - \Phi_A^2}. \end{aligned} \tag{S.4}$$

S.2 Concentration profile of $\boldsymbol{B}$ in spherical geometry

Mass balance equation for $\boldsymbol{B}$ in spherical geometry is

$$\frac{1}{\bar{r}^2}\frac{d}{d\bar{r}}(\bar{r}^2\frac{d\bar{C}_B}{d\bar{r}}) - \Phi_B^2\bar{C}_B = -\Phi_A^2\gamma\delta\bar{C}_A \tag{S.5}$$

with boundary conditions

$$\begin{cases} \bar{C}_B(1) = 1 \\ \bar{C}_B(\bar{r}) \text{ bounded as } \bar{r} \to 0. \end{cases}$$

Equation (S.5) is a non-homogeneous second order ODE. The solution will be of the form

$$\bar{C}_B(\bar{r}) = C_1(\bar{r})\frac{cosh(\Phi_B\bar{r})}{\bar{r}} + C_2(\bar{r})\frac{sinh(\Phi_B\bar{r})}{\bar{r}}. \tag{S.6}$$

Having already solved for $\bar{C}_A(\bar{r})$, we use variation of parameters to find $C_1(\bar{r})$ and $C_2(\bar{r})$. The Wronskian is

$$W = \begin{vmatrix} \frac{cosh(\Phi_B \bar{r})}{\bar{r}} & \frac{sinh(\Phi_B \bar{r})}{\bar{r}} \\ \frac{\Phi_B sinh(\Phi_B \bar{r})}{\bar{r}} - \frac{cosh(\Phi_B \bar{r})}{\bar{r}^2} & \frac{\Phi_B cosh(\Phi_B \bar{r})}{\bar{r}} - \frac{sinh(\Phi_B \bar{r})}{\bar{r}^2} \end{vmatrix} = \frac{\Phi_B}{\bar{r}^2}. \tag{S.7}$$

$C_1(\bar{r})$ and $C_2(\bar{r})$ are defined as

$$\begin{aligned} C_1(\bar{r}) &= -\int d\bar{r} \frac{sinh(\Phi_B \bar{r})}{W\bar{r}}(-\Phi_A^2 \gamma\delta \bar{C}_A) \\ &= \frac{\Phi_A^2 \gamma\delta}{2\Phi_B sinh(\Phi_A)} \left[\frac{1}{\Phi_B + \Phi_A} sinh((\Phi_B + \Phi_A)\bar{r}) - \frac{1}{\Phi_B - \Phi_A} sinh((\Phi_B - \Phi_A)\bar{r}) \right] + C_1' \end{aligned} \tag{S.8}$$

and

$$\begin{aligned} C_2(\bar{r}) &= \int d\bar{r} \frac{cosh(\Phi_B \bar{r})}{W\bar{r}}(-\Phi_A^2 \gamma\delta \bar{C}_A) \\ &= \frac{-\Phi_A^2 \gamma\delta}{2\Phi_B sinh(\Phi_A)} \left[\frac{1}{\Phi_B + \Phi_A} cosh((\Phi_B + \Phi_A)\bar{r}) - \frac{1}{\Phi_B - \Phi_A} cosh((\Phi_B - \Phi_A)\bar{r}) \right] + C_2'. \end{aligned} \tag{S.9}$$

Replacing these back into equation (S.6) gives

$$\bar{C}_B(\bar{r}) = \frac{\Phi_A^2 \gamma\delta}{\Phi_B^2 - \Phi_A^2} \frac{sinh(\Phi_A \bar{r})}{\bar{r} sinh(\Phi_A)} + C_1'' \frac{cosh(\Phi_B \bar{r})}{\bar{r}} + C_2'' \frac{sinh(\Phi_B \bar{r})}{\bar{r}} \tag{S.10}$$

and matching the boundary conditions we get C_1'' and C_2'' as

$$\begin{cases} C_1'' = 0 \\ C_2'' = \frac{1}{sinh(\Phi_B)} \left(1 - \frac{\Phi_A^2 \gamma\delta}{\Phi_B^2 - \Phi_A^2}\right). \end{cases}$$

Substituting these expressions back into equation (S.10) gives us the final solution

$$\begin{aligned} \bar{C}_B(\bar{r}) &= \left[1 - \frac{\Phi_A^2 \gamma\delta}{\Phi_B^2 - \Phi_A^2}\right] \frac{sinh(\Phi_B \bar{r})}{\bar{r} sinh(\Phi_B)} + \frac{\Phi_A^2 \gamma\delta}{\Phi_B^2 - \Phi_A^2} \frac{sinh(\Phi_A \bar{r})}{\bar{r} sinh(\Phi_A)} \\ &= \frac{sinh(\Phi_B \bar{r})}{\bar{r} sinh(\Phi_B)} - \gamma\delta\Phi_A^2 \frac{\frac{sinh(\Phi_B \bar{r})}{\bar{r} sinh(\Phi_B)} - \frac{sinh(\Phi_A \bar{r})}{\bar{r} sinh(\Phi_A)}}{\Phi_B^2 - \Phi_A^2}. \end{aligned} \tag{S.11}$$

S.3 Secondary effectiveness factor for the special case of $\Phi_A = \Phi_B = \Phi$

The secondary effectiveness factor (irrespective of the geometry) is given by

$$\eta_{\boldsymbol{B} \to \boldsymbol{C}} = \eta(\Phi_B) - \gamma\delta\Phi_A^2 \frac{\eta(\Phi_B) - \eta(\Phi_A)}{\Phi_B^2 - \Phi_A^2}. \tag{S.12}$$

In the limit where $\Phi_B \to \Phi_A = \Phi$ we have

$$\lim_{\Phi_B \to \Phi} \eta_{\boldsymbol{B} \to \boldsymbol{C}} = \eta(\Phi) - \gamma\delta\Phi^2 \lim_{\Phi_B \to \Phi} \frac{\eta(\Phi_B) - \eta(\Phi)}{\Phi_B^2 - \Phi^2}. \tag{S.13}$$

The limit on the right side of this equation is indeterminate. L'Hospital's Rule can be used here to give

$$\begin{aligned} \eta_{\boldsymbol{B} \to \boldsymbol{C}} &= \eta(\Phi) - \gamma\delta\Phi^2 \lim_{\Phi_B \to \Phi} \frac{\frac{d\eta(\Phi_B)}{d\Phi}|_\Phi}{\frac{d\Phi_B^2}{d\Phi}|_\Phi} \\ &= \eta(\Phi) - \gamma\delta\Phi^2 \frac{\frac{d\eta}{d\Phi}}{\frac{d\Phi^2}{d\Phi}} \\ &= \eta(1 - \frac{\gamma\delta}{2} \frac{d\ln(\eta)}{d\ln(\Phi)}). \end{aligned} \tag{S.14}$$