

Supplementary Data S1

The term appearing in (16) should be read as:

$$\begin{aligned} [diffc_f]_{i,k}^n &= \left(\frac{c_{f_{i,k+1}}^n - 2c_{f_{i,k}}^n + c_{f_{i,k-1}}^n}{\delta \xi^2} \right) \left\{ \frac{1}{R_i^2} + \varepsilon^2 \left(\frac{\partial \xi}{\partial z} \right)_{i,k}^2 \right\} + \left(\frac{c_{f_{i,k+1}}^n - c_{f_{i,k-1}}^n}{2\delta \xi} \right) \\ &\quad \times \left\{ \frac{1}{R_i \left\{ R_i (\xi_k - 1) + R_{tl_i} \right\}} + \varepsilon^2 \left(\frac{\partial^2 \xi}{\partial z^2} \right)_{i,k} + \frac{\varepsilon^2}{R_i^2} \left(\frac{dR}{dz} \right)_i \left((\xi_k - 1) \left(\frac{dR}{dz} \right)_i + \left(\frac{dR_{tl}}{dz} \right)_i \right) \right\} \\ &\quad + \varepsilon^2 \left(\frac{c_{f_{i+1,k}}^n - 2c_{f_{i,k}}^n + c_{f_{i-1,k}}^n}{\delta \xi^2} \right) + 2 \varepsilon^2 \left(\frac{c_{f_{i+1,k+1}}^n - c_{f_{i+1,k-1}}^n - c_{f_{i-1,k+1}}^n + c_{f_{i-1,k-1}}^n}{4\delta \xi \delta z} \right) \end{aligned}$$

The reaction term appearing in equations (17)–(18) can be written as:

$$[reac_{SR}]_{i,k}^n = Da_{SR} \left\{ \left(c_f \right)_{i,k}^n \left(c_{SR}^{\max} - \left(c_{SR} \right)_{i,k}^n \right) - \frac{\left(c_{SR} \right)_{i,k}^n}{k_{eq_{SR}}} \right\},$$

and

$$[reac_{ECM}]_{i,k}^n = Da_{ECM} \left\{ \left(c_f \right)_{i,k}^n \left(c_{ECM}^{\max} - \left(c_{ECM} \right)_{i,k}^n \right) - \frac{\left(c_{ECM} \right)_{i,k}^n}{k_{eq_{ECM}}} \right\}.$$

$$(Da_{ECM} = 8.0 \times 10^5, Da_{SR} = 32.0 \times 10^7, k_{eq_{ECM}} = 3.8 \times 10^2, k_{eq_{SR}} = 5.0 \times 10^6).$$