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Figure 1 Multiscale modelling framework.

Initialise bulk and lattice surface concentrations at time $t = 0$

Intrinsic kinetic modelling: surface concentration change over $\Delta t$

Effective diffusivity modelling: diffusive flux over $\Delta t$

Concentration gradient inside pore

Concentration gradient between bulk and pore

DRE solution (equation 1) over $\Delta t$

$t = t + \Delta t$

If $t \geq$ total time?

Yes

Stop

No

Update bulk and lattice surface concentrations at time $t$

Figure 2. A generic reactant concentration vs. time profile.

Concentration of feedstock (C)

$Slope = \left( \frac{dc}{dt} \right)_{t=t_0}$

$t_0, C_0$

$Slope = \left( \frac{dc}{dt} \right)_{t=t_1}$

$t_1, C_1$

$Slope = \left( \frac{dc}{dt} \right)_{t=t_2}$

$t_2, C_2$

$Slope = \left( \frac{dc}{dt} \right)_{t=t_3}$

$t_3, C_3$

Time (t)
Figure 3. Model mole fraction vs. time profiles and experimental data points of tributyrin, dibutyrin, monobutyrin and methyl butyrate.
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