Supporting Information

Ethylene polymerization via zirconocene catalysts and organoboron activators: an experimental and kinetic modeling study

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1. Population Balance Equations (PBEs)

The PBEs have been derived from the kinetic mechanism (Figure 2)

Active-Sites

$$C_{Act} = [Zr]_0 \tag{SI.1}$$

Deactivated- Sites

$$C_{Deact} = C_{Act} - Y_{0,1} - Y_{0,2} \tag{SI.2}$$

Active-Polymer of type 1, r = 1

$$\frac{d\left[P_{1,1}\right]}{dt} = k_{a2}[C_{Deact}][B] - \left(k_{p1}[M] + k_c\right)[P_{1,1}] + k_{tr1}[M]_l\left(\sum_{s=1}^{\infty}\left[P_{s,1}\right] - \left[P_{1,1}\right]\right) \tag{SI.3}$$

Active-Polymer of type 1, r >1

$$\frac{d\left[P_{r,1}\right]}{dt} = k_{p1}[M][P_{r-1,1}] - \left(k_{p1}[M] + k_c\right)[P_{r,1}] - k_{tr1}[M]_l\left[P_{r,1}\right] \tag{SI.4}$$

Active-Polymer of type 2, r = 1

$$\frac{d\left[P_{1,2}\right]}{dt} = k_c[P_{1,1}] - \left(k_{p2}[M]_l + k_{d2}\right)[P_{1,2}] + k_{tr2}[M]_l\left(\sum_{s=1}^{\infty}\left[P_{s,2}\right] - \left[P_{1,2}\right]\right) \tag{SI.5}$$

Active-Polymer of type 2, r >1

$$\frac{d\left[P_{r,2}\right]}{dt} = k_c[P_{r,1}] + k_{p2}[M]_l[P_{r-1,2}] - \left(k_{p2}[M]_l + k_{d2}\right)[P_{r,2}] + k_{tr1}[M]_l\left(\sum_{s=1}^{\infty}\left[P_{s,2}\right] - \left[P_{1,2}\right]\right) \tag{SI.6}$$

Dead polymer type 1, r =1,2,3,…

$$\frac{d\left[D_{r,1}\right]}{dt} = k_{tr1}[M]_l\left[P_{r,1}\right] \tag{SI.7}$$

Dead polymer type 2, r =1,2,3,…

$$\frac{d\left[D_{r,2}\right]}{dt} = \left(k_{tr2}[M]_l + k_{d2}\right)\left[P_{r,2}\right] \tag{SI.8}$$

2. Bubble-point (P_{bubl}) and (P_{Dew}) pressure of the binary system are calculated using the Equation

$$P_{Bubl} = \sum_{i=1}^{2} x_i P_i^{sat} \tag{SI.9}$$

$$P_{Dew} = \frac{1}{\sum_{i=1}^{2} \frac{y_i}{P_i^{sat}}} \tag{SI.10}$$

where x_i and y_i are the molar fraction of the component i (i = ethylene or toluene) in the liquid and vapor phase, respectively.