Supporting Information

Modeling of the ATRcoP Processes of Methyl Methacrylate and *2*-(Trimethylsilyl) Ethyl Methacrylate under Batch, Semi-batch, and Continuous Feeding: A Chemical Reactor Engineering Viewpoint

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In this work, Tables S1 and S2 are applied.

Table S1. Kinetic equations for reaction components.

Initiator

$$r(RX) = -k_a[RX][C] + k_{da}[R^{\bullet}][CX]$$

Activator

$$r(C) = k_{da}[R^{\bullet}][CX] - k_a[RX][C] + \sum_i \sum_{r=1}^{\infty} k_{da,i}[RM_{i,r}^{\bullet}][CX] - \sum_i \sum_{r=1}^{\infty} k_{a,i}[RM_{i,r}X][C]$$

Deactivator

$$r(CX) = -k_{da}[R^{\bullet}][CX] + k_a[RX][C] - \sum_i \sum_{r=1}^{\infty} k_{da,i}[RM_{i,r}^{\bullet}][CX] + \sum_i \sum_{r=1}^{\infty} k_{a,i}[RM_{i,r}X][C]$$

Primary radical

$$r(R^{\bullet}) = -\sum_i k_{in,i}[M_i][R^{\bullet}] - k_{da,0}[R^{\bullet}][CX] + k_{a,0}[RX][C]$$

Monomer

$$r(M_i) = -k_{in,i}[R^{\bullet}][M_i] - \sum_j \sum_{r=1}^{\infty} k_{p,ji}[RM_{j,r}^{\bullet}][M_i]$$

Living chain

$$r(RM_{i,r}^{\bullet}) = \sum_j k_{p,ji}[RM_{j,r-1}^{\bullet}][M_i] - \sum_j k_{p,ij}[RM_{i,r}^{\bullet}][M_j] + k_{a,i}[RM_{i,r}X][C] - k_{da,i}[RM_{i,r}^{\bullet}][CX]$$
$$-\sum_j \sum_{s=0}^{\infty} k_{t,ij}[RM_{i,r}^{\bullet}][RM_{j,s}^{\bullet}] - \sum_j k_{tr,ij}[RM_{i,r}^{\bullet}][M_j]$$

Dormant chain

$$r(RM_{i,r}X) = k_{da,i}[RM_{i,r}^{\bullet}][CX] - k_{a,i}[RM_{i,r}X][C]$$

Dead chain formed by coupling termination

$$r(RM_rR) = \frac{1}{2} \sum_i \sum_j \sum_{s=0}^{r} k_{tc,ij}[RM_{i,s}^{\bullet}][RM_{j,r-s}^{\bullet}]$$

Dead chain formed by disproportionation termination or chain transfer to monomer

$$r(RM_r) = \sum_i \sum_j \sum_{s=0}^{\infty} k_{td,ij}[RM_{i,r}^{\bullet}][RM_{j,s}^{\bullet}] + \sum_i \sum_j k_{tr,ij}[RM_{i,r}^{\bullet}][M_j]$$

Table S2. Differential moment equations for ATRcoP in a batch reactor.

Zeroth-order moments of living chains, dormant chains and dead chains

$$r(\mu_i^0) = k_{in,i}[R^{\bullet}][M_i] + \sum_{j \neq i} k_{p,ji}\mu_j^0[M_i] - \sum_{j \neq i} k_{p,ij}\mu_i^0[M_j] + k_{a,i}\lambda_i^0[C] - k_{da,i}\mu_i^0[CX]$$
$$-\sum_j k_{t,ij}\mu_i^0\mu_j^0 - \sum_j k_{tr,ij}\mu_i^0[M_j]$$

$$r(\lambda_i^0) = k_{da,i}\mu_i^0[CX] - k_{a,i}\lambda_i^0[C]$$

$$r(\psi^0) = \frac{1}{2}\sum_i \sum_j k_{tc,ij}\mu_i^0\mu_j^0$$

$$r(\phi^0) = \sum_i \sum_j k_{td,ij}\mu_i^0\mu_j^0 + \sum_i \sum_j k_{tr,ij}\mu_i^0[M_j]$$

First-order moments of living chains, dormant chains and dead chains

$$r(\mu_i^1) = k_{in,i}[R^{\bullet}][M_i] + \sum_j k_{p,ji}\mu_j^0[M_i] + \sum_{j \neq i} k_{p,ji}\mu_j^1[M_i] - \sum_{j \neq i} k_{p,ij}\mu_i^1[M_j] + k_{a,i}\lambda_i^1[C]$$
$$-k_{da,i}\mu_i^1[CX] - \sum_j k_{t,ij}\mu_i^1\mu_j^0 - \sum_j k_{tr,ij}\mu_i^1[M_j]$$

$$r(\lambda_i^1) = k_{da,i}\mu_i^1[CX] - k_{a,i}\lambda_i^1[C]$$

$$r(\psi^1) = \sum_i \sum_j k_{tc,ij}\mu_i^1\mu_j^0$$

$$r(\phi^1) = \sum_i \sum_j k_{td,ij}\mu_i^1\mu_j^0 + \sum_i \sum_j k_{tr,ij}\mu_i^1[M_j]$$

Second-order moments of living chains, dormant chains and dead chains

$$r(\mu_i^2) = k_{in,i}[R^{\bullet}][M_i] + \sum_j k_{p,ji}(\mu_j^0 + 2\mu_j^1)[M_i] + \sum_{j \neq i} k_{p,ji}\mu_j^2[M_i] - \sum_{j \neq i} k_{p,ij}\mu_i^2[M_j]$$
$$+k_{a,i}\lambda_i^2[C] - k_{da,i}\mu_i^2[CX] - \sum_j k_{t,ij}\mu_i^2\mu_j^0 - \sum_j k_{tr,ij}\mu_i^2[M_j]$$
$$r(\lambda_i^2) = k_{da,i}\mu_i^2[CX] - k_{a,i}\lambda_i^2[C]$$

$$r(\psi^2) = \sum_i \sum_j k_{tc,ij} (\mu_i^2 \mu_j^0 + \mu_i^1 \mu_j^1)$$

$$r(\phi^2) = \sum_i \sum_j k_{td,ij} \mu_i^2 \mu_j^0 + \sum_i \sum_j k_{tr,ij} \mu_i^2 [M_j]$$

Activator

$$r(C) = k_{da}[R\square][CX] - k_a[RX][C] + \sum_i k_{da,i} \mu_i^0 [CX] - \sum_i k_{a,i} \lambda_i^0 [C]$$

Deactivator

$$r(CX) = -k_{da}[R\square][CX] + k_a[RX][C] - \sum_i k_{da,i} \mu_i^0 [CX] + \sum_i k_{a,i} \lambda_i^0 [C]$$

Monomer

$$r(M_i) = -k_{in,i}[R\square][M_i] - \sum_j k_{p,ji} \mu_j^0 [M_i]$$

Initiator

$$r(RX) = k_{da,0}[R\square][CX] - k_{a,0}[RX][C]$$

Primary Radical

$$r(R\square) = -\sum_i k_{in,i}[M_i][R\square] - k_{da,0}[R\square][CX] + k_{a,0}[RX][C]$$