

Reaction templates in mcPolymer

Table: Reaction templates: M, M1 – monomer, P(n), Q(m) – macromolecular species, X, I, A, B – low molecular species; structure information: SCB – short chain branch, TDB – terminal double bond, MCR – mid-chain radical, MCRBB – mid-chain radical formed by backbiting, DRAD - dormant radical, IRAD – intermediate radical ; k – reaction rate coefficient

template	description	example	model file (.mcPolymer)
initiator $-k \rightarrow I + I$	initiator decomposition	AIBN $-k_i \text{AIBN} \rightarrow I + I$	Styrene
$I + M -k \rightarrow P(1)$	initiation	$I + \text{styrene} -k_p \rightarrow P(n)$	Styrene
$M + M + M -k \rightarrow P(1) + P(1)$	thermal initiation	$\text{styrene} + \text{styrene} + \text{styrene} -k_{th} \rightarrow P(1) + P(1)$	ATRP
$M + M -k \rightarrow P(1) + P(2)$	thermal initiation	$\text{BA} + \text{BA} -k_i \text{BA} \rightarrow \text{ECR}(1) + \text{ECR}(2)$	BA_HT
$P(n) + M -k \rightarrow P(n+1)$ $P(n) + M -k \rightarrow Q(n+1)$	propagation (homo- or copolymerization)	$P(n) + \text{styrene} -k_p \rightarrow P(n+1)$ $\text{PM1M1}(n) + \text{styrene} -k_{p112} \rightarrow \text{PM1M2}(n+1)$	Styrene MMA-S-SG1
$P(n) + Q(m, \text{TDB}) -k \rightarrow R(n+m)$	propagation with macromonomer	$\text{ECR}(n) + \text{MacroMS}(m, \text{TDB}) -k_{p\text{mac}} \rightarrow \text{MCRL}(n+m)$	BA-HT
$P(n) + M -k \rightarrow Q(n+1, \text{SCB})$	propagation + SCB	$\text{MCR}(n) + \text{BA} -k_{pt} \rightarrow \text{SPR}(n+1, \text{SCB})$	BA
$P(n) + P(m) -k \rightarrow D(n+m)$	termination by combination	$P(n) + P(m) -k_t \rightarrow D(n+m)$	Styrene
$P(n) + Q(m) -k \rightarrow D(n+m)$	termination by disproportionation	$\text{SPR}(n) + \text{MCR}(m) -k_{tsm} \rightarrow D(n+m)$	BA
$\text{ECR}(n) + \text{ECR}(m) -k_{td} \rightarrow D(n) + D(m, \text{TDB})$ $\text{ECR}(n) + \text{MCRS}(m) -k_{tdst} \rightarrow D(n) + D(m, \text{TDB})$	termination by disproportionation	$\text{PM1M1}(n) + \text{PM1M1}(m) -k_{td11} \rightarrow D(n) + D(m, \text{TDB})$ $\text{PM1M1}(n) + \text{PM2M2}(m) -k_{td12} \rightarrow D(n) + D(m, \text{TDB})$	BA_HT
$P(n) -k \rightarrow Q(n, \text{MCRBB})$	backbiting	$\text{SPR}(n) -k_{bb} \rightarrow \text{MCR}(n, \text{MCRBB})$	BA
$P(n) + X -k \rightarrow Q(n, \text{DRAD})$	transfer	$P(n) + N -k_c \rightarrow \text{PN}(n, \text{DRAD})$	NMP
$P(n) -k \rightarrow Q(n, \text{DRAD}) + X$		$\text{PN}(n) -k_d \rightarrow P(n, \text{DRAD}) + N$	NMP
$P(n) + X -k \rightarrow Q(n) + I$		$\text{SPR}(n) + \text{Solvent} -k_{ms} \rightarrow D(n) + I$	BA
$P(n) + M -k \rightarrow D(n) + Q(1)$	transfer to monomer	$P(n) + \text{styrene} -k_m \rightarrow D(n) + P(1)$	Styrene
$P(n) + D(m, M) -k \rightarrow D(n) + \text{MCRL}(m, M1)$	transfer to polymer	$\text{SPR}(n) + D(m, \text{BA}) -k_{mp} \rightarrow D(n) + \text{MCRL}(m, \text{BAX})$	BA
$P(n) -k \rightarrow Q(n-s) + D(s)$	fragmentation	$\text{PSCSP}(n) -k_{frac} \rightarrow P(n-m) + \text{PSCS}(m)$	RAFT

template	description	example	model file (.mcPolymer)
P(n,MCRBB) --k--> EQ(n-m) + R(m,TDB) P(n,MCR) --k--> EQ(n-m) + R(m,TDB)	beta scission	MCRS(n,MCRBB) --kbetasc--> ECRS(n-m) + MacroMS(m,TDB) MCRL(n,MCR) --kbetasc--> ECR(n-m) + MacroML(m,TDB)	BA_HT
A --k--> B + C	elementary reaction	RN --kd--> R + N	NMP
A + B --k--> C	elementary reaction	R + N --kc--> RN	NMP