Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Supporting Information for "Multi-scale reactive extrusion modeling approaches to design polymer synthesis, modification and mechanical recycling"

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Table S1: Parameters for Case study 3. Conventional epoxy-amine ones from De Keer *et al.*[1] Other parameters this work, which only considers intrinsic simulations results.

	Equation	*A*	E_a *(kJ/mol)*
Primary amine-acetoacetate - intermolecular	$-PA + -AA \xrightarrow{k_{VU,inter}} -VU + H_2O$	2.51 10^3	43.5
Primary amine curing – intermolecular	$-PA + -EP \xrightarrow{k_{PA,inter}} -SA + -OH$	2.51 10^3	60
Primary amine curing – intermolecular	$-PA + -EP + -OH \xrightarrow{k_{PA,inter,cat}} -SA + -OH$	1.26 10^3	60
Primary amine curing – intramolecular	$-PA + -EP + -OH \xrightarrow{k_{PA,intra,cat}} -SA + -OH$	2.51 10^3	60
Secondary amine curing – intermolecular	$-SA + -EP + -OH \xrightarrow{k_{SA,inter,cat}} -TA + -OH$	3.98 10^3	60
Secondary amine curing – intramolecular	$-SA + -EP + -OH \xrightarrow{k_{SA,intra,cat}} -TA + -OH$	3.98 10^3	60
Vinylogous Urethane - Primary amine – intermolecular	$-VU_1 + -PA_1 \xrightarrow{k_{VU-PA,inter}} -VU_2 + -PA_2$	2.51 10^3	60
Vinylogous Urethane - Primary amine – intramolecular	$-VU_1 + -PA_1 \xrightarrow{k_{VU-PA,intra}} -VU_2 + -PA_2$	2.51 10^3	60
Initial number of molecules so monomers			
Amine	3000		
Epoxy	2100		
Acetoacetate	1900		

Table S2: Parameters formally used in Case study 4 to illustrate the retardation caused by acrylate units during unzipping of an MMA-rich copolymer. A: MMA; B: acrylate unit. Note that $k_{\beta 4}$ is kinetically insignificant in this work as due to the low considered amount of B units in the copolymer (initially 5%) the probability for having both a terminal and penultimate B unit is very small. Hence, for simplicity $k_{\beta 4}$ is taken equal to $k_{\beta 2}$.

Reaction	Rate coefficient (in s^{-1})
$R_{i,AA} \xrightarrow{k_{\beta 1}} R_{i-1,A(B)A} + M_A$	10^5
$R_{i,BA} \xrightarrow{k_{\beta 2}} R_{i-1,A(B)B} + M_A$	10^2
$R_{i,AB} \xrightarrow{k_{\beta 3}} R_{i-1,A(B)A} + M_B$	10^8
$R_{i,BB} \xrightarrow{k_{\beta 1}} R_{i-1,A(B)B} + M_B$	10^2

1. De Keer, L.; Kilic, K. I.; Van Steenberge, P. H.; Daelemans, L.; Kodura, D.; Frisch, H.; De Clerck, K.; Reyniers, M.-F.; Barner-Kowollik, C.; Dauskardt, R. H., Computational prediction of the molecular configuration of three-dimensional network polymers. *Nature Materials* **2021,** 20, (10), 1422-1430.