Supporting information for:

Copolymerization of partly incompatible monomers: an insight from computer simulations.

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Influence of the polymerization scheme parameters on the obtained chain sequences

We investigated the effect of different parameters of the reaction scheme on the obtained chain sequences for the acrylic acid (A)-styrene (S) copolymerization model with $r_A = p_{AA}/p_{AS} = 0.13$ and $r_S = p_{SS}/p_{SA} = 0.38$ and $\varphi_A=0.5$. The initiator concentration was equal to 0.1%, which corresponds to the maximum average chain length of 1000. Four cases were studied: 1) $p_{SA} = p_{AS}=0.01$, no dormant ends ($\tau_A= \tau_S=0$) and no chain termination, $p_t=0$; 2) $p_{SA} =0.001$, $p_{AS}=0.01$, no dormant ends ($\tau_A= \tau_S=0$) and no chain termination, $p_t=0$; 3) $p_{SA} =0.0001$, $p_{AS}=0.01$, no dormant ends ($\tau_A= \tau_S=0$) and no chain termination, $p_t=0$; 4) $p_{SA} = p_{AS}=0.01$, $\tau_A=99$ (A-ends are in the dormant state 99% of time), $\tau_S=9$ (S-ends are in the dormant state 90% of time) and with chain termination, $p_t=1$. The first set of parameters corresponds to that studied in the main manuscript; the second and the third demonstrate the influence of the free parameters of the reaction probability matrix; finally, the fourth models a system with dormant ends and chain termination. The dependences of the dispersity Đ and triad fractions on the total monomer conversion for $\chi=0$ are presented in fig. S1 and S2.
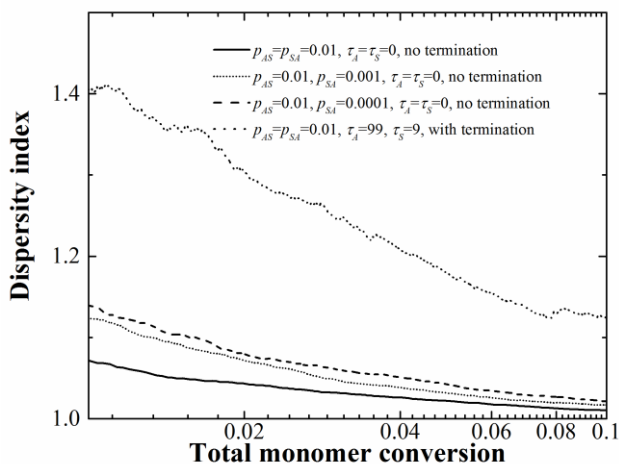

Fig. S1. Dependences of the dispersity Đ on the total monomer conversion for four different sets of reaction scheme parameters.

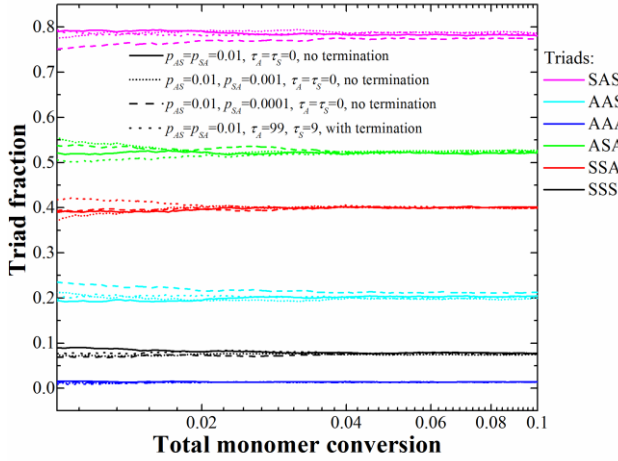[1] Corresponding author. E-mail: gavrilov@polly.phys.msu.ru

Fig. S2. Dependences of the triad fractions on the total monomer conversion for four different sets of reaction scheme parameters.

One can see that the dependences of Đ on total monomer conversion look rather different, especially at low total monomer conversions. The biggest difference is observed for the system with dormant ends and termination because due to the presence of dormant ends not all the chains are growing simultaneously but only the fraction being in the living state, which obviously leads to an increase in Đ; the termination process also increases Đ (at 0.1 total monomer conversion about 20% of chains were terminated). However, this effect becomes much less pronounced with growing total monomer conversion because on average all the chains stay in the living state exactly the same time.

Examination of the triad fractions reveals that the chain sequences are indistinguishable starting from rather small total monomer conversion of approximately 0.04-0.05, i.e. from the stage where the average chain length is much larger than 3 (i.e. the triad length). We will study the systems in the main text at total monomer conversion of 0.1 to be sure that the polymer chains are long enough for PDI not to affect the sequences.

The same is true for the case of nonzero χ. The dependences of the triad fractions on the total monomer conversion for $\chi=1.8$ (which is close to the critical point and therefore is a limiting case for realistic values of χ) is presented in fig. S3.
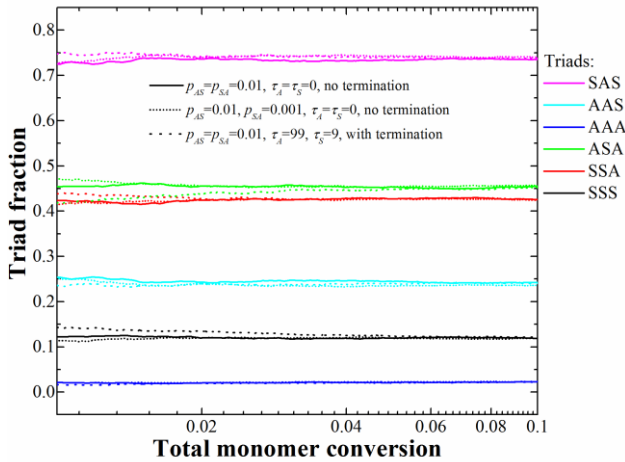

Fig. S3. Dependences of the triad fractions on the total monomer conversion for three different sets of reaction scheme parameters at $\chi=1.8$.

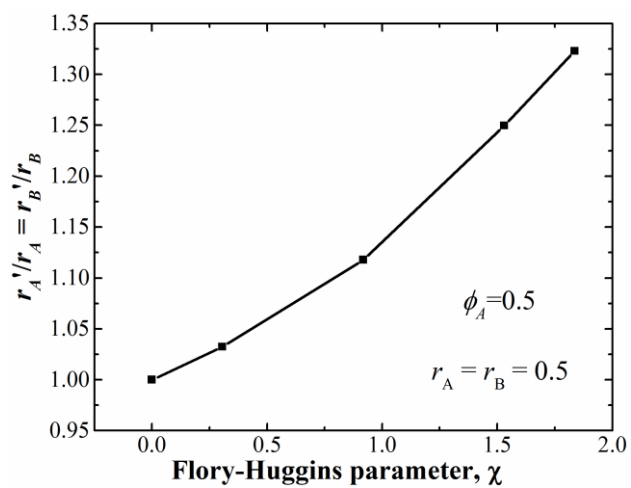**Dependence of the observable reactivity ratios on χ**

Fig. S4 Dependences of the relative increase of the "observable" reactivity ratios $r'_A=r'_B$ compared to the input ratios $r_A=r_B=0.5$ on the Flory-Huggins parameter χ for $\varphi_A=0.5$.