Role of a polymeric component in the phase separation of ternary fluid mixtures: A dissipative particle dynamics study

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Supplementary Information

In Fig. S1, we present the isosurface of the evolving system for chain length $L_p = 16,$ and 64 at two different times $t = 100$ and 500, whereas, the isosurface for $L_p = 32$ is already shown in Fig. 3a. After the quench, as expected for symmetric mixtures, we observe the formation of A-rich (open space), B-rich (blue patch), and C-rich (green patch) blobs with all three types of interfaces, namely AB, BC, and CA present. We plot the number density profiles of A-beads ($\rho_A(z)$) along the z-direction corresponding to $L_p = 16$ (in Fig. S1c), $L_p = 32$ (in Fig. 3d), and $L_p = 64$ (in Fig. S1d) at three different times ($t = 100, 300,$ and 500). The spreading of curves with time evidently supports the coarsening phenomenon. The density profiles (e.g., at $t = 500$) clearly demonstrate that the average domain size is larger for shorter polymer chain length ($L_p = 16$) as compared to that for other two chain lengths $L_p = 32$, and 64, respectively.

Next, we present the evolution snapshots (isosurfaces) at $t = 100$ and 500 for $k_a = 5$ (Fig. S2a) and 60 (Fig. S2b), respectively. The domain sizes are noticeably larger for the system with $k_a = 5$ as compared to that for $k_a = 60$, at a given instant of time. This can be anticipated as the polymer chains with a smaller value of k_a will be more flexible to move. In such systems, A and B- beads can be accommodated in their domains in a faster and easier way as compared to the system with larger k_a (more rigid/less flexible polymers). This is also apparent from Figs. S2c and S2d where we plot the number density profile of A-type beads along the z-direction for $k_a = 5$ and 60 at three different times as mentioned and indicated by the symbols.

In Fig. S3a, we compare $g_{AB}(r)$ of a critical simple ternary fluid (A:B:C=1:1:1) with the critical polymer-containing ternary fluids, for three different stiffness (k_a) values at $t = 200$. The shifting of the peak position of $g_{AB}(r)$ towards lower r validates that the average domain sizes of A- or B-type beads become smaller with increasing stiffness of the polymer chains. Further, we plot the scaled correlation, $D(r,t)$ vs. r/l_D at $t = 200$ to signify the domains of C-components in Fig. S3b. An apparent deviation of the scaling functions from each other in different cases (represented by various symbol types) confirms the dependence of scaling functions on the chain stiffness. Overall, the average domain size of A- or B-type beads changes clearly by replacing one simple fluid component (C) with a polymeric component in the phase separating ternary (ABC) fluid mixtures. The change in polymer chain stiffness also has a reasonably good effect on the domain size.

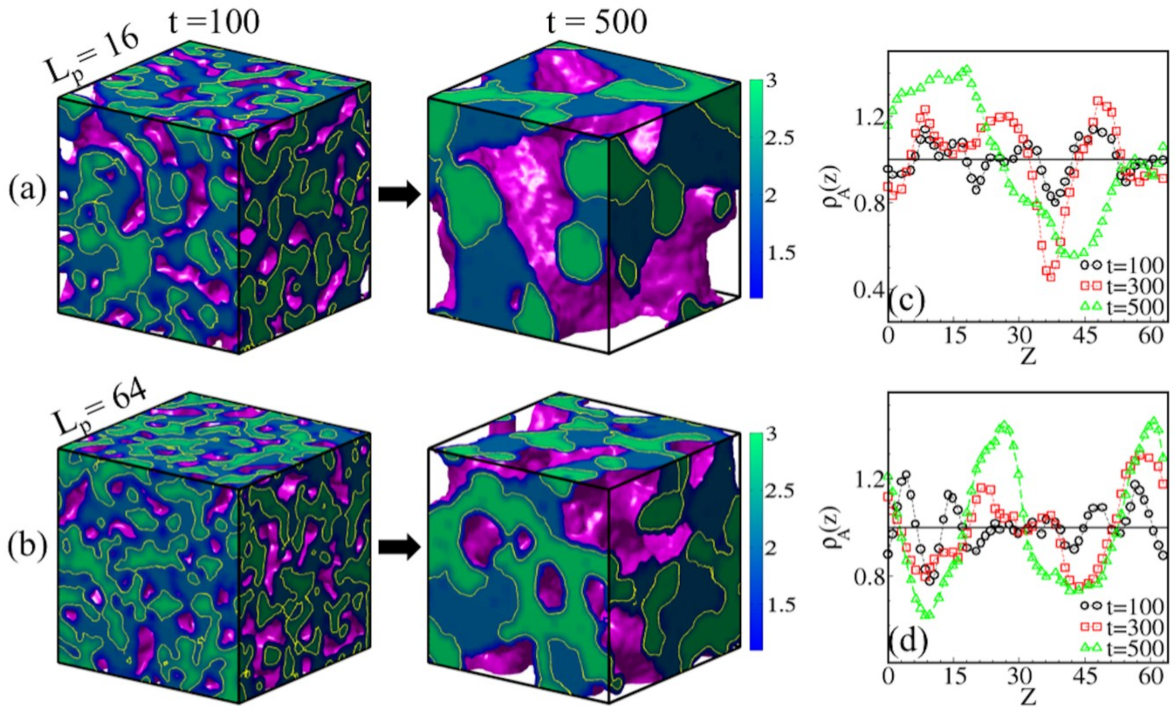

Figure S1: Evolution morphology of the ternary fluids corresponding to two different lengths of polymers (C-type molecules) for the case where $A{:}B{:}C = 1{:}1{:}1$ and $k_a = 20$. (a-b) represent evolution snapshots (isosurfaces) at $t = 100$ and 500 for $L_p = 16$ and 64 respectively. (c-d) Number density profile of A-type molecules along the z-direction, at three different times $t = 100$, 300, and 500 represented by the symbols for the respective chain lengths. The $L_p = 32$ case is already shown in Fig. 3a and 3d.

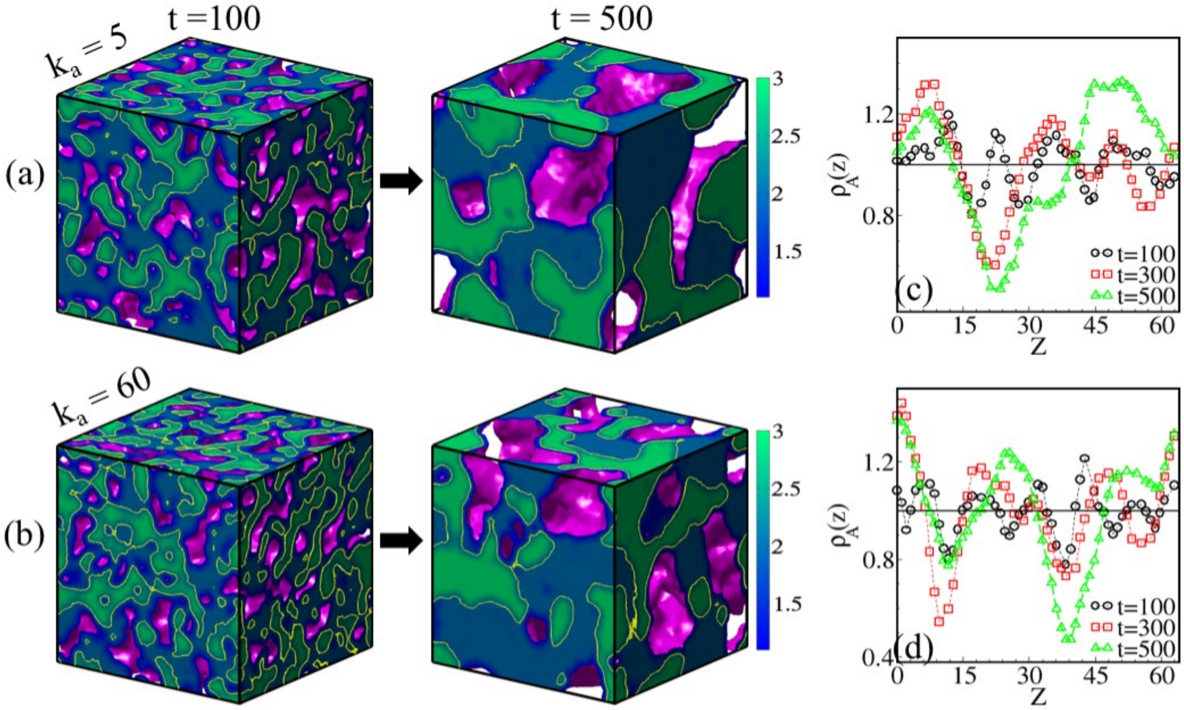

Figure S2: Evolution morphology of the ternary fluids (with one polymeric component) for $k_a = 5$ and 60 for the case where A:B:$C = 1$:1:1 and $L_p = 32$, in each case. (a-b) Display evolution snapshots at $t = 100$ and 500 for $k_a = 5$ and 60, respectively. (c-d) Number density profiles of A-type molecules at three different times, $t = 100$, 300, and 500 shown by the symbols for the respective k_a values of the polymers. For the case $k_a = 20$, Fig. 3a and 3d are referred.

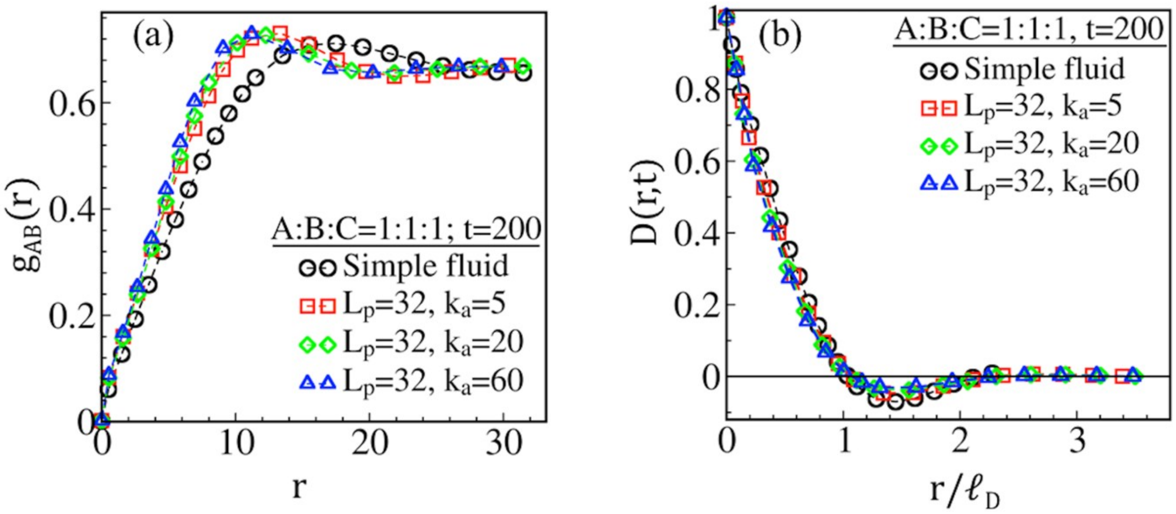

Figure S3: (a) Comparison of g_{AB} of simple fluid mixture and mixtures with one polymeric component for three different k_a values (shown by different symbol types) at $t = 200$. Here, we consider the critical mixtures (A:B:C=1:1:1) only. (b) Comparison of $D(r,t)$ vs. r/l_D at $t = 200$ shows a deviation of the scaling functions from each other in different cases represented by the various symbol types.