Model validation

Dissipative particle dynamics (DPD) was successfully used for modeling the dynamics of polymers and particles in incompressible Newtonian fluids.³ To further validate our model, we compare the results for cross-stream migration of nanoparticles and polymer chains in microchannels with numerical and experimental data from the literature. We carry out simulations for dilute suspensions in a quiescent fluid and in a Poiseuille channel flow with intermediate Reynolds numbers (Fig. S1). We find good agreement between the results of coarse-grained DPD simulations and molecular dynamics (MD) simulations of dilute polymer solutions,^{9b} which indicates that the DPD model properly captures the lateral migration of polymer chains in channel flows (Fig. S1a) and can predicts the polymers distribution at equilibrium (Fig. S1b). Insignificant discrepancy between the results can be attributed to the fact that we use bead density to characterize the polymer distribution, whereas the MD results are for the center of mass density distribution. Furthermore, our simulation for dilute suspension of rigid nanoparticles for Re ~ O(10) accurately captures the Segre-Silberberg effect.^{9a} Specifically, Fig. S1c shows that particles form a distribution with two concentration peaks at a distance ~ 0.28H from the center of the channel, as observed in experiments.^{9a}

Velocity flow field

To gain insight into the hydrodynamic effects leading to the lateral migration of rigid particles and polymer chains in microchannels with posted walls, we plot in Fig. S2 the circulating secondary flows arising inside microchannels. Here, we show the y and z components of fluid velocity averaged along the channel. Figure S2a shows that vertical posts do not create circulatory flow structures, whereas tilted posts introduce local circulatory flows shown in Figs. S1b and S1c. Furthermore, the posts with $\alpha = 45^{\circ}$ create fluid streams in which fluid in the gap between posts moves downwards (see Fig. S1b), whereas when $\alpha = -45^{\circ}$, fluid the gap moves upwards (see Fig. S1c). These secondary flows created by tilted posts give rise to the dissimilar cross-stream migration behavior of mixture entities, which in turn modifies the particle and chain distributions in microchannels.



Fig. S1 Chain distribution of a dilute polymer solution (a) in Poiseuille flow and (b) at equilibrium. Square and circle symbols represent, respectively, the bead density profile from the DPD simulations and the center of mass density distribution from MD simulations.^{9b} In these simulations, Re ~ O(10) and Pe ~ O(100). Panel (c) shows the bead density profile of a dilute suspension of rigid particles in a Poiseuille flow. The vertical dashed lines show the maximum of particle concentration observed in experiments.^{9a} Here, Re ~ O(10) and Pe ~ O(10).



Fig. S2 Cross-stream velocity field in a pressured-driven flow in microchannels decorated with arrays of regular rigid posts. Panel (a) shows the velocity field in a channel with posts normal to the channel surface. Panels (b) and (c) show the velocity fields in channels with posts tilted, respectively, along ($\alpha = 45^{\circ}$) and against ($\alpha = -45^{\circ}$) the flow direction. Velocities are averaged along the channel. The dashed lines show the outer contours of posts attached to the channel floor. The colors represent the magnitude of flow vorticity in the *x* direction.