Polymer gels, in particular polyacrylamide (PAM) preformed particles gels, are widely used in enhanced oil recovery (EOR) applications. We model the gel dynamics on multiple length scales. Using the Dissipative Particles Dynamics (DPD), we focus on the interactions of the PAM gel particle with the oil-water interface at the nanoscale; using a continuum three dimensional gel Lattice Spring Model (gLSM), we focus on the dynamics of the mm-scale thermoresponsive gels in temperature gradients.

**DPD simulations of PAM gels spreading at oil-water interfaces.** We developed a DPD framework to simulate PAM gel network interacting with the oil-water interface. We designed the gel matrix as a diamond-like lattice, where the lattice points are occupied by the tetrafunctional crosslinks (MBAM) connected by the acrylamide polymer chains. The details of the model are given in the Ref. and are based on the model of PAM polymer chains proposed in Ref. We performed DPD simulations using LAMMPS simulation package.

The dynamics of the gel adsorption onto the oil/water interface is shown in Fig. 1. Initially, we equilibrate the gel sample in water and place it within the water phase away from the interface. The gel and oil beads are shown in red and green, correspondingly, and for clarity water beads are not shown. Periodic boundary conditions are applied in all directions. The size of the sample is chosen to be 3x3x3 diamond-like cells (as defined in Ref. with \( N_x = 30 \) polymer beads between the crosslinks.

Gel first docks onto the oil interface from the water keeping its original shape close to spherical and then begins spreading over the interface minimizing the number of unfavorable contacts between the water and oil (Fig. 1a-c). The side (Fig. 1c) and the top (Fig. 1d) view of the gel show that it adopts a ‘pancake’-like shape at equilibrium.

To quantitatively characterize an extent of the gel spreading, we follow the evolution of its size and shape by calculating a radius of gyration, \( R_g \), and a shape anisotropy, \( \kappa^2 \) (Fig. 1e). The shape anisotropy, \( \kappa^2 \), is derived from the eigenvalues of the gyration tensor, \( S_g \), via its first and second invariants \( I_1 = \lambda_1 + \lambda_2 + \lambda_3 \) and \( I_2 = \lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1 \) as \( \kappa^2 = 1 - 3 \frac{I_2}{I_1^2} \). As long as the gel remains in the water phase, \( \kappa^2 \) remains close to zero, which corresponds to a shape close to spherical (Fig. 1e). As the gel approaches the interface and begins to spread over it, \( \kappa^2 \) increases until it reaches a value close to 0.25, which corresponds to a planar shape.

**Fig. 1.** Gel adsorption onto the oil/water interface at times: (a) 306 ns, (b) 452 ns, (c-d) 3646 ns. (e) Radius of gyration \( R_g \), black curve and shape anisotropy \( \kappa^2 \), blue curve.

![Fig. 2.](image-url) (a) The shape anisotropy, \( \kappa^2 \) (dashed curves, right axis) and the radius of gyration, \( R_g \), (solid curves, left axis) as a function of \( N_x \). The circles correspond to the gel with the matching number of polymer beads. (b) The number density of gel in x-z plane integrated in y-direction.
Different aspects of this work were presented by all the participants in the project: by O. Kuksenok at the invited lecture at ACS National Meeting, New Orleans, LA, March 18–22, 2018; by C. K. Choudhury at the MRS 2017 Fall Meeting, Boston, MA, Nov 26-Dec 1, 2017, and by Yao Xiong at the 2018 SEM Annual Conference, Greenville, SC, Jun 4-7, 2018.

References