First-Principles Based Models, Methods, and Experiments on Reversible Shear Thickening Fluids for Drilling, Stimulation, Conformance Control, and EOR Operations

Proposal Summary

We propose a **collaborative research effort on polymer colloidal science applied to enhanced and improved oil recovery technologies (EOR/IOR),** focused specifically on the application of unique first-principles based multiscale modeling and simulation methods, and novel experimental material synthesis and characterization capabilities, to: **understand, validate, steer design, and optimize synthesis of smart nano-polymeric fluids for EOR/IOR**.

The multiscale nature of our proposal enables us to develop improved understanding of the atomistic level mechanisms underlying shear induced modulation of viscosity of polymer fluids, and then to use this new understanding to design, synthesize, and validate new EOR/IOR fluids with controllable dynamic shear response.

The general expected outcomes include:

1. New multiscale simulation tools for simulating complex fluid phenomena
2. New validated materials providing controllable dynamic shear response
3. Improved research & education capacity on complex fluid phenomena at the CPG

More specifically, this effort will considerably enhance the fundamental understanding of the atomistic nanoscale mechanisms responsible for self-induced shear thickening/thinning in "smart" polymer fluid compositions applicable to EOR/IOR.

Key technologies developed at the MSC-Caltech will be optimized and applied, including: high-accuracy *ab initio* methods that capture electronic correlations; rule-based universal force fields to characterize the mechanics and conformational dynamics of crystalline and amorphous polymer blends as a function of shear and flow, including interaction with solvents and porous surfaces; first-principles based reactive force fields and reactive hyperdynamics methods for describing and characterizing reactive fluids, fluid-solid interfaces, aqueous phase reactions and surface chemistry, etc. over millions of atoms and multi-second timescales; coupled atomistic reactive dynamics with dissipative particle dynamics models to characterize the large-scale dynamic shear response mechanisms in nano-fluids to endogenous and exogenous stimuli and to understand reactive fluid formation, and electro-kinetics effects between solid and charged liquid phases; first-principles thermodynamic method to determine entropy and free energy flow information from short dynamics simulations capable of identifying nano-fluid compositions that meet the target reversible shear-thickening response; and a systematic multi-objective parameter optimization framework to couple the computational scales. We will connect the "self-adaptive thickening/thinning" feature of polymer fluids to fundamental atomic level information.

We will validate these new concepts from the theory and simulation by state-of-the-art rheological experiments relating polymer-fluid compositions to the response to internal or external stimuli, including the electro-kinetic interactions of the fluid in porous media, and reversibility mechanisms and triggers. Thus we will determine the correlation between the rheometer responses with the pressure-to-flow relationship in the porous media by using physical simulation in conjunction with numerical simulation.

We expect to design "smart" polymer agent solutions that would have both "fluid viscosifying" and "fluid diverting" functions when applied in the polymer-augmented water flooding EOR/IOR operations. In particular, such a novel polymer fluid will be able to show

shear thickening properties within the high-perm channels in reservoirs such that to divert fluids to oil-rich zones, yet will return to the base fluid viscosity when reaching the high shear regions of the injector and producer. Therefore, the desirable polymer additive would be able to automatically retard water flow in high-perm zone with less slowing down in the low-perm zone. Such "self-adaptive thickening/thinning" agent that could do both EOR/IOR and in-depth conformance control, so as to significant improve the volumetric sweep efficiency (VSE), is the cutting research focus of this proposal.

The key personnel: Goddard, Jaramillo-Botero, Tang, and Jiang bring more than 120 years of experience relevant to this project with expertise spanning fundamental theory, modeling, and experiments on complex polymer and nanoscale systems.

These advances should:

1. Put the CPG and their industrial sponsors at the forefront of developing the new generation of rheological fluids needed for EOR/IOR;
2. Leverage the MSC-Caltech and PEERi technologies in coupling simulation and experimental into a closed cycle and integrating them to rapidly advance petroleum research;
3. Prepare a new class of researchers at KFUPM, Saudi Armco, and other partners capable of incorporating the continuing advances in simulation and materials technology relevant to EOR/IOR into the KFUPM curriculum and into industrial practice.