

Dissipative particle dynamics simulation of wettability alternation phenomena in the chemical flooding process

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Abstract Wettability alternation phenomena is considered one of the most important enhanced oil recovery (EOR) mechanisms in the chemical flooding process and induced by the adsorption of surfactant on the rock surface. These phenomena are studied by a mesoscopic method named as dissipative particle dynamics (DPD). Both the alteration phenomena of water-wet to oil-wet and that of oil-wet to water-wet are simulated based on reasonable definition of interaction parameters between beads. The wetting hysteresis phenomenon and the process of oil-drops detachment from rock surfaces with different wettability are simulated by adding long-range external forces on the fluid particles. The simulation results show that, the oil drop is liable to spread on the oil-wetting surface and move in the form of liquid film flow, whereas it is likely to move as a whole on the water-wetting surface. There are the same phenomena occurring in wettability-alternated cases. The results also show that DPD method provides a feasible approach to the problems of seepage flow with physicochemical phenomena and can be used to study the mechanism of EOR of chemical flooding.

Keywords Wettability alternation · Dissipative particle dynamics · Enhanced oil recovery · Chemical flooding · Mesoscopic mechanics

1 Introduction

One of the most fundamental characteristics of an oil-bearing formation which determines the hydrocarbon production efficiency is its wettability [1–5]. The wettability of an oil formation can be alternated when some ampholytes are adsorbed on the rock surface, which usually occurs in the chemical flooding process with surfactant-aided fluids.

The microscopic origins of wetting alternation have not been well understood by now. What make the problem complex is the multiple scale associated with this physical phenomenon, of which both molecular and macroscopic effects are of importance and not all of which can be resolved by experimental studies [6, 7]. The traditional continuum-based approaches model the phenomenon on a macroscopic scale and ignore fully the microscopic effects. Microscopic molecular dynamics (MD), on the other hand, requires excessive CPU times and efforts before the macroscopic effects become visible. In fact, the scales of interest in this problem lie between the microscopic and macroscopic levels; consequently, a simulation method feasible on the mesoscopic scale is required. Since dissipative particle dynamics (DPD) was initially proposed by Hoogerbrugge and Koelman, and modified by Groot et al. [8–11], it is taken as a coarse-graining version of MD and becomes an appealing mesoscopic computational method. DPD has been used to study a wide range of physicochemical problems and flow problems of complex fluids including polymer or surfactant [12–14]. In our opinion, one of the obvious advantages of DPD is that, as a discrete particle method, it deals with interfaces in

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multiphase fluid and physicochemical phenomena occurring in multi-component fluid in a convenient way, and can be used to study the seepage flow problem in chemical flooding, where both the hydrodynamic and the physicochemical phenomena are described at the mesoscopic level.

This paper is organized as follows. An introduction of DPD model are given in Sect. 2 together with boundary condition and integration scheme used in our simulation. In Sect. 3, DPD simulation results are presented for wettability alternation, wetting hysteresis phenomena and the process of oil-drop detachment from rock surface, followed in Sect. 4 by a brief summary.

2 Methodology

In the model of DPD, the system is represented by particles, each corresponding to a cluster of real molecules. The system is specified by the position and momentum of each particle and the motion of each particle are governed by Newton's Law. The particles interact with each other via pairwise conservative, random, and dissipative forces that locally conserve momentum and lead to a correct hydrodynamic description. The force exerted on particle i is given by

$$F_i = \sum_{j \neq i} [a_{ij}(1-r_{ij}/r_c) + \sigma w^R \xi_{ij} - \gamma w^D (\mathbf{r}_{ij} \cdot \mathbf{v}_{ij})] \check{\mathbf{r}}_{ij},$$

where three parts of the sum represent the conservative, dissipative and random forces acting on particle i by particle j , respectively, and the sum runs over all other particles within a certain cutoff radius r_c , which is usually taken as the unit of length. Here, a_{ij} is an interaction parameter between particle i and particle j , and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the separation vector of the particles with distance r_{ij} and unit vector $\check{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$. σ and γ are random and dissipative coefficient, respectively, and w^R and w^D are the fluctuation and dissipation weight function, respectively. The random variable ξ_{ij} is selected from a Gaussian distribution with zero mean and unit variance and independent for each ij pair of particles and time step. $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity between particle i and particle j .

One of the two weight functions w^R and w^D can be chosen arbitrarily and the other function is determined by this choice, and there is also a relation between the two

coefficients σ and γ . In summary:

$$w^D = [w^R]^2 = (1 - r_{ij}/r_c)^S, \quad \text{and} \quad \sigma^2 = 2\gamma K_B T,$$

where K_B is Boltzmann constant, T is the Kelvin temperature of the system, and $K_B T$ is taken as the unit of energy. The Schmidt number S is set at 2 in our simulation.

For the molecules constructed by connecting several DPD particles together, a spring force F_i^S should be added. There are several types of spring forces adopted in literatures, and Hookean spring force is the simplest one, which is given by

$$F_i^S = \sum_j K_s (r_{ij} - r_{eq}) \check{\mathbf{r}}_{ij},$$

where the sum runs over all particles to which particle j is connected, K_s and r_{eq} are the spring constant and equilibrium spring distance, respectively, and r_{eq} is set at 0 in our simulation. Nonlinear spring models, including finite extensible nonlinear elastic (FENE) springs model, are used for the polymer [15, 16].

There are two main forms of boundary conditions: periodic and enclosed. Periodic boundary conditions (PBC) are used to model an infinitely-sized system, whereas, enclosed boundary conditions reduce the particles' freedom of movement to the extents of the system. There are many possible approaches [17–20] to what may happen to a particle when it contacts a wall boundary, depending on the category of application. In this simulation, the boundary condition with bounce-back reflection is adopted.

The feature that dissipative forces depend on the relative velocities in DPD makes the equations of motion nonlinear. This, in turn, implies that a self-consistent time-integration scheme should be employed, otherwise numerical artifacts would be produced. In our simulation, Leap–Frog integration scheme is adopted [21].

3 Simulation and discussion

There are totally five kinds of DPD particle in the simulation. Herein, the surfactant, that is sodium dodecylbenzene sulfonate (SDS) used broadly in oilfield, is divided into two DPD particles as shown in Fig. 1. The structures on the left of the solid line in SDS molecular are selected as the hydrophobic tail (denoted with “T”), in which we use the hydrogen atoms instead of the tails. Accordingly, the right part is selected as the hydrophilic head (denoted with “H”). Dodecane, water

Fig. 1 DPD particle structure models of SDS (H and T), dodecane (O) and water (W)

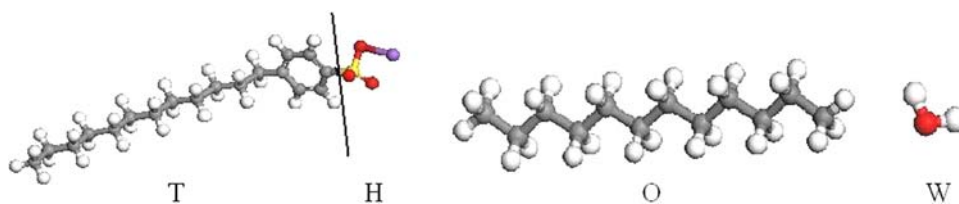


Table 1 The interaction parameter in DPD simulation

	W	O	H	T
W	30.0			
O	61.8	30.0		
H	32.4	47.2	30.0	
T	67.1	32.1	48.3	30.0

and solid are represented by one particle denoted by “O”, “W” and “S”, respectively.

The interaction parameters between two kinds of DPD particle can be evaluated according to the mixing energy and Flory–Huggins interaction parameters, which can be obtained by Blend simulation based on Monte Carlo methods [22]. The calculated conservation parameters a_{ij} are given in Table 1 (temperature $K_B T$ is set at 1.2 and particle density is set at 3).

The simulations are performed on dual-core CPU (2.8GHz) and software developed in terms of FORTRAN 95. The computation domain is a cube with sizes $10r_c \times 17r_c \times 20r_c$, and solid wall boundary conditions are imposed along Y -axis direction and PBC are imposed on the other directions. The random and dissipative forces are defined by the parameters $\sigma = 3$ and $\gamma = 3.75$, respectively. The time step Δt and spring force coefficient K_s are set at 0.02 and 4, respectively. In order to maintain the flow, an external body force F_e can be imposed in the simulation.

Fig. 2 DPD simulation of wettability alteration of water-wet to oil-wet, the oil drop is surrounded by surfactant particles (water particles are hidden in all the results)

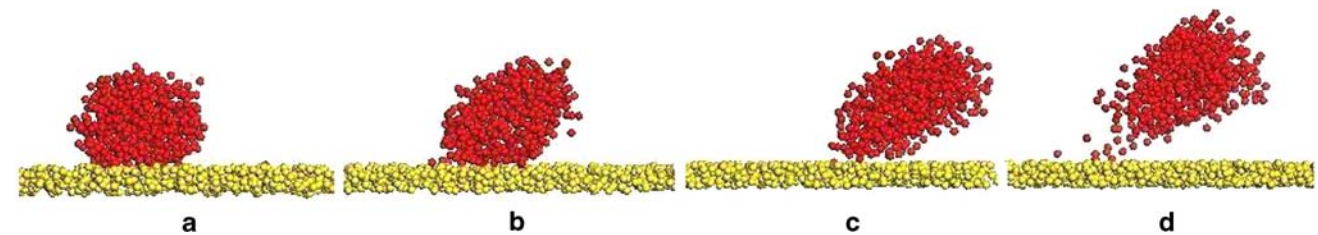
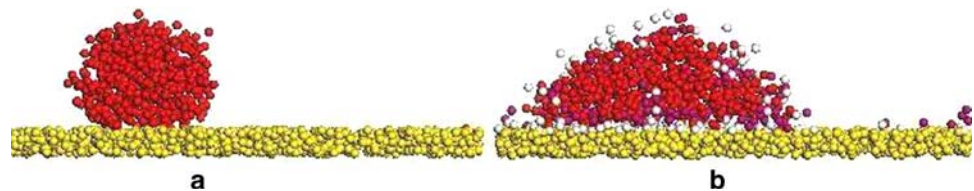


Fig. 3 DPD simulation of the process of oil drop detachment from a water-wetting surface, the oil drop is finally removed as a whole. **a** Initial time; **b** after 1,200 steps; **c** after 2,400 steps; **d** after 3,600 steps

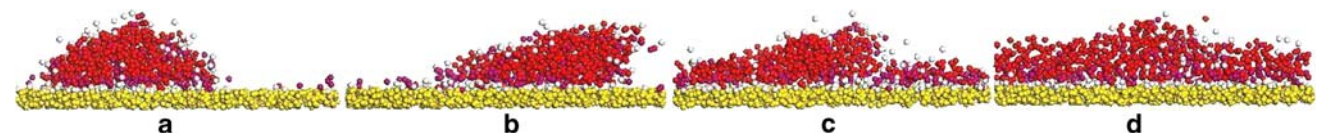


Fig. 4 DPD simulation of the process of oil drop detachment from a water-wet to oil-wet wettability-alternated surface, the oil drop is finally removed in the form of liquid film flow. **a** Initial time; **b** after 2,400 steps; **c** after 5,200 steps; **d** after 10,000 steps

3.1 Wettability alternation of water-wet to oil-wet

In this section, DPD simulation results are presented, in which the equilibrium contact angle of oil drops situated on a water-wetting solid interface is modeled, as shown in Fig. 2a. It is reasonable to choose proper values that can lead to results in good agreement with real physical pictures (e.g. the contact angle). The interaction parameter between particles W, O and particle S are set at 35 and 55 in our simulation, respectively. The wettability alternation phenomena are simulated for surfactants-added fluids, as shown in Fig. 2b, where the interaction parameter between particles H, T and particle S are set at 10 and 40, respectively. Here, the ratio of particles in the simulations are $W/O = 14/1$ and $W/O/H-T = 134/10/3$, respectively.

By adding an external body force $F_e = 0.02$ in Z -axis direction, the processes of oil droplet detachment from a water-wetting and a water-wet to oil-wet wettability-alternated surface are shown in Figs. 3 and 4, respectively. It is worth mentioning that the wetting hysteresis phenomenon, which is presented by advancing angle and receding angle, is clearly shown in the process.

3.2 Wettability alternation of oil-wet to water-wet

A simulation of wettability alternation of oil-wetting to water-wetting is shown in Fig. 5, where the interaction parameters between particles W, O and particle S are set at 55 and 35,

Fig. 5 DPD simulation of wettability alteration of oil-wet to water-wet, the oil drop is surrounded by surfactant particles

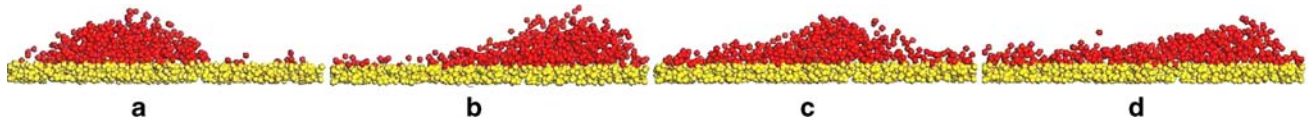
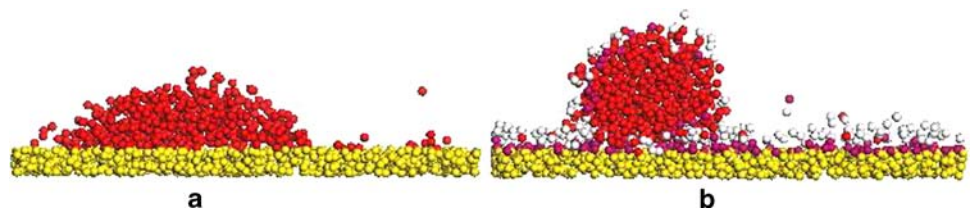


Fig. 6 DPD simulation of the process of oil drop detachment from an oil-wetting surface, the oil drop is finally removed in the form of liquid film flow. **a** Initial time; **b** after 2,400 steps; **c** after 5,200 steps; **d** after 10,000 steps

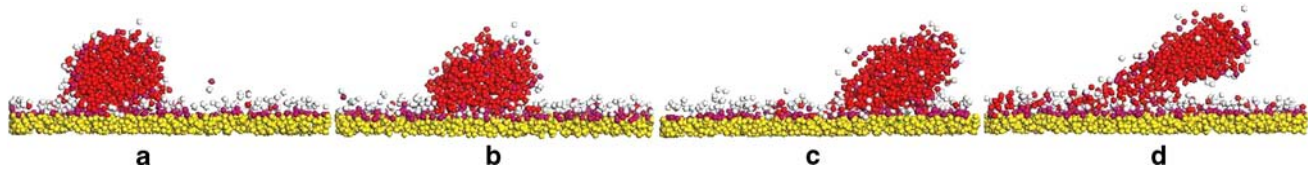


Fig. 7 DPD simulation of the process of oil drop detachment from an oil-wet to water-wet wettability-alternated surface. **a** Initial time; **b** after 1,200 steps; **c** after 2,400 steps; **d** after 4,400 steps

respectively, and the interaction parameter between particles H, T and particle S are set at 40 and 10, respectively. By adding an external body force $F_c = 0.02$ in Z-axis direction, the processes of oil droplet detachment from an oil-wetting and an oil-wet to water-wet wettability-alternated surface are, respectively, shown in Figs. 6 and 7.

3.3 Discussion

In general, water-wetting formations favor oil production over water. An oil drop situated on a rock surface can be removed as a whole under hydrodynamic actions, as shown in Figs. 3 and 7, when the solid surface is water-wetting including the case of oil-wet to water-wet wettability alternation. There would be some differences when the heterogeneities of porous media are considered. Entrapment of oil drops dispersed in water is liable to occur when the fluid passes through throats, building up pressure due to Jamin effect [4]. Opposite to the case of water-wetting, oil drops would spread on the oil-wetting surface to form an oil film which can move in the form of liquid film flow, as shown in Figs. 4 and 6. Therefore, it is now recognized that an appropriate mixed wettability could provide maximum oil production efficiency [1], especially for low-permeability oil reservoirs.

It is necessary to mention that the effect of surfactant concentration on the simulation results is crucial, and detailed descriptions will be given in other papers.

4 Summary

DPD simulation results are presented for wettability alternation induced by the adsorption of surfactants on solid surface, and the wetting hysteresis phenomena and the process of oil-drop detachment from solid surface are also simulated. These results show that the mesoscopic DPD model can be successfully used to assess the performance of surfactant-aided oil-recovery fluid. More systematic studies on the application of DPD to seepage flows with physico-chemical phenomena in the chemical flooding will be presented in the near future.

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