Abstract

We present a framework for the application of multiscale science and technology to Enhanced Oil Recovery [EOR] by propagating physical models for wetting and flow from the molecular scale to the scale of pore networks in reservoir rock. The framework contains dedicated, computational and experimental platforms for performing calibrations at critical length scales. The approach enables us to scientifically investigate and validate liquid-solid interactions from the nanometer to the micrometer scale and to deploy experimentally calibrated, multi-scale flow simulations in a digital representation of a given rock pore network. Built on reservoir-specific data input such as measured rock tomographies and chemical compositions, the nanoscience-based flow simulations are expected to predict with higher accuracy the efficiency of a specific EOR agent for improving oil displacement in a pore network with feature sizes spanning six orders of magnitude on the physical length scale. We discuss a conception that integrates the experimentally calibrated, multiscale flow simulations with a computational system for providing reservoir-specific EOR strategies. In particular, we report progress in the research and development of the computational and experimental platforms and discuss the challenges and opportunities related to their application within future EOR solutions.

1. Introduction

Enhanced Oil Recovery [EOR] comprises a set of exploration technologies and practices for increasing oil production. A key challenge is to scientifically understand and accurately predict the efficiency of a particular EOR technique for a given reservoir. The chemical and physical processes that promote oil displacement occur on the length scale of nanometers, i.e. twelve orders of magnitude smaller than the scale of a typical reservoir. In order to create an accurate EOR simulation technology, the interactions between reservoir constituents, such as rock and oil, and EOR materials, such as polymers and nanoparticles, need to be quantitatively captured and linked across the physical length scales. As discussed by Feger et al. (2014), in order to validate the interaction models for their correctness, it is necessary to perform dedicated experimental measurements at critical length scales. In a rigorous physical bottom-up conception of EOR, quantitative models of molecular scale interactions between solids and liquids need to be implemented and validated for capturing the liquid wetting behavior at the nanoscale under well-defined conditions. The critical physical parameters that define the system’s behavior at the nanoscale are then identified, extracted, and incorporated into multi-scale models for quantifying fluid flow properties. In a next step, the multi-scale flow model is deployed and tested in a computational representation of the reservoir’s connected pore network at the micrometer scale. Ultimately, the validated microscopic flow properties can be aggregated and transformed into macroscopic quantities for prediction and evaluation of production scale effects.

To simulate fluid flow properties across scales, one challenge is to sum over cubic meters or kilometers the flow contributions from all the individual pores, in which nanoscale phenomena control behavior. Another is to reconcile the characteristic differences between the various simulation methods: at the nanoscale are discrete molecules driven individually by forces, and at the macroscale is the continuum of the bulk oil and gas. In between are various hybrid pictures, such as Lattice Boltzmann methods based on particle kinetics as discussed by Chen and Doolen (1998), pore network models as proposed by Fatt (1956) in which representative pores can be modeled with high resolution and then
linked together to represent porous media, and mesh-free methods such as Smoothed Particle Hydrodynamics as discussed by Müller et al. (2003). One key to simulating across scales is to find appropriate links, informed by both the relevant phenomena to be simulated as well as by the type of output that is needed to connect to the next simulation in the sequence. Another key that is essential for overall accuracy is to identify simulations that can be verified by experiments and vice versa.

![Figure 1. The Big Picture: From Nanoscale Science to Enhanced Oil Recovery Technology and Solutions.](image)

In Figure 1, we show the roadmap from EOR nanometer scale science via computational flow simulation technologies to EOR advisory solutions. The main scientific challenges are the quantification of nanoscale wetting properties, the quantification of multiphase flow in nanoscale porous media, including surface interactions, and the inclusion of novel functional materials for enhanced oil recovery, including the computational design of nanoparticles and polymers. All scientific core challenges need to be addressed by suitable combinations of experimental and theoretical research approaches. By using appropriate model linkage techniques, the nanoscale wetting and flow models are then scaled and integrated within a computational representation of reservoir rock. The computational rock representation is obtained from measured, reservoir-specific rock data having feature sizes ranging from the nanoscale to the microscale. The computational rock representation together with an experimentally calibrated, nanoscale flow model form the Nano-EOR flow simulation platform. This platform can now be connected to additional data sources and deliver physically and chemically consistent, high-accuracy predictions of key metrics, such as permeability, through an EOR advisor solution to the reservoir engineer. Ultimately, the provision of reservoir-specific EOR strategies will improve planning, decision making, and risk management in exploration and production. In the following, we discuss in more detail the progress in the research and development of individual platform components and their relation to the Nano-EOR flow simulation platform.

2. The Nanowetting Platform and Nanoparticle Design & Optimization

For quantifying the interactions between solid and liquids at the nanometer scale, we have developed a combined experimental and simulation platform. The nanowetting platform is suited for quantifying the wettability of various surfaces and to analyze how wettability is affected by e.g. chemical additives for EOR. In order to simulate nanoscale oil droplet shapes, we use appropriate molecular scale modeling techniques that account for effects such as the local surface roughness. The simulations are validated within this approach by well-defined experimental procedures. For the experimental verification of liquid droplet shapes at the nanometer scale, we apply atomic force microscopy [AFM] and high-resolution optical microscopy at a dedicated device surface. As demonstrated by Steiner et al. (2015), the experimental nanowetting platform allows to determine topography and contact area of sessile nanoscale oil droplets having volumes of the order of attoliters.
In order to simulate the interaction of attoliter-sized oil droplets situated at nanoscale glass surfaces surrounded by nitrogen, we have used Classical Molecular Dynamics [CMD] and Coarse-Grained Molecular Dynamics [CGMD] as discussed in detail by Giro et al. (2015). The motivation for choosing CMD and CGMD approaches is twofold: [i] coverage of length scales ranging from a few nanometers to several hundreds of nanometers and [ii] inclusion of surface roughness effects. CMD is a suitable method for simulating systems at the molecular level, i.e. nanometers in length and nanoseconds in time, in an all-atom fashion. We have simulated a flat glass surface sized 30nm x 30nm in x and y directions, see Figure 2a. After t=3ns, the CMD simulation reaches a steady state and we obtain a decane droplet with a base diameter of 18.3nm and a height of 4.2nm. This model system constitutes a physically consistent, molecular scale representation of nanoscale surface wetting. The CMD simulated decane droplet contains 2257 decane molecules.

In order to scale up the model system with the CGMD method, we have grouped a set of atoms in an artificial bead, capturing the interaction between them with an effective pair potential obtained by mapping from CMD simulations, see Figure 2b. In Figure 2c, we show a CGMD decane droplet with a base diameter of 130nm and a height of 32nm. On this larger scale, the surface corrugations modify the droplet tails at the three phase contact line by about 3 nm. As a result, for droplets with base radii of 100nm and above the deviation in droplet height determination, due to surface roughness, can be of the order of 10%. For smaller droplets, the surface topography in the immediate local vicinity of the droplet is relatively smooth and can thus be represented by a flat surface in a good approximation.

Figure 2. Nanowetting and Nanoparticle Design for Enhanced Oil Recovery. (a) A decane droplet (in light blue) at a glass surface (in red/yellow) surrounded by nitrogen gas (represented in dark blue). The droplet has a base diameter of 18.3 nm, a height of 4.2 nm, and contains 2257 decane molecules. (b) Schematic representation of coarse-grained (CG) mapping from the all-atom molecular dynamics model system depicted in (a). CG beads are represented as transparent spheres. (c) A decane droplet (light blue) at a rough glass surface (red/yellow) surrounded by nitrogen gas (dark blue). The droplet has a base diameter of 130 nm, a height of 32 nm, and contains 591,657 decane molecules. (d) 3D decane droplet profiles obtained from AFM measurements. (e) Topography measurement of a decane droplet at a glass surface and droplet shape fit by a Bessel Function expansion (lower panel); data and fit profile along y=0μm (upper panel). The gray shaded area represents an effective surface potential in the coarse-grained thermodynamical model discussed in the text. (f) Hydroxylated silicon nanoparticles (spheres represented in red, yellow) at the water/decane interface (water represented in red/white; decane represented in blue/white). The nanoparticles have diameters of 3nm, 5nm, and 7nm, respectively (from left to right).

In Figure 2d we show a three-dimensional droplet profile obtained by performing AFM measurements on spatially isolated, nanometer scale decane droplets deposited at an amorphous glass surface. To link experimental measurements and molecular dynamics simulations to mesoscale models, we have developed a coarse-graining technique based on thermodynamics, which allows us to bridge the gap in scales, from nanoscopic to macroscopic. In addition, it allows us link molecular-level kinetics to bulk phenomena. At the nanoscale, a droplet's non-trivial curvature and its ratio of surface area to volume are significant indicators of the underlying molecular scale interactions. We analyze both experimental and simulated droplet shapes by fitting a measured or simulated droplet's surface to a Bessel Function expansion and thereby extract the droplet's shape information. In the example shown in Figure 2e, lower panel, the measured droplet is well-represented by four Bessel terms. Having a droplet's shape captured in a model fit, we identify in a next step an effective surface potential that reproduces the same shape within the thermodynamical model. The shaded area in the droplet cross sectional view shown in Figure 2e, upper panel, represents this effective potential. Next, by using the thermodynamical droplet model, we calculate a droplet's binding energy which we expect to be a key
metric for the wettability or affinity of the droplet to a particular surface at the nanoscale. It is important to note that, because of the complex droplet shapes, the assessment of contact angle at the nanoscale can be highly ambiguous, which favors a thermodynamic model as this relies on the entire droplet shape and not on contact angle. Furthermore, the thermodynamic model allows to straightforwardly include temperature and chemical effects which is desirable for extrapolations towards reservoir conditions. From a model linkage perspective, we can use the thermodynamic model also to tune the effective interaction terms to reproduce experimentally validated droplet shapes and profile inflection points within Lattice Boltzmann [LBM] simulations as discussed by Wolf et al. (2009). Overall, we obtain good agreement between simulated and experimental droplet shapes and the nanoscale wetting properties can now be scaled up within the thermodynamic model approach.

In order to design and investigate novel functional materials such as nanoparticles for their efficiency as EOR agents, nanoscale materials modeling capabilities need to be developed and integrated within the nanowetting computational platform. For optimizing important nanoparticle parameters such as material compositions, size, and shape we have performed molecular dynamics simulations with hydroxylated silicon nanoparticle; see Figure 2f. By changing the nanoparticle diameter from 3nm to 7nm, we significantly modify the nanoparticle wettablity at the decane/water interface. The larger nanoparticle penetrates much deeper into the decane oil which, for example, results in higher stability of nanoparticle based oil-in-water emulsions. We are currently calculating key parameters with molecular scale simulations that quantify nanoparticle diffusion as well as nanoparticle-nanoparticle, nanoparticle-fluid, and nanoparticle-rock surface interactions for integration within a mesoscale Smoothed Particle Dissipative Dynamics model as discussed by Español and Revenga (2003). With this procedure, we expect to predict how nanoparticles change the surface wettability and emulsion formation in a multiscale porous network representation of reservoir rock.

3. The Nanofluidics Platform

![Image of nanofluidics platform](image)

Figure 3. Nanofluidics Platform for Enhanced Oil Recovery. (a) Photograph of a silicon-based nanofluidic chip encapsulated with a glass cover; the chip dimensions are 4cm x 4cm. (b) Scanning electron micrograph displaying one fluidic channel within the chip. The intra-channel features are an array of nanoscale pillars (pillar width, height=400nm). (c) Cross-sectional scanning electron micrograph showing the fluidic channel with intra-channel features and the glass cover. (d) Snap shot of fluid flow taken with an optical camera. The intra-channel flow is visualized by laser-excited fluorescent beads. The overlay shows the experimental velocity distribution within the channel. (e) Corresponding LBM flow simulation performed within the same channel geometry.
In order to validate the linkage of nanoscale wetting to microscale flow, we have developed combined experimental and computational platform that involves Lab-on-Chip devices with nanoscale intra-channel features. The devices contain a channel system with constrictions that allow to study liquid flow properties with well-defined geometrical boundaries from the nanoscale to the microscale. High flexibility in chip design allows us to implement various geometrical representations of reservoir rock with device surfaces that can be modified through chemical functionalization. The dedicated flow chips are built on silicon wafers using CMOS semiconductor process technology discussed by Nishi and Doering (2000). This approach enables fabrication of intra-channel features with dimensions smaller than 1µm, see Figure 3b. The fluidic chip is enclosed by a glass cover that enables the application of high-resolution optical microscopy for the investigation of flow behavior within the device channels. The glass cover contains access ports which can be connected to an external liquid injection/flow control system. Flow in the devices is characterized with a measurement setup by optically exciting fluorescent beads in the liquid with a LED and recording the fluorescence signature of the beads with a CCD camera. Correlation analysis between successive fluorescence images allows quantification of flow velocity distributions, similar to the method reported by Taylor et al. (2010), inside the fluidic channel, see Fig.3d. The measured flow properties in the device channel are then used to calibrate multiscale flow simulations such as the LBM simulations shown in Figure 3e which are performed within the same geometrical boundaries. The nanofluidics platform is currently being used to investigate flow at small scales and to perform permeability studies with liquids relevant to EOR. The validated flow models will be deployed in the computational representation of a reservoir rock’s porous media network which is discussed in the following section.

4. The Digital Rock Analysis Platform

An accurate computational representation of a reservoir rock’s pore network at the micro- and nanoscale can be established based on tomographic imaging data as discussed in and provided by the following references (Dong and Blunt, 2009; Madonna et al., 2013; Prodanovic et al., 2015). The microscopic structure of the rock is represented by a three-dimensional x-ray attenuation map where different phases [rock matrix, pore space, mineral inclusions] appear as different gray levels and/or textures. Typically, image processing techniques are used to localize the phases in a given tomographic rock sample, defining the geometry of the pore network. Subsequently, a morphological analysis is performed to extract key parameters such as connectivity, surface-to-volume ratio, curve skeleton, and fractal dimension that characterize the porous network. Finally, based on the computational representation of the connected pore network, fluid flow simulations are performed to assess the rock’s porous flow properties.

In order to generate a digital reconstruction of a rock sample and characterize its pore network, we have used the computational workflow depicted in Figure 4a. The workflow starts by loading a grayscale micro-tomography image...
from an open library as provided by Prodanovic et al. (2015). In a next step, a 2-voxel radius mean filter is applied which is followed by an image segmentation step as reported in the following references (Glasbey, 1993; Shanbhag, 1994; Li and Tam, 1998). The procedure delivers a binary rock representation as the one shown in Figure 4b. Subsequently, the enhanced Hoshen-Kopelman algorithm introduced by Hoshen et al. (1997) is used to locate all pore clusters and eliminate the non-connected pores. This enables to establish the connected porous network fraction that enables flow across the rock. Finally, morphological properties of the pore network such as the surface-to-volume ratio, fractal dimension, porosity, and skeleton can be extracted and quantified. The example shown in Figure 4 is that of a Berea Sandstone with 400³ voxels at 5.345 µm resolution. We estimate that 19.5% of the voxels are associated with pore space [porosity], up to 75% of which are at the surface [surface-to-volume ratio], as shown in Figure 3c for different algorithm parameters reported by Neumann et al. (2016). This result quantifies the impact of liquid-solid interactions on fluid flow. The mass-radius fractal dimensions following Landini and Rippin (1993), the pore space, and the pore surface of the rock matrix in Figure 4d are found to be very close to 3, as expected. Finally, the pore skeleton is obtained and the spatially-dependent pore size distribution is shown in Figure 4e.

Based on the computational representation of the connected pore network of a given reservoir rock sample, we are currently embedding multi-scale flow simulations with experimentally validated nanoscale liquid-solid interactions for assessing the influence of EOR additives such as polymers or nanoparticles on permeability and oil displacement. Ultimately, as shown in Figure 1, the Nano-EOR flow simulation platform will form the core module of a system for providing EOR strategies as an advisory service to the reservoir engineer.

5. Summary and Conclusions

In summary, we have presented a framework for the application of multiscale science and technology to enhance oil recovery based on computational and experimental platforms at nanoscopic and microscopic length scales. We have introduced a computational system that leverages the experimentally calibrated, multiscale flow simulations for providing reservoir-specific EOR strategies. Specifically, we have discussed the progress made in the research and development of the computational and experimental platforms for application within future EOR solutions. In conclusion, the approach enables us to [i] scientifically investigate and validate liquid-solid interactions from nanometer to micrometer scales, [ii] deploy and test experimentally calibrated, multi-scale flow simulations in a digital representation of a reservoir-specific rock pore network, and [iii] to accurately predict the efficiency of a particular EOR material for oil displacement, ultimately allowing us to devise EOR strategies for a given field. A novel multiscale science-enabled flow simulation technology with higher prediction accuracy, if provided as an advisory service to the reservoir engineer, will enable reservoir-specific EOR strategies for better planning, decision making, and risk management in O&G exploration and production.

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7. References


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