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Smart Water flooding: Part 2

Important input parameters for modeling and upscaling workflow

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Smart Water flooding: Part 2 - Important input parameters for modeling and upscaling workflow

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Important input parameters for modeling and upscaling workflow



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Objective and target audience

This document presents some guidelines on how to conduct numerical investigations of the physicochemical effects of Smart Water flooding on different length scales.

The National IOR Centre of Norway (NIORC) has developed several simulation tools. The objective of this report is to describe how three NIORC-developed simulation tools BADChIMP, IORCoreSim, and IORSim, can be used to investigate Smart Water effects on different length scales. We present which input parameters are needed by the simulation tools, and we discuss which processes these tools are suited to study.

When working with different length scales, one of the challenges is how to upscale results obtained from smaller scales, i.e., pore and core scale experiments or simulations, to the field scale. Here, three relevant questions are: 1) how far do the Smart Water effects propagate into a reservoir? 2) What is the effect of reservoir temperature on Smart Water behavior? 3) How is the oil release, observed on core scale, related to the oil production from a field?

This document targets research scientists planning to perform either pore scale simulations, core scale simulations, or field scale simulations for Smart Water studies.

The technical level of the document is targeting an industry engineer.

Introduction

In this recommended practice, we will define Smart Water as an injection fluid, with waterlike viscosity, that has a different ionic composition than the formation water, thus "Low Salinity" is a subset of Smart Water.

Upscaling of Smart Water requires knowledge of the flow functions, relative permeabilities and capillary pressure, at different scales (see Figure 1). Traditional upscaling deals with how to translate core scale flow properties to grid block scale. In this process one use core scale data or a geo-model to populate a fine gridded reservoir simulation block. The upscaling task is to determine average properties of the large block, such as saturation, porosity, permeability, and flow functions, that are consistent with the fine gridded blocks. The goal is to get the same relationships between flow rate and pressure drop for the homogenous block, as the fine gridded block. This process can be done in a mathematical consistent way in the capillary or viscous limit. Upscaling of relative permeabilities and capillary pressure is a well-known process in the industry and therefore not a topic in this report. We recommend that one uses one of the existing upscaling procedures on lab data or experience-based data to determine or estimate flow functions that represents the state when the porous media is flooded with an inert (formation water) brine and the state when a modified (Smart Water) brine is flooded through the core.



Figure 1 Illustration of different system sizes, from a single pore (left), via a network of pores and core scale, to field scale (right).

The focus in this report is on what we call "chemical upscaling of Smart Water effects". Then the relevant questions become:

- 1. How long does the injection water stay "smart"? When the injection water enters the reservoir in the near well zone, it will interact with the formation and the composition will change.
- 2. How does the reservoir temperature impact Smart Water performance? The injection water usually has a temperature much lower than the reservoir, thus the brine will heat up as it flows from the injector to the producer. Is the historical flooding of the reservoir important (beyond the cooling effect)? Injecting seawater into the reservoir will lead to mineralogical changes in the reservoir. If Smart Water is injected in tertiary mode, the secondary water flooding with seawater might impact the performance of Smart Water.
- 3. Are the mechanisms for oil release on the core scale important? If a core scale measurement of Smart Water injection gives, e.g., 10% additional oil, will the positive (or potentially negative) effect on the field be dependent on the actual underlying pore scale mechanism?

Our strategy to answer these questions has been to study processes on the pore-, core- and reservoir-scales. Hence, the length scales involved span from nm to km. To successfully include a process on the core scale we must first understand it on the pore scale. In this recommended practice report, we will describe the numerical approaches to investigate the questions above.

The report does not have all the answers, but it tries to highlight important features to be aware of when trying to obtain such answers.

The experimental study of Smart Water is described in the recommended practice report "Smart Water flooding: Part 1 – Laboratory workflow for screening EOR potential" (Mamonov, Strand, Puntervold, & Piñerez Torrijos, 2021).

Methodological approach and validation

In general, a fluid, not in equilibrium with the reservoir it is injected into, will start to equilibrate with the formation. These processes will change the chemical composition of the injected fluid. The interaction with the formation can lead to changes in the wetting state, dissolution and precipitation of minerals, and redistribution of fluids due to osmotic effects. Among these, we have focused on changes in wetting state and the mineralogical changes. Fluid chemistry and temperature are the two most important variables to describe and understand these changes. We therefore need to model both the transport of chemical species and temperature changes.

The two main transport mechanisms for fluid systems are advection and molecular diffusion. On scales where the interaction between rock and fluid is modeled by Darcy's law, one would also include dispersion to effectively model the complex flow paths in the pore space. On the pore scale (nm-mm scale), diffusion is the dominating transport mechanism under reservoir conditions. On the core scale (cm scale) one needs to include all three transport modes, while on the field scale (m-km scale) advection and dispersion are the dominating modes of transport.

Wettability alterations are linked to changes in surface energies. On the pore scale, these alterations are given as changes in contact angles between the fluid interfaces and the pore walls. On the core and field scales, wettability changes are effectively modeled as changes in relative permeability and capillary pressure curves.

Mineralogical changes are slow developing processes. They do not cause gradients in the chemical species concentrations on the pore scale but will slowly change the pore geometry. On the core scale, or even field scale, these changes are governed by a rate constant that gives a typical time scale for fluid and rock to reach equilibrium.



Figure 2 Schematical representation presenting the levels of physical details in the numerical models and at what length scales the simulators are applied.

The NIORC has developed numerical tools for simulating the physicochemical effects of Smart Water flooding behavior on different length scales. The simulators developed for this purpose include BADChIMP, a lattice Boltzmann (LB) based pore scale fluid dynamics solver, and the continuum scale based IORCoreSim and IORSim. These simulation tools span from the pore scale, describing the behavior in the nm (10⁻⁹ m) to mm (10⁻³ m) range, all the way up to reservoir scale, describing the behavior in the m to km range (see Figure 2).

On the pore scale, the flow behavior is described by classical laws of nature. Pore scale simulations may to a large degree be set up as numerical experiments. These simulations are therefore a great tool to

understand the exact mechanisms resulting in the overall flooding behavior. In principle, these simulations are valid on all scales and are only limited by length scales where atomistic behavior becomes important and molecular dynamics need to be accounted for. However, the fine spatial resolution needed in these simulations make them computationally heavy and sets a practical limit on the system size. Given state-of-the-art computational power, it is currently realistic to simulate multiphase flow systems ~1 mm³.

The customary go-to method to capture the behavior on a larger scale is to utilize effective multiphase flow and transport simulators taking effective quantities such as relative



Figure 3 Schematics presenting how different Smart Water experiments and simulations relate.

permeability curves as input. These models, contrary to the pore scale models, rely on other methods, e.g., core flooding experiments, to obtain the necessary flow functions. Ideally, pore scale simulations would directly provide the necessary input to the larger scale simulators. However, core flooding experiments are typically conducted on \sim 7 cm long cores with a diameter of \sim 3 cm, while pore scale simulations use samples of \sim 1 mm³. This discrepancy in length scales means, for instance, that boundary conditions applied in the core experiments are not directly transferable to the pore scale system. In other words, it is not possible, at present, to set up a numerical pore scale experiments. Figure 3 shows a schematical representation of how Smart Water experiments and simulations may be related.

The Geochemical model

One of the strengths in the set of software presented in this report is that all of them have implemented the same geochemical solver. The geochemical solver is an extended model based on the HKEF EOS (Helgeson, Kirkham, & Flowers, 1981). The original HKEF EOS does not consider interactions between ions and surfaces, but this is rectified in our current model. A technical and detailed description of the model is given in (Hiorth, Jettestuen, Cathles, & Madland, 2013). The geochemical solver has been benchmarked with other state-of-the-art geochemical solvers, such as PHREEQC (Hiorth, Cathles, & Madland, 2010). We have used it to predict changes in surface charge on carbonates and silicates and successfully compared the results with data.

The geochemical model can predict changes in reservoir chemistry, given appropriate input. The geochemical solver require input that is consistent with mineralogical data obtained at the core scale. To some extent, one may use information from the formation water composition to check the model. The strategy is then to use core scale information to give an appropriate mineralogical composition of the rock. The geochemical solver will, based on the mineralogical data, temperature, and reservoir pressure, predict the composition of the formation water. If the predicted composition compares well with observations, this can serve as a quality assurance of the mineralogical data.

The geochemical solver can also predict how the water chemistry changes when a brine with a different composition than the formation water is injected. These changes could cause minerals to precipitate or dissolve, and the geochemical solver calculates the flux of mass between the fluid phase and the rock. From the mass flux it is possible to estimate changes in porosity. In many cases, models can predict how the surface area changes with mineral precipitation. These changes can, for instance, be directly related to permeability changes. This is the approach we apply to model precipitation of silica gel in water-shut-off operations. Silicate is injected and when the temperature increases, the pH is lowered and/or the salinity is changed, silicate precipitates. And, in turn, the permeability is reduced.

Pore scale simulations

All the physical and chemical behavior observed on the larger scales have its origin at the pore scale. To truly understand larger scale behavior, one must understand the dynamics of the cooperative pore scale mechanisms. Simulations and micromodel experiments give qualitative insight into physical and chemical mechanisms. This is used to construct conceptual models that can be implemented in the core scale simulator. In the following sections, we point out different effects to be aware of, and the situations commonly encountered, when doing pore scale simulation of Smart Water systems.

Simulating advection-diffusion in compressible fluid flow

The standard LB fluid models have finite sound speeds, as is common to most forward computational fluid dynamics (CFD) numerical schemes. This gives rise to density changes (compressibility effects) in the simulations that can cause unphysical gradients in the chemical species concentrations using standard LB advection-diffusion solvers. If the system is far from equilibrium, this effect is usually insignificant. However, for systems close to chemical equilibrium, these spurious numerical effects can be enough to make an oversaturated solution undersaturated. This could have major implications for the simulated results. In our pore scale simulations, we have addressed this by modelling the absolute concentration as a product of fluid density and relative concentration, since the relative concentration is the governing variable for chemical reactions. This method reduces compressibility effects by many orders of magnitude and yields reliable simulation results (Aursjø, Jettestuen, Vinningland, & Hiorth, 2017).

Dissolution/Precipitation on the pore scale

The seepage velocities for reservoir flow at the Norwegian Continental Shelf (NCS) are in the range of cm to meters per day. In this flow regime, we know that diffusion dominates on the pore scale. However, on the core scale, advection cannot be disregarded, maintaining transport of chemical species out of the core. In the pore scale model, we can mimic this fluid advection by including a source-term expression in the effective diffusion equation describing the evolution of the chemical species concentrations in the system. This source term is derived from known core scale quantities. Say we inject fluid into a core sample, with cross sectional area of *A* and length *L*, at a volumetric injection rate *Q*, and the core has a porosity of $\varphi = V_p/(AL)$. The average flow velocity in the pore space will, assuming incompressible fluids, then be $\langle u \rangle = Q/(\varphi A)$. Or, equivalently, $\langle u \rangle = u_D/\varphi$, where $u_D = Q/A$ is the Darcy velocity in the system. The injected fluid has a constant molar concentration of φ_{in} . If diffusion dominates on pore scale, the fluid going out of our simulated volume will have a molar concentration equal that of the bulk average concentration $\langle \varphi \rangle$ in the system. We can therefore approximate the average concentration gradient over our system, of length *l*, to be $(\langle \varphi \rangle - \varphi_{in})/l$. Putting this all together and rearranging, we end up with a source term

$$R(\varphi) = \frac{u_{\rm D}}{\varphi l} (\varphi_{\rm in} - \langle \varphi \rangle) = \frac{QL}{V_p l} (\varphi_{\rm in} - \langle \varphi \rangle).$$

This replaces the advective term in the full advective-diffusion equation (Vinningland, Jettestuen, Aursjø, Madland, & Hiorth, 2017). And this gives an efficient model where end-effects are avoided.

It is difficult to obtain reliable values for the rate constants for use in rate equations for precipitations and dissolution of minerals. Values from the literature can be orders of magnitude different from each other, even for quite simple systems. In core scale experiments, it also observed that using standard rate constants give a poor match with experiments. One

reason for this is that when secondary minerals precipitate, they will, on the pore scale, do so in a heterogeneous manner. Here, some nucleation sites could completely dominate the precipitation process. Another effect is that precipitated minerals will shield the principal mineral leaving it unaffected. Finally, microporosity contribute to mass exchange only through Fickian diffusion. Figure 4 shows the changes in microstructure in chalk cores flooded with MgCl₂.



Figure 4 SEM micrographs of two chalk cores. To the left, an unflooded core and, to the right, a core flooded with MgCl₂.

By matching simulations to long-term flooding experiments, running over several years, it was observed that the effluent concentrations from only the first days of the experiments could be matched well using literature values for the rate constant. When simulating later stages of the experiment, it was necessary to effectively reduce the rate constant for dissolution by a factor of 10⁴. To deal with these complications we suggest partitioning the rate equation for dissolution into three terms, so that

$$\frac{\Delta m}{\Delta t} = (A_{\text{fast}} + k_{\text{cov}}A_{\text{cov}} + k_{\text{slow}}A_{\text{slow}})J.$$

Here, $\Delta m/\Delta t$ is the rate of change in mass of the dissolving mineral, *J* is the mass flux given in the literature, A_{fast} represents the fast-dissolving part of the surface, A_{slow} is the slow–dissolving part of the surface, and A_{cov} is the part of the surface that is covered by the secondary precipitated mineral. k_{cov} and k_{slow} are dimensionless factors (typically \ll 1) that reduce the rate of dissolution. These surface area variables are time dependent and must be included in the simulations. The values for the parameters can now be found by history matching the effluent concentrations or by targeted pore scale simulations. A similar expression is found for the precipitated minerals and is described in more detail in (Pedersen, et al., 2016).

Relative permeability simulations

The ideal situation for obtaining relative permeability curves from pore scale simulations would, of course, be to simulate a complete core sample. From our experience with one-to-one comparison between microfluidic two-phase experiments and simulations, there is little reason to doubt that such a simulation would produce a good approximation to measured relative permeability curves. However, the computational demands for such a simulation make it unfeasible.

The common approach to extract relative permeability curves from pore scale simulations is to impose periodic boundary conditions on a smaller geometry. Without periodic boundaries, one must specify both inlet and outlet boundary conditions. This would introduce unwanted boundary effects that could dominate the behavior for small geometry simulations. But even simulations of smaller geometries suffer from high demand on both temporal and spatial resolution. To obtain a set of relative permeability curves, it is necessary to run a single twophase flow simulation for each fixed saturation level. In these simulations, the overall flowrate is maintained at a prescribed value through a time-varying spatially constant body force. This body force is, together with the resulting Darcy velocity of the individual fluid phase, used to determine the relative permeabilities of the fluid phases. Changing saturations are accomplished by modifying the initial fluid configurations. To assure that the final flow dynamics, and subsequently the measured relative permeability, are not correlated to the initial fluid configuration, the simulations must run sufficiently long. What "sufficiently long" means in this context is a topic for continued research. A minimum would be to let the fluid flow through at least 1 pore volume.

The typical creep-flow encountered in a reservoir is described by a low Capillary number $Ca = \mu u/\sigma \sim 10^{-5}$, where μ is a measure of the viscosity, σ is the surface tension between the oil and water phase, and u is the typical velocity of the flow. One characteristic feature of low-capillary-number flows are the large speed differences related to the creep-flow in a reservoir and the local movement of oil-water interfaces. Even though the overall creep-flow is slow, the momentary movement of capillary interfaces overcoming local capillary thresholds are typically rapid. To correctly capture these rapid movements, it is necessary to have a small simulation timestep. In the LB pore scale simulator, we have parameters σ_{LB} and μ_{LB} which numerical values are limited upwards and downwards, respectively. An optimistic value for $\sigma_{LB}/\mu_{LB} \sim 10$. Comparing to the typical Ca $\sim 10^{-5}$, would give us a LB velocity $u_{LB} \sim 10^{-4}$ grid units per timestep.

Given a segmented representation of a $1000 \times 1000 \times 2000 \ \mu\text{m}^3$ large porous system, consisting of ~ 50 × 50 × 100 pores, with a voxel resolution of $1 \ \mu\text{m}^3$, each pore will be represented by ~ 20 grid cells in each direction. With a capillary number in the range described above, it will take ~ $2 \cdot 10^7$ timesteps for the fluid to flow 1 pore volume. Even with state-of-the-art computational resources, this is both very time-consuming and very computationally expensive.

Three-dimensional imaging of carbonate rocks

In collaboration with Sandia National Laboratory (SNL), a total of 11 chalk pore geometries with resolutions of 10 nm and sample sizes ranging from 5 - 10 μ m were obtained using the FIB-SEM imaging technique. In FIB-SEM, a focused ion beam (FIB) repeatedly slices off very thin layers of the sample to expose new surfaces to the SEM. Series of SEM images yield a detailed description of the geometry of the solid surfaces and pore volumes. These digital pore samples have been used in our numerical models to investigate how the pore space evolve under various conditions.

Samples were obtained from four different unflooded outcrop chalk types (Kansas, Liege, Mons, and Stevns-Klint), and one flooded chalk sample (Liege). The pore samples showed large variations in flow properties, and some of the samples had absolute permeability values close to values measured in core-scale experiments. Other samples displayed values well below experimental core-scale values, which indicates that we need to increase the size of the pore samples well beyond 5-10 μ m to approach a core-scale permeability. This is particularly important for chalk where pore sizes may range over at least one order of magnitude.

The raw gray-scale SEM images undergo a segmentation process to distinguish solid and void regions. This is a critical stage of the imaging process that can lead to large variations in the resulting geometry. As an example, two different segmentations based on the same set of SEM images, one performed at SNL and the other at Utrecht University, resulted in two quite different pore geometries with a 60 % difference in measured permeability. Figure 1 shows the

Sandia geometry in a) and the Utrecht geometry in b), together with the respective porosities and permeabilities.

A recommendation for future FIB-SEM imaging would be to fill the pore space with a substance that solidify prior to the FIB slicing. This would consolidate the sample and avoid small pieces of rock material to break off during the FIB slicing. A pore space filled with a solid of contrasting color would also simplify the segmentation between solid rock and pore space.



Figure 5: *Variability of segmentation: pore geometries of a flooded Liege chalk sample segmented from the same set of FIB-SEM images yield different results.*

Core scale simulations

Although the actual mechanisms behind increased oil recovery with Smart Water are not fully understood, core scale simulations may still be a useful tool for interpretation of experiments by testing assumptions regarding the mechanisms and investigate implications on the larger scale (field).

IORCoreSim is specifically designed to simulate laboratory experiments. The two main types of Smart Water experiments used are forced displacement of oil by injecting water trough core plugs, and spontaneous imbibition where the oil is displaced by an imbibing brine. Most of the Smart Water experiments are spontaneous imbibition addressing fractured (chalk) fields such as the Ekofisk field. Very little is published on simulating the Smart Water processes. This might partly be due to the somewhat awkward process of setting up such models with commercial simulators. In IORCoreSim, especially designed boundary conditions are assigned to the spontaneous imbibition system and modelling this kind of experiment is therefore straightforward. Other relevant models implemented in IORCoreSim are listed in Table 1.

 $Table \ {\it 1} \ {\it Models} \ in \ {\it IORCoreSim} \ relevant \ for \ Smart \ Water.$

Geochemical model

- Ion exchange (both cations and anions).
- Dissolution/precipitation of minerals.
- pH and surface potential + flash calculation of produced brine pH at measured temperature.
- Allow CO₂ partitioning between water and oil.

Interpolation of saturation functions (kr and Pc)

- Handles the Smart Water effects on oil recovery.
- Linear or logarithmic relative permeability interpolation.
- Interpolation based on specie concentration or adsorption, capillary number, pH or surface potential. Linear or tabular variation of interpolation parameter.

Diffusion

- Potential important transport mechanism for ions and other species at the core scale.
- Saturation and porosity dependent diffusion using Archie's resistance model.
- Diffusion across surfaces (appropriate option for spontaneous imbibition experiments). Temperature model
- Allows simulating experiments with changing temperatures.
- Temperature effects included in all relevant models.
- Corrects for thermal expansion.

Spontaneous imbibition boundary conditions

- Easy representation of different experimental setups with spontaneous imbibition over all or selected parts of the core surface.
- Core plug placed in a flow-through imbibition cell. Diffusive and advective exchange of ions between core plug and surrounding brine is tracked and cell effluent history is reported.

The Smart Water models developed and used in IORCoreSim can be validated using the experimental workflow described in the recommended Smart Water EOR workflow", where changes in minerology, wettability alteration, oil production curves and effluent chemistry are measured as function of influx water chemistry, oil type and acid number, core mineralogy and surface reactivity.

Displacement experiments

If an increased oil recovery is observed in the laboratory, what does this imply on the field scale? To scale the results to field conditions, we need to determine two things: (1) the travelling velocity of the Smart-Water front, and (2) the length effect on the magnitude of the Smart Water response.

A natural choice will be to link the speed of the smart-water front to observed effluent production of different ions and pH. This is because the actual mechanism taking place must be in response to some changes in the bulk properties. However, the Smart Water response may trail behind, e.g., the observed pH front, simply because the "wettability alteration" process itself is slow compared to experimental residence times. In this case, one would need experimental data from longer cores and/or results obtained at lower flow rates to correct for such a delay. Possible reasons for such a delay may be slow kinetics in processes like chemical reactions, adsorption, desorption or equilibration of osmotic pressure.

The magnitude of the increased oil recovery must obviously be corrected for eventual capillary effects. Smart Water effects on the capillary pressure may give promising results at low rates in short cores, but at high rates, or in long cores, the effect of capillary pressure diminishes and only the Smart Water effect on relative permeability remains. Length effects may also be a result of slow geochemical reactions. And again, experiments with sufficient variations of residence time should be made available.

One may also use the simulator for testing various assumptions. Increased pH is typically observed in laboratory experiments when Smart Water brines are injected. The simulations, shown in Figure 6, indicate that if increased pH is considered a necessary condition for increased oil recovery, then fields containing CO_2 above some limits, could be removed from the list of candidates for Smart Water brine injection. To validate or reject such an assumption, additional experiments including CO_2 should be performed.



Figure 6 Time evolution (From top to bottom) of two IORCoreSim scenarios showing how the amount of CO_2 in the oil affects the pH during water injection. After 600 days the injection fluid is changed from seawater to low sal.

Spontaneous imbibition experiments

Spontaneous imbibition experiments are mostly done by placing the core plug drained to irreducible water saturation S_{wi} in an imbibition cell filled with the imbibing brine so that all surfaces of the core are exposed. Oil produced in response to the imbibing brine floats up to the top of the cell where it is measured. The "smartness" of a brine is ranged by comparing the oil recovery with that obtained using formation water as imbibing fluid. The experiment may be done by first imbibing formation water for some time until the oil production stops, and then replace the brine in the imbibition cell with Smart Water, or by using a new core plug for each brine composition imbibing from the start.

The information available from such spontaneous imbibition experiments are limited to the oil production history, and history matching relative permeability, capillary pressure, and geochemical models to single experimental results in non-unique solutions. To do a proper interpretation, one should have supplementary experiments with separate measurements of capillary pressure and relative permeability. One might increase the geochemical information by measuring changes in ion composition of the brine surrounding the core, but a better solution is to do Smart Water brine displacement experiments with measured effluent ion and pH profiles for validation of the simulations.

Figure 7 demonstrates the use of IORCoreSim for numerical investigation of how laboratory results will scale to larger dimensions. The experimental data obtained with the reference brine (SWoNaoS) was first matched using some reasonable capillary pressure and relative permeability functions for chalk. The effect of the Smart Water (SW) was matched with an upward shift of the capillary pressure curve in presence of sulphonate, similar to that reported in (Webb, Black, & Tjetland, 2005). The timescale for the Smart Water response was found to be controlled by the ion diffusion velocity, and no information regarding Smart Water effects on relative permeability could be extracted from the results. The experimental data were obtained in small core plugs (L=7.2 cm, D=3.8 cm). Figure 7 shows the predicted results if the core diameter is increased to 1 m (L=1.9 m, D=1 m). The simulation with gravity turned off (left figure) matches the experimental results when the time axis is scaled with L^2 . In the laboratory, it took approximately one month to fully produce the incremental oil injecting Smart Water. In the larger mode, l it will take 700 months (58 years). If we include gravity in the simulations, more oil is produced at a much faster rate. But the difference between Smart Water and the reference brine is reduced.



Figure 7 Scaling of laboratory spontaneous imbibition from core with D=3.8 cm to D=1m. Time axis for experimental results are scaled with L^2 ; $t = t_{lab} \cdot (100/3.8)^2 \approx t_{lab} \cdot 700$. To the left, simulations with gravity turned off and to the right gravity turned on. Data from (Sandvik, 2018; Puntervold, Strand, Ellous, & Austad, 2015)

Reservoir scale simulations

The IORSim software

It was recognized quite early in the NIORC that there are, and most likely always will be, many potential chemical mechanisms that could explain why Smart Water flooding releases additional oil. In some cases, it could be a change in reservoir pH that is the controlling factor, and in other cases it might be the change in salinity. A choice was made to implement a complete description of all the possible geochemical reactions in the water phase that could take place in the reservoir: mineral dissolution/precipitation, surface complexation, ion

exchange and release of CO_2 to and from an oil phase. A change in relative permeability and capillary pressure can then be linked to one or several of these chemical mechanisms.

These chemical reactions are implemented in IORCoreSim which is capable of simulating core floods, and smaller field scale models. However, to simulate a large field, with wells being introduced at various times, requires a commercial reservoir simulator. IORSim is based on the same geochemical model as IORCoreSim, which makes IORSim well suited for upscaling results from core scale to field scale. The idea behind IORSim is to add chemical reactions to a commercial reservoir simulator without altering the simulator code. The reservoir simulator predicts where oil and water are flowing, and then IORSim piggyback the chemical species on the flow fields from the reservoir simulator. At each time step IORSim calculates changes in water chemistry due to rock fluid chemistry and keeps track of where in the reservoir the chemical changes are occurring. The change in chemistry can then be linked to a change in relative permeability. IORSim dynamically chooses relative permeability curves for Eclipse based on ionic composition, pH, or surface potential calculated in IORSim. IORSim may also perform local grid refinement, thus allowing for much less numerical errors when transporting species.

Back-coupling IORSim data dynamically to Eclipse

IORSim has mainly been used together with Eclipse which can communicate with external programs via interface-files using the keyword READDATA. At every report step, IORSim communicates back to Eclipse which flow functions to use, by modifying the SATNUM value for the grid blocks. Hence, IORSim and Eclipse run in an alternating sequence where Eclipse is paused while IORSim reads the Eclipse output and prepare a new interface-file. IORSim is then paused, and Eclipse resume by reading the updated interface-file with new SATNUM values. This back-coupling loop is facilitated by a Python script with a graphical user interface (GUI) that makes running IORSim more user-friendly.

Silicate injection on Snorre modeled by IORSim

In 2013, Equinor injected 240 000 m³ of sodium silicate at the Snorre field in a water diverging operation to improve the reservoir sweep. With minor modifications of the original Eclipse model used at Snorre in 2013, we used IORSim to model the complete injection history and predict the formation of the sodium silicate plug (see Figure 8). The reservoir permeability is dynamically updated by IORSim based on chemical and physical relations of gelation (Stavland, Jonsbråten, Vikane, Skrettingland, & Fischer, 2011) and permeability (by the Carman-Kozeny equation).



Figure 8 Tracer concentration of the silicate model compared to a reference model. The location and extent of the silicate plug is clearly visible.

Only minor changes were necessary to make the original Eclipse model for the Snorre case compatible with IORSim. In short, these changes included adding READDATA at the end of the .DATA-file and ensure restart files are written at every report step. IORSim used the original Eclipse schedule file (.SCH-file) to control the well-rates. To save computation time, IORSim used the Eclipse restart file for the 10-years prior to the silicate injection to get correct reservoir conditions.

Conclusions and recommendations

Based on the work done in the IOR Centre we have the following recommendations:

- 1. To evaluate Smart Water flooding on a field, a case-by-case study is needed. It is important that the effect of Smart Water is studied on cores with a representative wettability (see the DF report on Core restoration). Smart Water is dependent on reservoir mineralogy, temperature, formation water composition, and reservoir flooding history all of which varies from field to field.
- 2. The chemical mechanisms for release of additional oil must be identified (see the report on Smart Water EOR workflow for how to approach this experimentally). The mechanisms are important because the effect on oil release propagate at a different speeds on the field scale. Broadly speaking one can group the mechanisms in two classes: i) chemical interactions that only interact with the pore surface (e.g., adsorption) ii) chemical interactions that interacts with the grains (e.g., dissolution/precipitation, many pH effects). The first group typically travels with a fractional speed of the water (lagging behind the water and salinity front). The second group travel much slower and in some cases, it could be like an exponential decay, only reaching a very limited part of the reservoir.
- 3. To achieve a realistic oil recovery potential for Smart Water flooding, one needs a simulator that can calculate geochemical changes to the minerals, adsorption of ions (and changes in surface potential), reservoir pH (including the effect of CO₂ in the oil phase). The typical models in reservoir simulators where one interpolates between salinity gradients, will in most cases give a too high potential as it implicitly assumes that the Smart Water does not change composition as it travels from injector to producer.
- 4. Smart Water should be considered as an injection fluid in secondary mode as it will mix with less formation water before it interacts with the oil, alternatively one should consider injecting Smart Water in the oil zone.
- 5. If low salinity water is considered as a Smart Water fluid, one should investigate potential positive effects of combining low salinity water with polymer injection. If polymers can be injected together with low salinity, less polymer is needed, the polymer is more stable, and it adsorbs less. Less low salinity water is needed to be injected as polymer flooding (done properly) will produce the same amount of oil from the reservoir with less water injected.

In this report we have highlighted that there are a vast number of chemical mechanisms observed in core scale experiments that could explain the release of oil (e.g., changes in pH in sandstone cores, amount of sulphate in chalk core experiments, alteration of the pore space due to dissolution or precipitation). We have suggested to relate changes in relative permeability to the change in the local pore chemistry. Although this approach is probably flexible and quite robust for field simulation and evaluation of potential for Smart Water flooding, it still based on correlations. The chemical processes should ultimately be related to a physical process that describes the wettability alteration. Is the pH alteration related to changes in surface charge which creates an osmotic pressure for the release of oil? Is pH affecting the charge and number of charges at the oil water interface? More work should be focused on relating the change in pore chemistry to a holistic description of wettability change. If this was successful one could use the simulation tools developed in the NIORC to predict the effect of Smart Water based on the core properties and fluid compositions alone, brines could be optimized, and the model predictions could be controlled by additional experiments. The dissolution/precipitation kinetics were found to be at odds with measurements from powder

experiments. Here we will suggest that controlled experiments conducted on solid chalk samples conducted with measurements on surface topology (Neuville, et al., 2017) would be a good complimentary experimental activity to support the extraction of core scale rate model parameter from core scale experiments.

The wetting behavior, on the pore scale, is described by a contact angle between the oil-water interface and the mineral surface. The contact angle will change with alterations in water chemistry as it will perturb the thermodynamic equilibrium between water, oil, and rock. These changes will be dependent on the changes in surface energy. We lack the experimental data that can supply this information. One such method is measurements of the streaming potential which is closely related to the surface charge in a fully water-saturated system, and in simple geometries one can derive the surface charges from zeta-potential measurements. As the system becomes more complex one will need more detailed simulations to interpret the data, but the models will then be based on a sound experimental setup.

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