Experimental Investigation and High Resolution Simulator of In-Situ Combustion Processes

Quarterly Report

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Abstract

Accurate simulation of in-situ combustion processes is computationally very challenging because the spatial and temporal scales over which the combustion process takes place are very small. In this fifth quarterly report of our DoE funded research, we continue the discussion of the design of a new simulation tool based on an efficient Cartesian Adaptive Mesh Refinement technique that allows much higher grid densities to be used near typical fronts than current simulators. We have now developed an appropriate upscaling technique for our grids, based on the local-global upscaling approach. We show preliminary results on two-dimensional test cases.
On the experimental side, we continued experiments to measure the rates and kinetics of combustion in the presence and absence of metallic additives. In this quarter, we developed a better understanding of the cation replacing power of the various additives that affect combustion performance positively, and obtained a preliminary reactivity series. We also resumed our experimental investigation into the cyclic solvent-combustion process using crude oil from the Hamaca Region of Venezuela. Various measurements were made including oxygen consumption as a function of temperature. Preliminary results show that the temperatures for the onset of combustion are a function of the solvent injected.

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1. Introduction

In-situ combustion, or air injection, is the process of injecting oxygen into oil reservoirs to oxidize the heaviest components of the crude oil and enhance oil recovery through the heat and pressure produced. The emphasis of this work is to study and model numerically in situ combustion processes. The ultimate objectives are to provide a working accurate, parallel in situ combustion numerical simulator and to better understand the in-situ combustion process when using metallic additives and/or solvents combined with in situ combustion. For this purpose, experimental, analytical and numerical studies are conducted.

This report presents results of the first quarter of the second year of this project.

2. Executive Summary

2.1. Personnel

Current personnel include Prof. Margot Gerritsen (PI), Prof. Tony Kovscek (Co-PI), Dr. Louis Castanier (Technical manager), Dr. Jonas Nilsson (postdoctoral fellow), Mr. Rami Younis (PhD student), and Mr. Qing Chen (MSc student). Mr. Jean Cristofari (MSc student) is also working on the project, albeit paid from departmental sources.

2.2. Important accomplishments

2.2.1 A novel multi-level upscaling technique for CCAR grids

In the previous quarterly reports, we described the Cartesian Cell-based Adaptively Refined (CCAR) grids and appropriate finite volume methods for these grids that we are developing for our in-situ combustion simulator. CCAR grids allow very aggressive refinement near important features, such as the combustion front, and are efficient because of their underlying Cartesian structure. In this quarter, we developed an appropriate upscaling technique for CCAR grids.

Grid adaptation strategies

We distinguish two grid adaptation strategies: static and dynamic. Static grid adaptation is adaptation determined before the simulation is started, based on geological data and simplified flow problems. The refinement criterion should ideally be based on an estimation of the upscaling errors. In other words, the grid should be coarsened up from the geo-cellular level only to a level at which the upscaling errors are below a predefined tolerance. Currently, we apply as a first static refinement indicator, based on a 'leaky' connected-set approach (developed by Younis and Caers[1]) that delineates clusters of fine cells with similar permeability. Heuristic measures are used to color each connected set, indicating the level of the importance of capturing the set by refinement. Refinement flags are then obtained by explicit boundary detection. An illustration of the process appears in Figure 1. In the current implementation, maximum and minimum levels of refinement are set, and a CCAR grid is generated by iteration until these level constraints are met.

We use gradient-based adaptivity indicators to dynamically adapt the statically refined base grid to important flow features such as shocks and regions of steep gradients. Gradient based indicators can be easily obtained as local estimates of the directional gradient of flow variables on the CCAR topology. The refinement criteria are evaluated frequently, and the grid is adapted accordingly. The frequency with which to adapt the grid is problem dependent. It is determined by the speed with which the features to be resolved propagate, and the costs of grid adaptation compared with the costs of extending locally refined regions to keep the features from propagating out of the refined areas between grid updates.

The static and dynamic indicators are combined, and the CCAR adaptivity algorithm is then applied. Figures 2a, b and c show a statically refined grid and adapted grids to the gradient indicator for a two-phase immiscible test problem (water flowing into an oil saturated reservoir) driven by pressure boundary conditions). More concretely, we solve the problem

$$\nabla\left[\left(\lambda_o + \frac{b_o}{b_w}\lambda_w\right)\kappa\cdot\nabla p\right] = 0$$
$$\frac{\partial S_o}{\partial t} + \frac{1}{\phi b_w}\nabla\left[\lambda_w \kappa\cdot\nabla p\right] = 0 \quad ,$$

with the boundary conditions p=350 at the top boundary (y=64), p=1 at the bottom boundary (y=0), and no-flow boundary conditions at the left (x=0) and right (x=64). We set $b_o = b_w = 1$, and $\phi = 0.45$, and compute the relative permeabilities according to

$$k_{ro} = 0.9\left(\frac{S_o - S_{or}}{1 - S_{or} - S_{wr}}\right)^2,$$
$$k_{rw} = 0.75\left(\frac{S_w - S_{wr}}{1 - S_{or} - S_{wr}}\right)^2,$$

with $S_{or} = S_{wr} = 0.1$. Finally, the oil viscosity is set to 2, and the water viscosity to 1. We solve the equations on the permeability field shown in Figure 1a. This is given on a uniform fine grid with 64x64 (4096) grid cells.

An IMPES scheme is applied with volume weighted first-order upwinding for mobility terms suitable for CCAR grids. Saturation fronts are shown at two different times in 2d and 2e for a fine CCAR grid with a total of 1400 grid cells (30% of the uniform fine grid). The permeability field is that shown in figure 1a.

Effective upscaling for CCAR grids

Populating adapted CCAR grids with permeability values using those on the fine-scale geo-cellular grid is an upscaling problem. Naturally, the upscaling method should be appropriate for the grid topology used. For coarse Cartesian methods, for example, static or local upscaling methods are not attractive. In static upscaling, the permeability in a coarse cell is computed from algebraic averages of underlying fine-scale permeability values. When a coarse grid cell is not aligned with, but rather straddles a strong permeability contrast, this averaging results in a strong smoothing of the permeability field. The same holds true for local or extended local methods. For flow-based grids on the other hand, these local upscaling methods may lead to good results provided the grids capture the reservoir heterogeneity well.

It has been shown that for Cartesian methods, the local-global method leads to improved results as compared to local, or extended local, methods [2]. The local-global method was in fact inspired by an AMR approach. For each coarse grid cell, an effective permeability is computed by solving a local flow problem on the fine geo-cellular grid directly around the coarse cell. This local flow problem is driven by boundary conditions interpolated from a coarse global solve. The resulting coupling between the local flow problems and the coarse global solve leads to an iterative scheme that generally converges rapidly.

As mentioned in the previous section, the base grid is designed with the aim to minimize upscaling errors. Thus, upscaling and base grid generation are coupled processes. The local-global method fits very naturally into this coupled process.

In the general procedure we are developing, we start with an initial CCAR grid found using the leaky connected set approach. We populate this grid with an initial permeability field determined by static averaging of the geo-cellular permeability values.

After these initial steps, we apply local-global upscaling to all grid levels sequentially, starting at the finest level. When appropriate permeability values have been found on a level, we fix them and continue on to the next coarser level. The global solves in this local-global upscaling procedure are always performed on the full CCAR grid. This multi-level local-global procedure is repeated until the permeability field on the CCAR grid has converged. At that time, we assess the upscaling errors on the CCAR grid. If they exceed a specified tolerance, a new CCAR grid is generated to reduce the upscaling errors (for example by further local refinement, or extension of refined regions). In the results below, we estimate upscaling errors by comparing with a fine grid solution. In practice, this is of course not possible. We are currently working on good upscaling errors indicators and will report on these in a forthcoming quarterly report.

In the simulations shown in figure 2, the permeability values used on the CCAR grids are generated using this new approach. The global flow for this challenging channel problem is computing within 5% accuracy. For comparison, we computed the global flow errors for a 32x32 uniform coarse grid (comparable density) using the local-global upscaling method[2], which was shown to give much improved upscaling errors compared to local methods. This grid gave approximately 11% error in global flow as compared to the fine uniform grid. This suggests that upscaling errors can be controlled effectively by local grid refinement.

Figure 3 shows a comparison of the water cut between the uniform grids with resolutions 64x64, 32x32, 16x16 and 8x8, the fine CCAR grid mentioned above and a coarse CCAR grid with 440 grid cells. The CCAR grids predict the correct water breakthrough time, and follow the fine grid curve closely.

2.2.2 Experimental in-situ combustion

The experimental program is focused on the proof of concept for (i) water-soluble metallic salts to improve fuel lay down and enhancement of combustion performance as well as (ii) a new recovery concept that combines cyclic solvent injection and in-situ combustion to remove any solid precipitation resulting from the solvent.

Metallic Additives

Previous reports detailed experiments in a kinetics cell to measure the rates and kinetics of combustion in the presence and absence of metallic additives. Water-soluble, metallic additives such as these improve combustion by affecting cracking, low temperature oxidation, and pyrolysis reactions thereby improving fuel laydown. The mechanism of catalysis by metallic additives is not yet known. It is our working hypothesis that the cationic metals ion exchange with ions residing in the clay to create an activated site that acts in a manner analogous to a heterogeneous catalyst.

Progress on this task centered on developing a better understanding of the cation replacing power of the various additives that affect combustion performance positively. Based on the work above, and former research employing metallic additives and Huntington Beach oil[3,4], a preliminary

reactivity series is obtained by a series of standards. These standard include the increase in the extent of oxidation reactions, oxygen utilization efficiency, peak temperature and temperature profile, and heat of combustion. The series reads:

$$Sn^{2+} > Fe^{3+} > Al^{3+} > Zn^{2+} > Mg^{2+} > Cu^{2+} > Cd^{2+}$$

That is tin is a more effective additive than iron, and so on. This ranking is developed from experiments with specific crude oils and clays. Further work is needed to verify that the series is general. Nevertheless, the rankings originate from a rather large set of data.

An accepted method to compare the adsorption strength of cations onto clay surfaces is to compute the ratio of the cation valance upon the hydrated radius of the ion[5]. Thus, both electrical charge as well as the hydrated ion size are taken into account. The greater the ratio, the greater is the likelihood of the cation to exchange. Table 1 summarizes valence, ionic radius, and hydrated ionic radius for the reactivity series above. No values of hydrated radius for Sn^{2+} could be found in the literature. The remaining cations follow the trend of decreasing charge to hydrated radius ratio with decreasing combustion reactivity (compare the column labeled CHIRR).

This result supports the hypothesis above that metallic additives ion exchange into clays to create activated sites that improve combustion. Clays generally have a great affinity for such polar, oxygenated compounds. The organic molecules likely wedge directly into the clay interlayer structure. Removal of the partially oxygenated products from the reaction disrupts the equilibrium of the LTO reaction and shifts the oxidation reaction towards the products. In this way, clay with metallic additive has a positive effect on the LTO reaction.

Table 1. Summary of cation replacing power.

	valence	ionic radius[25] (Å)	hydrated ionic radius[26,27] (Å)	CHIRR* ($Å^{-1}$)
Sn^{2+}	2	1.19	-	-
Fe^{3+}	3	0.55	4.28	0.701
Al^{3+}	3	0.54	4.75	0.632
Zn^{2+}	2	0.74	4.3	0.465
Mg^{2+}	2	0.72	4.28	0.467
Cu^{2+}	2	0.73	4.19	0.477
Cd^{2+}	2	0.95	4.26	0.469

* CHIRR = valence: hydrated ionic radius

Solvent-Combustion Process

We have proposed cyclic injection of solvents to upgrade oil in situ, followed by in-situ combustion of a small part of the reservoir to increase the temperature near well bore and also to clean the well bore region of all residues left by the solvents. Alternate slugs of solvent and air are injected and allowed to soak. Production is after each slug. The process is repeated until economic limit is reached. Both solvent injection and in-situ combustion are technically effective in a variety of reservoirs. The combination of the two methods has, however, never been tried to our knowledge.

Our experimental investigation into the cyclic solvent-combustion process resumed in October of 2004. We have been trying to obtain a sample of heavy, Alaskan crude oil through an industrial contact since the beginning of this contract. They have encountered numerous problems during sample collection, such as pumps sanding up. Rather than wait any longer for a sample, we decided to proceed with crude oil from the Hamaca region of Venezuela as discussed in section 3 below. Experiments have shown to date that the temperatures for the onset of combustion are a function of the solvent injected. Work continues in this area.

3. Experimental

Our laboratory work this quarter focused on an investigation into the cyclic solvent-combustion process as discussed in section 2.2.2. We used crude oil from the Hamaca region of Venezuela. It is a 10.5 °API oil with 11.3 wt% asphaltenes. The solvents employed were pentane, decane, and kerosene.

The experimental procedure was to saturate a sandpack with crude oil, inject a slug of solvent, and then subject the sandpack to a ramped temperature oxidation kinetics test. Various measurements were made including oxygen consumption as a function of temperature.

4. Results and discussion

This report covers the fifth quarter of our research grant. The quarter was used primarily to further design the computational algorithms, with increased emphasis on the three-dimensional simulator, and to continue our experimental work. We have made very good progress in these areas again this quarter. Our papers on the work presented at the Society of Petroleum Engineers Reservoir Simulation Symposium, to be held early 2005, and the Society of Petroleum Engineers Western Regional Meeting in March 2005, are attached to this quarterly report.

Numerical simulations – upscaling

We have developed a promising and appropriate upscaling technique for our adaptive grid framework. In essence it is a multi-level extension of the local-global upscaling approach developed by Chen, Gerritsen and Durlofsky[2]. When the grids are adapted dynamically, to refine near moving fronts for example, the upscaling method can be applied to adjust the permeability values retaining consistency with global flow. Downscaling strategies are not needed.

Experimental work

Our work this quarter has improved our understanding of the cation replacing power of the various additives that affect combustion performance positively. We obtained a preliminary reactivity series is obtained by a series of standards, including the increase in the extent of oxidation reactions, oxygen utilization efficiency, peak temperature and temperature profile, and heat of combustion. Further work is needed to verify that the series is general.

We resumed our experimental investigation into the cyclic solvent-combustion process. Experiments performed this quarter have shown that the temperatures for the onset of combustion are a function of the solvent injected.

5. Conclusions

We have nearly finished the development of the three-dimensional flow solver for incompressible flows using anisotropic refined grids in heterogeneous media. Although it is too early to conclude that our approach is entirely successful, early indications are that the proposed methodology will improve both robustness and efficiency of the pressure solver. Our next step will be to extend the methodology to compressible cases. We expect this to be finished before the end of the second year of our grant.

On the experimental side, we will continue to focus on understanding how the additives work during combustion. Our work confirms the working hypothesis that metallic ions create activated sites within the solid substrate where combustion processes are enhanced. We have found an appropriate indicator (CHIRR) that can be used to rank metallic additives. This indicator is in

agreement with existing experimental data. The current results are a step forward to improving the design of in-situ combustion processes using metallic additives.
We will also continue our experimental investigation into the cyclic solvent-combustion process.

References

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[3] Shallcross, D.C., Rios, C.F. De Los, Castanier, L.M. 1991. "Modifying In-Situ Combustion Performance by the Use of Water-Soluble Additives", *SP*

[4] He, B.: 2004. "The Effect of Metallic Salt Additives on In-Situ Combustion Performance", M.S. Report Stanford University. Online at http://ekofisk.stanford.edu/pereports/web /default.htm

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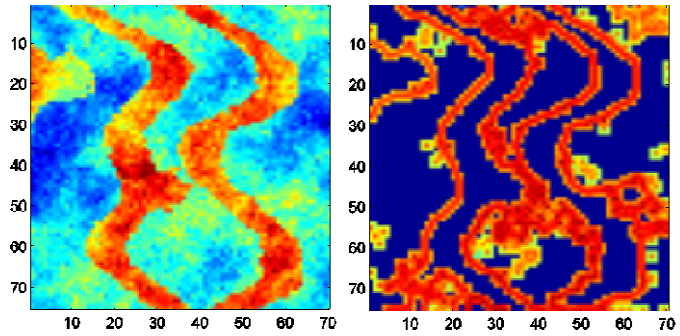

Figure 1: a) Permeability field, ranges from 1mD (dark blue) to 8D (dark red);

b) Refinement flags

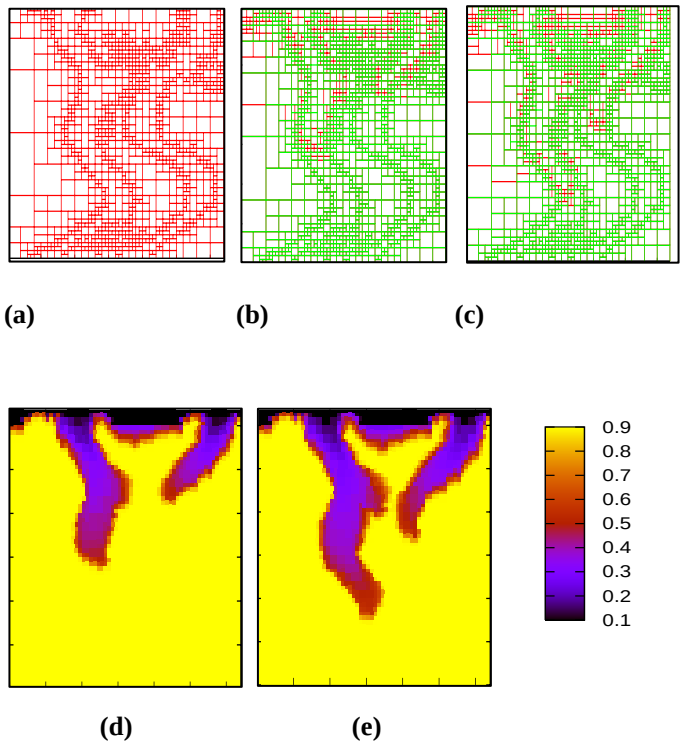

Figure 2: a) Base grid; b) Grid at 0.03 PVI; c) Grid at 0.05 PVI; d) Saturation at 0.03 PVI e) Saturation at 0.05 PVI

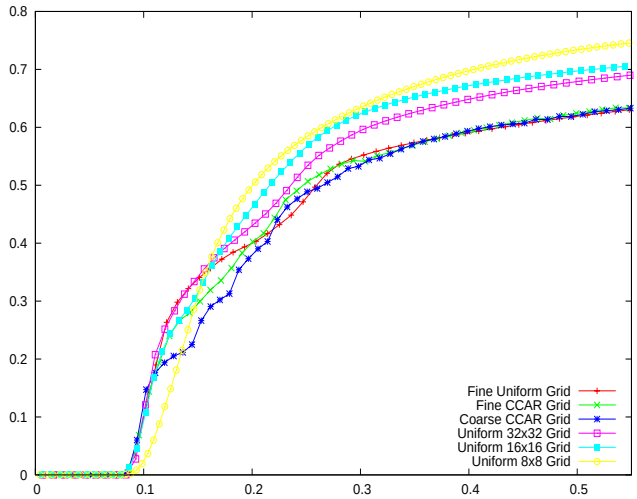

Figure 3. Water cut as a function of time in PVI.