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Fully compositional and thermal reservoir simulation

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ABSTRACT

Fully compositional and thermal reservoir simulation capabilities are important in oil exploration and production. There are significant resources in existing wells and in heavy oil, oil sands, and deep-water reservoirs. This article has two main goals: (1) to clearly identify chemical engineering sub-problems within reservoir simulation that the PSE community can potentially make contributions to and (2) to describe a new computational framework for fully compositional and thermal reservoir simulation based on a combination of the Automatic Differentiation-General Purpose Research Simulator (AD-GPRS) and the multiphase equilibrium flash library (GFLASH). Numerical results for several chemical engineering sub-problems and reservoir simulations for two EOR applications are presented. Reservoir simulation results clearly show that the Solvent Thermal Resources Innovation Process (STRIP) outperforms conventional steam injection using two important metrics – sweep efficiency and oil recovery.

1. Introduction

Modeling and simulation to predict long-term performance of oil recovery methods (i.e., reservoir simulation) is a topic studied for over 50 years (see Douglas et al., 1959; Price & Coats, 1974; Todd et al., 1972). Early reservoir models (e.g., black-oil reservoir models) were typically based upon rigorous mass-balance equations for key species (oil, water, and gas), but only used approximate phase equilibria (e.g., no oil dissolved in the water phase) and/or neglected energy balances. By the 80's, reservoir simulation had reached a level of maturity to warrant the first Society of Petroleum Engineers (SPE) Comparative Solutions Project on 3-D Black Oil Reservoir Simulation (Odeh, 1981) in which seven different companies participated. To date, there have been ten separate comparative solution projects sponsored by the SPE with topics that include three-phase behavior, steam injection, horizontal wells, and effective grid-generation and up-scaling techniques. These Comparative Solutions Projects papers are useful for readers new to reservoir simulation or those simply interested in learning more about challenging issues in this area.

Today, reservoir simulation has reached a point where advanced concepts such as dual-porosity models, rigorous phase behavior, energy-balance considerations, fully implicit time stepping with Newton's method to solve the reservoir model equations at each time step, iterative linear solvers, finite difference, and/or analytical Jacobian matrices (to name a few) are available as modeling components.

There remains considerable oil in place (OIP) in many reservoirs that are either in current operation or have been shutdown (often with infrastructure remaining in place). There are also large amounts of fossil fuels in heavy oil, oil sands, and deep-sea reservoirs – but these hydrocarbons are more challenging and more costly to produce. An increase in production at a standard oil field of just 1% can represent a $25 B opportunity. Many oil producers are considering enhanced oil recovery (EOR) methods such as steam injection and in situ CO_2 + steam injection (i.e., Solvent Thermal Resource innovative Process or STRIP) as a means of increasing recovery. Modeling STRIP, and other advanced EOR methods necessarily requires both fully compositional and thermal reservoir flow simulation capabilities, something that remains challenging.

Perhaps it is not surprising that various aspects (or subproblems) of fully compositional and thermal reservoir modeling and simulation are, in many ways, similar to modeling and equation-solving task associated with the kinds of chemical processes with which the process systems engineering (PSE) community and readership of Computers & Chemical Engineering are familiar. These sub-problems include

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Nomenclature

a_{ij}	number of atoms j in molecule i
A_j	total amount of atom j
B_{oil}	oil surface-to-reservoir formation volume factor
c_1,c_2,c_3,c_4	coefficients of cubic EOS
$[c]$	equilibrium ion solubility limit
C	total number of components
$C_{p,i}$	ideal gas heat capacity for ith component
f_i	partial fugacity of component i in solution
F	total density
g	acceleration due to gravity
G	heat conduction flux
ΔG_f^0	standard Gibbs free energy of formation
H	enthalpy
ΔH_f^0	standard heat of formation
ΔH_R^0	standard heat of reaction
K,K^k	intrinsic rock or soil permeability, thermal conductivity
K_{sp}	equilibrium solubility product
k_{ij}	binary interaction parameters
M	mass source or sink term
MW	molecular weight
n,n_i	vector of mole numbers, ith component mole number
p,p_c	pressure, critical pressure
P	total number of phases
Q	energy source or sink term
Q_{sp}	ion solubility product
r	oxygen-to-methane ratio
R	universal gas constant, relative permeability
S	saturation or amount of salt precipitate
t	time
T,T_c,T_{jm}	absolute temperature, critical temperature, transmissibility coefficient
U	internal energy
V	volumetric flow, volume of grid block
x,x_i	vector of liquid phase mole fractions, ith component liquid mole fraction
z	coordinate in direction of gravity, compressibility factor, vector of feed compositions

Greek symbols

ϕ	porosity
φ_i,φ_M	partial fugacity coefficient of component i, mixture fugacity coefficient
Φ	geometric part of flux
γ	mass density at interface
η	sweep ratio
κ	permeability
λ	mobility
μ	viscosity, chemical potential
ρ	density

Superscripts

k	phase index
L	liquid
V	vapor
0	standard state

Subscripts

c	critical property
C	number of components
i	component or summation index
M	porous media

1. Multi-phase equilibrium or flash.
2. Chemical reaction equilibrium.
3. Combined chemical and phase equilibrium.
4. Adiabatic flame temperature determination.
5. Heat and mass transfer in porous media.
6. Models consisting of differential algebraic equations (DAEs).
7. Nonlinear equation-solving using Newton and trust region methods.
8. Iterative linear equations solving.

Thus it is our opinion that chemical engineers, particularly those in the process systems engineering (PSE) community, are in a unique position to make significant contributions to various aspects of reservoir simulation.

In this paper, we present an advanced reservoir modeling and simulation framework for fully compositional and thermal reservoir simulation and subsequently apply this simulation framework to a comparative study of steam injection and STRIP in EOR applications. We also identify those sub-problems to which the PSE community can contribute. Accordingly, this work is organized as follows. Section 2 gives an overview of the relevant literature. In Section 3, a generalized reservoir model is presented; it includes model equations for both the reservoir and the bulk-phase length scales. Coupling between the reservoir and other constitutive equations needed to close the model (e.g., multiphase equilibrium flash, viscosity correlations, Darcy's law, heat conduction, etc.) are also described. In Section 4, details that describe how model equations are formulated and solved at various computational levels are given. Specific algorithmic features of the coupled methodology are also presented. In Section 5, steam injection and STRIP are introduced along with common metrics used to evaluate thermal EOR techniques. In Section 6, several relevant sub-problems are presented and solved prior to the application of this new reservoir simulation framework to two reservoir examples that demonstrate modeling and simulation capabilities and quantify the reliability and computational efficiency of the approach. A quantitative comparison of steam injection and STRIP is provided for the first reservoir simulation example using common performance metrics. The second example compares the performance of a modified compositional space adaptive tabulation (CSAT) with the conventional multiphase flash approach. Finally, in Section 7 conclusions of this work are drawn and future needs are highlighted while in Section 8 some additional sub-problems of interest to the PSE community are identified.

2. Literature survey

The focus of this article is numerical reservoir simulation, which comprises a vast body of literature and thus it is not possible to survey all relevant scientific papers. Therefore in this section only a summary of those papers and numerical methods directly relevant to the modeling and simultaneous solution of numerical reservoir models is presented. We refer the reader to the book by Peaceman (2000) for an introduction to the fundamentals of reservoir modeling and simulation and a description of some of the foundational numerical methods that have been developed. A secondary focus of this manuscript is to identify sub-problems within a larger reservoir