INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 9, Number 3, Pages 529–542

NUMERICAL SIMULATION OF RESERVOIR MULTICOMPONENT FLUID MIXING

ZHANGXIN CHEN AND HONGSEN CHEN

(Communicated by Kenneth H. Karlsen)

This paper is dedicated to the memory of Professor Magne S. Espedal.

Abstract. This paper presents numerical results on the development of compositional fluid mixing simulators in porous media. These simulators integrate geological processes (source rock maturation, hydrocarbon generation, migration, charge/filling, etc.) and reservoir processes (fluid mixing through Darcy's flow, advection, and diffusion, gravity segregation, etc.). The model governing equations are written with a proper choice of solution variables so that numerical mass conservation is preserved for all chemical components. The approximation procedure uses the finite volume method for space discretization, the backward Euler scheme in time, and an adaptive time stepping technique. The traditional simulator for solving the isothermal gravity/chemical equilibrium problem is deduced as a special example of the simulators presented here. Extensive numerical experiments are given to show segregation and instability effects for multiple components.

Key words. compositional gradients, reservoir simulation, fluid mixing, advection, diffusion, gravity segregation, numerical experiment, instability

1. Introduction

Compositional variations with depth have been observed in hydrocarbon reservoirs. These variations result from a variety of sources and typically indicate nonequilibrium states. They can be observed in systems in equilibrium when chemical potential gradients are balanced by gravitational potential gradients [8, 10, 13, 14, 21, 22, 24]. Temperature gradients can also contribute to compositional variations. Compositional variations in hydrocarbon reservoirs play an important role in reservoir delineation. The ability to forecast horizontal compositional variations helps the petroleum engineer to determine whether a given pair of producing wells drain the same reservoir, for example. Their other important applications include the study of the interplay of heterogeneity, advection, diffusion, gravity, viscosity, reservoir segmentation, and other forces that may affect the distribution of chemical components in reservoirs [4, 15].

In particular, the application to reservoir segmentation has increasingly become important due to exploration demands of new energy resources. Common assumptions are that there is a high chance of reservoir connectivity if

- Reservoir fluids are in pressure equilibrium;
- Fluids have similar or continuous PVT (pressure, volume, and temperature) properties;
- Fluids have similar geochemical compositions;

Received by the editors February 20, 2011 and, in revised form, May 14, 2011.

2000 *Mathematics Subject Classification.* 35Q10, 65N30, 76D05.

This research was supported in part NSERC/AERI/Foundation CMG Chair and iCORE Chair Funds in Reservoir Simulation.

- There are no significant changes in lithological characteristics from core and well log interpretation;
- Seismic reflectors are continuous;
- There is a common hydrocarbon-water contact.

Thus one needs to understand how similarities and differences can be interpreted from these diverse data sets when assessing reservoir segmentation. On one hand, multiple processes that affect fluid properties include reservoir charge/filling, fluid mixing through Darcy's flow, advection, and diffusion, gravity segregation, biodegradation, fractionation, and differential leakage of gas vs. oil. On the other hand, distinct time scales (key to understanding the relative significance of fluid data to reservoir segmentation studies) occur for different processes:

- Charge/filling of reservoirs: geological time–several millions of years;
- Biodegradation: thousands to hundreds of thousand of years;
- Molecular diffusion: 1 to 100 million years;
- Pressure diffusion: hundreds or even thousands of years;
- Convective flow: thousands to million years.

Therefore, one needs process-driven simulators to isolate the effects of each of these processes to evaluate reservoir fluid data in the interpretation of compartmentalization. We have been developing a software package that will integrate geological processes (source rock maturation, hydrocarbon generation, migration, charge/filling, etc.) and reservoir processes (fluid mixing through Darcy's flow, advection, and diffusion, gravity segregation, etc.). In the current paper instability problems (fingering phenomena) due to the interplay of advection, diffusion, and gravity are especially studied for multiple components. The literature is rich in the study of instability problems [9, 20, 23]. However, most of the studies dealt with viscous fingering and gravity segregation for two fluid components in a different setting.

The model equations governing the flow and transport of chemical components are written with a proper choice of solution variables so that numerical mass conservation is preserved for all these components. The approximation procedure here uses the finite volume method for space discretization, the backward Euler scheme in time, and an adaptive time stepping technique. Extensive numerical experiments are given to show segregation and instability effects for multiple components.

The rest of the paper is organized as follows. In the next section, we present the governing differential equations. Then, in the third section, we show that Gibbs' formulation can be treated as a special example of the mathematical formulation developed here. In the fourth section, the choice of the primary variables is given, and remarks about the approximation procedure used are made. In the fifth section extensive numerical experiments are presented. Finally, we draw several concluding remarks in the last section. Nomenclature is provided at the end of this paper.

2. Governing Differential Equations

We consider a gas or liquid phase that consists of N_c chemical species, where there is no viscous dissipation and chemical reaction and the only external force is due to gravity. Conservation of mass of each component in the fluid mixture is

$$\frac{\partial(\phi x_i \xi)}{\partial t} = -\nabla\cdot(x_i\xi\mathbf{u} + \mathbf{J}_i) + q_i, \qquad i = 1, 2, \ldots, N_c, \tag{2.1}$$

where ϕ is the porosity, ξ and $\mathbf{u}$ are the fluid molar density and velocity, and x_i, q_i, and $\mathbf{J}_i$ are the mole fraction, the source/sink term, and the diffusive mass flux