Simulation of Multiphase and Compositional Flow in Porous Media
R. Huber & R Helmig
Institute of Applied Mechanics, Chair of Numerical Methods and Information Processing, Technical University of Braunschweig, D-38106 Braunschweig, Germany
E-mail: r.huber@tu-bs.de

Abstract

Ground contaminations by non-aqueous phase liquids have become in recent years a problem of increasing concern. To get a better understanding of the processes and to develop in-situ remediation techniques numerical simulations of such multiphase and compositional flow problems are necessary. We will show a family of multiphase-multicomponent simulators which are based on a new consistent finite volume (box) scheme formulation with an efficient multigrid algorithm.

The concept of global mass fractions is incorporated into the system of equations. For the simulation of multiphase flow there are several options for the choice of primary variables. This is because a Newton–Raphson iterative scheme is used to solve the system of equations which is combined with a numerical differentiation of the partial derivatives with respect to the primary variables.

Several two- and three-dimensional example problems are investigated. First, to show the physical processes which take place and, second, to demonstrate the performance of the different simulators. In one example the validity of the passive air phase assumption in the case of a LNAPL infiltration is investigated.

1 Introduction

In the following the full three-phase formulations box3p and box3p3c of the numerical simulator MUFTE–UG are presented. DNAPL and LNAPL infiltrations into the unsaturated–saturated zone are simulated. In contrast to other investigations (e.g., Faust and Panday...
et al.\textsuperscript{2}) which analyse shallow systems, the vadose zone in the presented problem is of a larger vertical dimension. Usually the passive air phase assumption is used which makes the air phase conservation relation redundant. This assumption neglects the influence of air phase pressure gradients (e.g., Richards (1931)\textsuperscript{3}). Here, full three-phase formulations with pressure-dependent relations are used.

2 Governing Equations

Three-phase systems in the subsurface typically consist of two liquid phases (water (w) and a non-aqueous phase liquid (n), in short NAPL) and one gaseous phase (g). Conservation of each phase $\alpha \in \{w, n, g\}$ is described by the following continuity equation (e.g., Aziz & Settari\textsuperscript{4}):

$$\frac{\partial (\phi \rho_\alpha S_\alpha)}{\partial t} = -\text{div} [\rho_\alpha v_\alpha] + q_\alpha, \; \alpha \in \{w, n, g\}$$

where $S_\alpha$, $\rho_\alpha$, $v_\alpha$, $q_\alpha$ is the saturation, the density, the Darcy velocity, the mass source rate of each phase $\alpha$, respectively, and $\phi$ is the porosity.

The generalized Darcy’s law for multiphase flow in porous media is described by:

$$v_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} K (\text{grad} p_\alpha - \rho g), \; \alpha \in \{w, n, g\}$$

where $k_{r\alpha}$ is the $\alpha$–phase relative permeability, $K$ the absolute permeability tensor, $\mu_\alpha$ the viscosity, and $g$ the gravitational acceleration vector.

These two laws are supplemented by the constraint that the sum of all phases is always one, i.e., $S_w + S_n + S_g = 1$, and the following constitutive relationships: The relative permeabilities are assumed to be functions of the phase saturations. The differences of the phase pressures of the three-phase system are described by capillary pressure–saturation relations. The water phase is the most wetting phase and forms a film along the pore walls. NAPL is the intermediate wetting phase and separates the water and gas phases.

3 Numerical Formulations

Substitution of Darcy’s law (eqn (2)) into the conservation equations (eqn (1)) and a finite volume (box) discretization with backward Eu-
ler time discretization and mass lumping of the accumulation terms yields the discrete formulation of box3p (see, e.g., Helmig):  

\[ \frac{L_{\alpha i} := |B_i|}{\Delta t} \left\{ \left[ \frac{\phi \, q_\alpha \, S_{\alpha}}{\Delta t} \right]_{t^+}^{t} - \left[ \frac{\phi \, q_\alpha \, S_{\alpha}}{\Delta t} \right]_{t}^{t} \right\} - \sum_{j \in \eta_i} \left( \frac{\phi \, \lambda_\alpha}{\Delta t} \right)_{\text{ups}(i,j)} \gamma_{\alpha ij} - |B_i| q_{\alpha i} = 0, \quad \alpha \in \{w, n, g\} \]  

(3)

where \( \eta_i \) is the set of all neighbor boxes which have a mutual box boundary face with box \( i \), or in other words, all indices \( j \) with \( |\gamma_{\alpha ij}| > 0 \). \(|B_i| = \int_{B_i} dx\) is the volume of box \( B_i \). The transmissivity term for the box scheme which represents the discrete flux between neighboring boxes is given by

\[ \gamma_{\alpha ij} = - \sum_{e:i,j \in e} \left[ K (\text{grad} \, \bar{p}_\alpha - \phi \, q_\alpha \, g)]_{x=P_{ij}^e} \cdot \bar{n}(l_{ij}^e) \cdot A(l_{ij}^e) \right. \].

(4)

\( \bar{n} \) is the outward unit normal vector with respect to box \( i \). In the case of quadrilateral elements each element is divided into four subcontrol-volumes each of which belongs to a box associated with an element node (see Fig. 1). The term in brackets in eqn (4) is evaluated at the midpoint \( P_{ij}^e \) of the dividing line \( l_{ij}^e \) between the two subcontrol-volumes of the boxes \( i \) and \( j \) inside of element \( e \). \( A(l_{ij}^e) \) is the area of this box boundary segment.

Figure 1: Finite volume (box) scheme for a rectangular element \( e \).

The mobilities \( (\lambda_\alpha = k_{\alpha}/\mu_\alpha) \) and densities in the flux term in eqn (3) are upstream weighted. The \( \alpha \)-phase upstream direction at the interface between boxes \( i \) and \( j \) is determined by

\[ \text{ups}(i, j) = \begin{cases} i & \text{if } \gamma_{\alpha ij} \geq 0 \\ j & \text{if } \gamma_{\alpha ij} < 0 \end{cases} \]

(5)
This upstream weighting of saturation dependent terms is necessary to obtain a stable solution, especially in the case of convection-dominated processes where the equations are essentially hyperbolic (e.g., Forsyth\(^6\)).

The discrete phase conservation equations for the box3p3c simulator are obtained from eqn (3) using the following equality

\[ \phi \varrho_{\alpha} S_{\alpha} = \phi Z_{\alpha} \sum_{\beta} \varrho_{\beta} S_{\beta} \quad . \quad (6) \]

The discrete equations for box3p3c have then the following form:

\[
L_{\alpha i} := \frac{|B_i|}{\Delta t} \left\{ \left[ \phi Z_{\alpha} \sum_{\beta} (\varrho_{\beta} S_{\beta}) \right]_{i}^{t+\Delta t} \right. \\
- \left. \left[ \phi Z_{\alpha} \sum_{\beta} (\varrho_{\beta} S_{\beta}) \right]_{i}^{t} \right\} \\
- \sum_{j \in \eta} (\varrho_{\alpha} \lambda_{\alpha})_{wps(i,j)} \gamma_{\alpha ij} \quad - |B_i| q_{\alpha i} = 0, \quad \alpha \in \{ w, n, g \} \quad . \quad (7)
\]

\( Z_{\alpha} \) in the equations above is the global mass fraction of the \( \alpha \) phase.

The three-phase simulator box3p uses as primary variables two phase saturations and the phase pressure of the third phase, and they are fixed for the entire simulation, i.e., the set of primary variables is one out of the following set of triplets: \{ \( (p_w, S_n, S_g) \), \( (S_w, p_n, S_g) \), \( (S_w, S_n, p_g) \) \}.

In contrast to the first two methods the choice of primary variables for box3p3c depends on the set of phases resident at the corresponding location (box) during the numerical simulation.

Table 1 shows for each possible phase state (combination of resident phases) the corresponding set of primary variables. \( V_{\alpha i} \) is the (nodal) primary variable associated with the \( \alpha \)-phase conservation equation \( L_{\alpha i} \) for box \( B_i \).

A variable substitution is done in the case of a local phase appearance or disappearance. These transitions are recognized when during the iteration process negative saturations appear, or when the global mass fraction of an absent phase becomes positive.

Both multiphase simulators utilize the Newton–Raphson concept to solve the discrete system equations. The Jacobian is constructed with a chord slope technique. The partial derivatives are obtained by central finite difference approximations.
Table 1: Phase states and primary variables of box3p3c

<table>
<thead>
<tr>
<th>Resident Phases</th>
<th>Primary Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>water, NAPL, gas</td>
<td>$S_w$, $S_n$, $p_g$</td>
</tr>
<tr>
<td>water, NAPL</td>
<td>$Z_g$, $S_n$, $p_g$</td>
</tr>
<tr>
<td>NAPL, gas</td>
<td>$Z_w$, $S_n$, $p_g$</td>
</tr>
<tr>
<td>water, gas</td>
<td>$S_w$, $Z_n$, $p_g$</td>
</tr>
<tr>
<td>water</td>
<td>$Z_g$, $Z_n$, $p_g$</td>
</tr>
<tr>
<td>NAPL</td>
<td>$Z_w$, $Z_n$, $p_g$</td>
</tr>
<tr>
<td>gas</td>
<td></td>
</tr>
</tbody>
</table>

In the following computations the $(S_w, S_n, p_g)$–primary variable set is employed for the box3p formulation. For both methods the BICGSTAB matrix solver is used.

4 NAPL Infiltration Problem

In Fig. 2 the set-up of this NAPL infiltration problem is given. It is an axisymmetric problem with a constant NAPL infiltration source on the surface at the center. A cross–sectional area of dimension 16.9 m x 6 m is taken as the model domain. The water table is located at a depth of 3 m. At the ground surface a constant recharge of water is prescribed. Constitutive relationships are taken from Forsyth.

![Figure 2: Configuration of NAPL infiltration problem.](image)

A more precise description of the problem is given in Huber & Helmig.
Before the NAPL infiltration starts the system has been allowed to reach from a fully-saturated state an equilibrium state. The vadose zone is then almost entirely at residual saturation. Infiltrating NAPL is moving due to gravitation mainly downwards. At the water table LNAPL ($950 \text{ kg/m}^3$) is pooling and its principle propagation is now lateral (see Fig. 3). In contrast to LNAPL the DNAPL ($1460 \text{ kg/m}^3$) is still moving downwards (see Fig. 4).

**Figure 3:** LNAPL saturations after 1883 days of infiltration.

**Figure 4:** DNAPL saturations after 1830 days of infiltration.

DNAPL are difficult to remediate because they accumulate at great depths. LNAPL are easier to assess and applicable for a clean-up by excavation or in–situ techniques. Once NAPL phase is resident in the ground, they represent a long-term contamination source. Solution processes of NAPL components into the surrounding phases take place. Organic compounds of the NAPL phase can migrate within the soil air and groundwater long distances.
Table 2: Runtime statistics (simulation of 1800 days)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>box3p</th>
<th>box3p3c</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNAPL problem:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total cpu time*</td>
<td>s</td>
<td>1881</td>
<td>2505</td>
</tr>
<tr>
<td>No. of time steps</td>
<td>-</td>
<td>407</td>
<td>383</td>
</tr>
<tr>
<td>LNAPL problem:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total cpu time*</td>
<td>s</td>
<td>1419</td>
<td>1841</td>
</tr>
<tr>
<td>No. of time steps</td>
<td>-</td>
<td>371</td>
<td>374</td>
</tr>
</tbody>
</table>

*: on a Pentium MMX 233 MHz.

Table 2 shows that box3p is computationally more efficient than the box3p3c formulation. However, in certain cases box3p3c is the more robust algorithm.

5 Conclusions

The two presented full three-phase simulators give accurate and stable solutions for a wide range of three-phase flow problems. The presented infiltration problem shows the high sensitivity of LNAPL migration to the assumed constitutive relationships and the resulting initial conditions within the vadose zone. E.g., Faust\textsuperscript{1} got results which indicate that LNAPL migrates mainly in lateral direction at very small depths, and that the pooling assumption of LNAPL above the water table is not always valid. Croisé et al.\textsuperscript{9} investigated the propagation behavior of NAPL using different numerical models with different presumed constitutive relations. Their conclusions which have been based on passive air phase simulations were similar to ours: The constitutive relations have a major impact on the numerical results. One conclusion of the present investigation is that an accurate simulation of a real contamination scenario requires very good and detailed knowledge of the soil characteristics.

References


