Finite volume approximation of a diffusion–dissolution model and application to nuclear waste storage[☆]

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Abstract

The study of two phase flow in porous media under high capillary pressures, in the case where one phase is incompressible and the other phase is gaseous, shows complex phenomena. We present in this paper a numerical approximation method, based on a two pressures formulation in the case where both phases are miscible, which is shown to also handle the limit case of immiscible phases. The space discretization is performed using a finite volume method, which can handle general grids. The efficiency of the formulation is shown on three numerical examples related to underground waste disposal situations.
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1. Introduction

A large community of scientists is concerned with understanding the mechanical and hydraulic behaviour of deep repository radioactive waste, in reason of its large impact on environment and human safety. This implies to be able to model and simulate complex phenomena such as the de-saturation and re-saturation of geological media, gas production induced by the corrosion of steel containers, within complex 3D heterogeneous and anisotropic domains including singular zones such as galleries and cells intersections. Moreover, materials with highly contrasted physical properties are involved in long time phenomena (from thousand to millions of years).

Hence the simulation of these physical features happens to be a complex task, and their validation is a major concern for the safety improvement of the industrial devices. Computational benchmarks, such as the Couplex Gaz benchmark [18], are useful for the definition of relevant physical models and numerical methods. Indeed, the Couplex Gaz benchmark has shown that the Darcy flow of two immiscible phases, the first one being an incompressible liquid phase and the second one the gaseous phase, can lead, in presence of high capillary pressures, to unphysical situations and to drastic numerical difficulties. This model implies the displacement of a free boundary between zones where the

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Nomenclature

$\mathcal{E}_K$	Set of all faces of control volume K
$\mathcal{M}$	Mesh
$\mathbf{F}_p$	Mass flux for phase $p = l, g$
$\mathbf{g}$	Gravity acceleration
$\mathbf{J}_p^c$	Mass diffusive flux for component $c = h, w$ in phase p
$\mathbf{k}$	Absolute permeability
$\mathcal{C}(P)$	Capacity function
μ_p	Viscosity of phase $p = l, g$
$\mathbf{n}_{K,\sigma}$	Unit vector normal to σ outward to K
ϕ	Porosity
ρ_p	Density of phase $p = l, g$
σ	Face of a control volume
$\mathbf{x}_\sigma$	Barycentre of face σ
$\mathbf{x}_K$	Centre of control volume K
C_p	Molar concentration of phase $p = l, g$
C_p^c	Molar concentration of the component $c = h, w$ in phase $p = l, g$
D_p^c	Diffusion coefficient of component $c = h, w$ in phase $p = l, g$
$d_{K,\sigma}$	Orthogonal distance between point $\mathbf{x}_K$ and face σ
$D_{l,K,\sigma}^h$	Approximation of diffusion flux of component h in phase l outward to K at face σ
$F_{K,\sigma}$	Approximation of normal gradient outward to K integrated over face σ
$F_{p,K,\sigma}^c$	Approximation of Darcy flux of component $c = h, w$ in phase $p = l, g$ outward to K at face σ
g	Subscript for gaseous phase
H	Henry's law constant at the temperature of the domain
h	Superscript for gaseous component
K	Control volume, element of $\mathcal{M}$
K_σ	Cone with vertex $\mathbf{x}_K$ and basis σ
k_{rp}	Relative permeability of phase $p = l, g$
L	Control volume, element of $\mathcal{M}$
l	Subscript for liquid phase
m	Parameter of Van Genuchten–Mualem law
M^c	Molar mass of component $c = h, w$
m_p^c	Volumic mass of component $c = h, w$ in phase $p = l, g$
n	Parameter of Van Genuchten–Mualem law
P_c	Capillary pressure
P_p	Pressure of phase $p = l, g$
P_r	Parameter of Van Genuchten–Mualem law
R	Ideal gas constant
S_p	Saturation of phase $p = l, g$
S_{gr}	Parameter of Van Genuchten–Mualem law
S_{lr}	Parameter of Van Genuchten–Mualem law
T	Temperature
w	Superscript for water component
X_p^c	Molar fraction of component $c = h, w$ in phase $p = l, g$

two fluid phases are simultaneously present (called in this paper the "under-saturated" zone) and zones where the only present fluid phase is the liquid phase (called in this paper the "saturated" zone). In an unexpected way, it can lead to the existence of zones where the liquid phase has been removed because of capillary forces and cannot be instantaneously replaced by the gaseous phase, hence creating a vacuum volume. It is interesting to exhibit the origin of such behaviour