Advances in Water Resources 51 (2013) 52–66

Contents lists available at SciVerse ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

Model coupling for multiphase flow in porous media

Rainer Helmig [a], Bernd Flemisch [a,*], Markus Wolff [a], Anozie Ebigbo [b], Holger Class [a]

[a] Department of Hydromechanics and Modelling of Hydrosystems, University of Stuttgart, Pfaffenwaldring 61, 70569 Stuttgart, Germany
[b] Laboratoire Environnement, Géomécanique et Ouvrages (LAEGO), Ecole Nationale Supérieure de Géologie, Institut National Polytechnique de Lorraine, Rue du Doyen Marcel Roubault, BP 40, 54501 Vandœuvre-lès-Nancy, France

ARTICLE INFO

Article history:
Available online 31 July 2012

Keywords:
Model coupling
Multiphase flow
Multiphysics
Multiscale

ABSTRACT

Numerical models for flow and transport in porous media are valid for a particular set of processes, scales, levels of simplification and abstraction, grids etc. The coupling of two or more specialised models is a method of increasing the overall range of validity while keeping the computational costs relatively low. Several coupling concepts are reviewed in this article with a focus on the authors' work in this field. The concepts are divided into temporal and spatial coupling concepts, of which the latter is subdivided into multi-process, multi-scale, multi-dimensional, and multi-compartment coupling strategies. Examples of applications for which these concepts can be relevant include groundwater protection and remediation, carbon dioxide storage, nuclear-waste disposal, soil dry-out and evaporation processes as well as fuel cells and technical filters.

1. Introduction

The description of the flow of multiple fluid phases through a material which consists of a solid and interconnected pore space is highly relevant in several fields of application. This includes environmental and geological applications such as groundwater protection and remediation, (enhanced) oil recovery, nuclear-waste disposal, carbon dioxide storage, dry-out and evaporation processes etc., but also technical systems such as the flow of water and gas in fuel cells or filters. In all of these examples, a quantitative prediction of flow and transport on strongly varying spatial and temporal scales is required and typically achieved with mathematical and numerical models. A need for model coupling arises for two basic reasons: (i) The relevant spatial and temporal scales, in particular for some geological applications such as CO_2 storage and nuclear waste disposal, are very large, and computational costs need to be reduced by adapting the complexities of the applied (sub-) models. (ii) The processes of the overall problem are in some cases described by different sets of equations, for example, if different compartments of hydrosystems interact with each other. An example is the problem of water evaporation and dry out of soils due to wind in arid regions.

This paper gives a review of coupling concepts and multi-scale approaches with a focus on the authors' contribution in this field.

1.1. Scales

As outlined in Helmig et al. [61], several characteristic length scales can be identified on which the relevant flow processes can be described. A basic differentiation is made here between (i) the pore scale, at which the fluids, solid, and interfaces can explicitly be accounted for, (ii) the REV (or fine) scale, at which effective properties and functions are sufficient to describe flow in a representative elementary volume (REV), and (iii) the macro (or coarse) scale, which is typically determined by the size of grid blocks of a computational simulation – see Fig. 1. The models considered in this article are based on the REV scale and the macro scale, which will also be referred to as the fine and coarse scales, respectively.

1.2. Modelling challenges

The modelling applications mentioned previously pose several challenges to numerical models, some of which are listed below:

- Geological applications are often characterised by their very large spatial and temporal scales. For example, geological formations relevant for oil recovery or CO_2 storage may extend several hundreds of kilometres; in the storage of nuclear waste, processes of interest continue even after millennia.
- They are usually also characterised by a small region in which complex physical processes take place as compared to the simpler processes in the rest of the domain.
- Heterogeneities exist on all the scales considered here. Obviously, the effects of fine-scale heterogeneities have to be accounted for on the coarse scale.

* Corresponding author.
E-mail address: bernd.flemisch@iws.uni-stuttgart.de (B. Flemisch).

0309-1708/$ - see front matter
http://dx.doi.org/10.1016/j.advwatres.2012.07.003

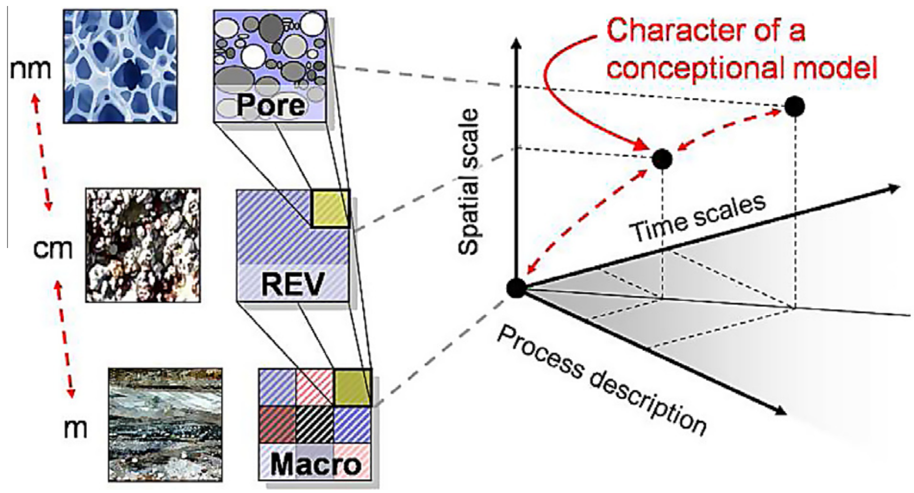

Fig. 1. Several characteristic length and time scales can be identified when considering flow and transport in porous media. Model concepts need to be developed with respect to the temporal and spatial scales at which the flow processes occur.

- The rate at which processes occur can vary significantly. For the underground storage of CO_2, there is a strong difference in flow velocities during and after injection.
- Due to a general scarcity of geological data, there is a high degree of uncertainty. Methods for the quantification of uncertainties require several possible realisations of the underlying deterministic numerical model.

Due to computational-cost constraints, efficient methods are necessary if the above modelling challenges are to be met. One way of improving efficiency is specification. Making a model concept specific to a problem of given complexity and/or scale can boost efficiency without affecting accuracy. Such models can then be coupled to address a complex and realistic problem.

1.3. Outline

This article gives an overview of the model-coupling strategies which are currently in the focus of research. Before describing coupling strategies, the basic mathematical models which describe multiphase and compositional flow in porous media are given in Section 2. Then the coupling strategies are divided in Section 3 into various categories which are partly overlapping or in a smooth transition to each other: spatial coupling methods (volume coupling, surface coupling, see Fig. 2), in which case regions of the spatial domain are identified with differing characteristic model complexities or where equations of different character are solved on different scales etc. Section 4 focuses on temporal coupling where processes have different characteristics in time such that model complexity can be adapted in the entire domain (or in parts, if multiple coupling approaches are useful) over time. Finally, Section 5 summarises the perspectives of model coupling for future research and application to current challenging engineering problems.

2. Mathematical models for multiphase flow

Mathematical and numerical formulations of the equations which govern multiphase flow in porous media are briefly introduced with the aim of setting a basis on which the coupling strategies operate.

2.1. Governing equations

The governing equations are generally derived by balancing such quantities as mass, momentum, and energy. These equations are given on the REV (fine) scale. The pore scale is not considered, and the macro (coarse) scale is achieved by upscaling. More comprehensive descriptions of these equations have been given, e.g. by [61,22,96,51].

Balance equations for the mass of a component in a system which consists of more than one fluid phase generally have the following form:

$$\frac{\partial}{\partial t}\left(\varrho_\alpha \phi S_\alpha X_\alpha^\kappa\right) + \nabla \cdot \left(\varrho_\alpha \phi S_\alpha X_\alpha^\kappa \mathbf{u}_\alpha + \mathbf{J}_\alpha^\kappa\right) = I_\alpha^\kappa + q_\alpha^\kappa, \tag{1}$$

where ϱ is density, ϕ is porosity, S is fluid-phase saturation, X is mass fraction, $\mathbf{u}$ is velocity, $\mathbf{J}$ is diffusive flux, I is interphase mass exchange, and q stands for external sources and sinks. The subscripts κ and α denote the component and the phase, respectively. In addition to the solid phase, a general system may consist of an aqueous (w), a non-aqueous (n), and a gas (g) phase as well as N components:

$$\kappa \in \{1, 2, \ldots, N\}; \quad \alpha \in \{\mathrm{w}, \mathrm{n}, \mathrm{g}\}. \tag{2}$$

Given the constraints and definitions

$$\begin{aligned} &\sum_\kappa \mathbf{J}_\alpha^\kappa = 0, \ \sum_\kappa X_\alpha^\kappa = 1, \ \sum_\kappa I_\alpha^\kappa = I_\alpha, \ \sum_\kappa q_\alpha^\kappa = q_\alpha, \\ &\sum_\alpha I_\alpha^\kappa = 0, \ \sum_\alpha S_\alpha = 1, \ \sum_\alpha q_\alpha^\kappa = q^\kappa, \end{aligned} \tag{3}$$

it is convenient to sum up the balance equations either over all components in each phase, which gives one equation for each phase

$$\frac{\partial}{\partial t}\left(\varrho_\alpha \phi S_\alpha\right) + \nabla \cdot \left(\varrho_\alpha \phi S_\alpha \mathbf{u}_\alpha\right) = I_\alpha + q_\alpha, \tag{4}$$

or over all phases, which gives one equation for each component

$$\sum_\alpha \frac{\partial}{\partial t}\left(\varrho_\alpha \phi S_\alpha X_\alpha^\kappa\right) + \sum_\alpha \nabla \cdot \left(\varrho_\alpha \phi S_\alpha X_\alpha^\kappa \mathbf{u}_\alpha + \mathbf{J}_\alpha^\kappa\right) = q^\kappa. \tag{5}$$

The extended Darcy equation. As noted by Miller et al. [96], a separate momentum balance equation is usually not considered. Instead, the flux of a fluid phase $\mathbf{v}_\alpha$ is approximated with the extended Darcy equation