INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 12, Number 3, Pages 476–515

FLOW AND TRANSPORT WHEN SCALES ARE NOT SEPARATED: NUMERICAL ANALYSIS AND SIMULATIONS OF MICRO- AND MACRO-MODELS

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Abstract. In this paper, we consider an upscaled model describing the multiscale flow of a single-phase incompressible fluid and transport of a dissolved chemical by advection and diffusion through a heterogeneous porous medium. Unlike traditional homogenization or volume averaging techniques, we do not assume a good separation of scales. The new model includes as special cases both the classical homogenized model and the double porosity model, but it is characterized by the presence of additional memory terms which describe the effects of local advective transport as well as diffusion. We study the mathematical properties of the memory (convolution) kernels presented in the model and perform rigorous stability analysis of the numerical method to discretize the upscaled model. Some numerical results will be presented to validate the upscaled model and to show the quantitative significance of each memory term in different regimes of flow and transport.

Key words. Upscaled model, double-porosity, memory terms, solute transport, non-separated scale, stability.

1. Introduction

We are concerned with advection-diffusion-dispersion equations when studying the flow of a single-phase incompressible fluid and transport of contaminant through heterogeneous porous media. The heterogeneities are represented by two different porous materials. In particular, we do not assume a good separation of scales. In [15], Peszyńska and Showalter derived a discrete version of the double-porosity model with various memory (convolution) terms for the coupled flow-transport equation without assuming a well-defined separation of scales in the porous medium. This model has been numerically studied in [20], where different tailing effects due to the memory terms were observed and the quantitative significance of each memory term in different regimes of flow and transport was studied. However, no analysis for the numerical methods used for the upscaled model was presented in [20]. The main purpose of this paper is to present a rigorous mathematical analysis of the numerical methods that are used to discretize the upscaled model proposed in [15].

For the numerical discretization of the upscaled model with convolution terms, we used the cell-centered finite difference (CCFD) method combined with the product integration rule for the convolution terms in which both the primary and secondary advection terms are approximated using the upwind method. Moreover, the (primary) advection was treated explicitly while the (primary) diffusion and all of the memory terms are treated implicitly in time. Our stability analysis will be given only for the 1d version of the upscaled model.

Received by the editors July 2, 2014 and, in revised form, November 23, 2014.
2000 *Mathematics Subject Classification.* 35B27, 35R09, 75S05, 74Q15, 65M12, 65M06.
This work was supported by the U.S. Department of Energy, Office of Science, Multiscale Mathematics Initiative under Award 98089. Research by Peszyńska was also partially supported by the National Science Foundation under Grant DMS-0511190 R.E. Showalter was partially supported by the U.S. Department of Energy, Office of Science under Award 98089 and Award 9001997.

Known results on numerical analysis of integro-partial differential equations and more general problems with memory terms include those in [18, 9, 10, 19, 12, 11]. All of these papers deal with memory terms of the form $\beta * Lu$, where L is a self-adjoint spatial differential operator. Moreover, all but [10] assume that the kernels β are bounded and monotone. On the other hand, in [13], Peszyńska considered a weakly singular memory term of the form $\beta * u_t$ in a parabolic equation with a self-adjoint elliptic part. Later, in [14], she also considered a memory term with weakly singular β in a first order hyperbolic equation.

For our analysis, we first investigate the qualitative behavior of the convolution kernels present in our model. We carefully represent the kernels in series representations and study their qualitative properties analytically. Unlike the monotone double-porosity and secondary advection kernels, the secondary diffusion kernel is found to be only piecewise monotone. Our mathematical findings on the properties of the convolution kernels will be confirmed numerically.

Using some assumptions on the convolution kernels based on the above findings, we perform stability analysis of our numerical methods for the upscaled model. First, we perform von-Neumann analysis for the upscaled model defined on an infinite domain $\mathbb{R}$. We study a simple version of the problem with only the double-porosity term first, then include additional memory terms, *i.e.*, the secondary advection and secondary diffusion terms, one by one. It is shown that the upwind-memory scheme we employ for our 1d upscaled model with all memory terms is (ultra-) weakly stable. We also discuss stability using the method of lines (MOL).

The rest of the paper is organized as follows: in Section 2, we describe the model problem for a heterogeneous system with combined fast and slow flow regimes. Then, in Section 3, we present the upscaled model with various memory terms for the coupled flow-transport equation that was developed in [15]. In Section 4, we investigate the qualitative properties of the memory kernels using Fourier series representations. Section 5 is devoted to stability analysis of the numerical discretization of the upscaled model using von-Neumann stability analysis and MOL. Finally, in Section 6, we present some numerical results.

2. The Model Problem

Let Ω be a two-dimensional heterogeneous porous medium containing two disjoint flow regimes. The subscripts f and s are associated with the fast and slow regions Ω_f and Ω_s, respectively. These are disjoint open sets covering Ω, $\overline{\Omega} = \overline{\Omega_f} \cup \overline{\Omega_s}$, with an interface $\Gamma_{fs} = \partial\Omega_f \cap \partial\Omega_s$. The region Ω_f is connected, but $\Omega_s = \cup_{i=1}^{N_{\text{incl}}} \Omega_{is}$ is a union of disjoint connected regions Ω_{is}.

Assume that Ω is covered by a union of rectangular subdomains Ω_i, $i = 1, \ldots, N_{\text{incl}}$, with each Ω_i containing exactly one inclusion Ω_{is}. Let $\Omega_{if} = \Omega_i \cap \Omega_f$ be the fast part surrounding Ω_{is} and let $\Gamma_i = \partial\Omega_{is} \cap \partial\Omega_{if}$ denote the local interfaces so that $\Omega_i = \Omega_{is} \cup \Omega_{if} \cup \Gamma_i$ and $\Gamma_{fs} = \cup_i \Gamma_i$. Let us assume that each Ω_i is congruent to a generic cell Ω_0 which contains the fast flow region Ω_{0f} surrounding the slow flow region Ω_{0s}. We also denote the volume fraction of the fast part by $\theta_f = \frac{|\Omega_{0f}|}{|\Omega_0|}$ and analogously $\theta_s = \frac{|\Omega_{0s}|}{|\Omega_0|} = 1 - \theta_f$.

Now, we describe the microscopic model of the flow and solute transport in the heterogeneous porous medium, with porosity and permeability discontinuous across