Correspondence Between One- and Two-Equation Models for Solute Transport in Two-Region Heterogeneous Porous Media

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Abstract In this work, we study the transient behavior of homogenized models for solute transport in two-region porous media. We focus on the following three models: (1) a time non-local, two-equation model (2eq-nlt). This model does not rely on time constraints and, therefore, is particularly useful in the short-time regime, when the timescale of interest \( t \) is smaller than the characteristic time \( \tau_1 \) for the relaxation of the effective macroscale parameters (i.e., when \( t \leq \tau_1 \)); (2) a time local, two-equation model (2eq). This model can be adopted when \( t \) is significantly larger than \( \tau_1 \) (i.e., when \( t \gg \tau_1 \)); and (3) a one-equation, time-asymptotic formulation (1eq\( _\infty \)). This model can be adopted when \( t \) is significantly larger than the timescale \( \tau_2 \) associated with exchange processes between the two regions (i.e., when \( t \gg \tau_2 \)). In order to obtain insight into this transient behavior, we combine a theoretical approach based on the analysis of spatial moments with numerical and analytical results in several simple cases. The main result of this paper is to show that there is only a weak asymptotic convergence of the solution of (2eq) towards the solution of (1eq\( _\infty \)) in terms of standardized moments but, interestingly, not in terms of centered moments. The physical interpretation of this result is that deviations from the Fickian situation persist in the limit of long times but that the spreading of the solute is eventually dominating these higher order effects.
Keywords  Porous media · Homogenization · Volume averaging · Dispersion · Spatial moments

List of Symbols

Variables

- $b_{ij}$: Closure mapping vector in the $i$-region associated with $\nabla \langle c_j \rangle$ (m)
- $c_i$: Pointwise solute concentration in the $i$-region (mol m$^{-3}$)
- $\langle c_i \rangle$: Superficial spatial average of $c_i$ (mol m$^{-3}$)
- $\langle c_i \rangle^i$: Intrinsic spatial average of $c_i$ (mol m$^{-3}$)
- $\langle c \rangle_{\gamma\omega}$: Weighted spatial average concentration (mol m$^{-3}$)
- $\tilde{c}_i$: Solute concentration standard deviation in the $i$-region (mol m$^{-3}$)
- $D_{ij}$: Dispersion tensor in the two-equation models associated with $\partial_t \langle c_i \rangle^i$ and $\Delta \langle c_j \rangle^j$ (m$^2$ s$^{-1}$)
- $D_{ij}$: Dispersion coefficient in the 1-D two-equation models associated with $\partial_t \langle c_i \rangle^i$ and $\Delta \langle c_j \rangle^j$ (m$^2$ s$^{-1}$)
- $D^\infty$: Dispersion tensor of the one-equation time-asymptotic model (m$^2$ s$^{-1}$)
- $D^\infty$: Dispersion coefficient of the 1-D one-equation time-asymptotic model (m$^2$ s$^{-1}$)
- $\exp$: Exponentially decaying terms ($\cdots$)
- $h$: Transient effective mass exchange kernel (s$^{-1}$)
- $h_\infty$: Effective mass exchange coefficient (s$^{-1}$)
- $\tilde{j}_i$: Deviation of the total mass flux for region $i$ (mol m$^{-2}$ s$^{-1}$)
- $J_i$: Average of the total mass flux for region $i$ (mol m$^{-2}$ s$^{-1}$)
- $L$: Characteristic length of the field-scale (m)
- $\ell_i$: Characteristic length of the $i$-region (m)
- $m^n_i$: $n$th-order centered moment associated with $\langle c_i \rangle^i$ for the two-equation model (m$^n$ mol)
- $m^n_{\gamma\omega}$: $n$th-order centered moment associated with $\langle c \rangle_{\gamma\omega}$ for the two-equation model (m$^n$ mol)
- $m^n_\infty$: $n$th-order centered moment associated with $\langle c \rangle_{\gamma\omega}$ for the one-equation asymptotic model (m$^n$ mol)
- $M^n_{\gamma\omega}$: $n$th-order standardized moment associated with $\langle c \rangle_{\gamma\omega}$ for the two-equation model ($\cdots$)
- $M^n_\infty$: $n$th-order standardized moment associated with $\langle c \rangle_{\gamma\omega}$ for the one-equation asymptotic model ($\cdots$)
- $n_{ij}$: Normal unit vector pointing from the $i$-region towards the $j$-region ($\cdots$)
- $p_k$: Three lattice vectors that are needed to describe the 3-D spatial periodicity (m)
- $Q^i(x, t)$: Macroscopic source term in the $i$-region (mol m$^{-3}$ s$^{-1}$)
- $Q^\gamma\omega$: Weighted macroscopic source term (mol m$^{-3}$ s$^{-1}$)
- $R$: Radius of the REV, (m)
- $S_{ij}$: Boundary between the $i$-region and the $j$-region ($\cdots$)
- $S_{ij}$: Area associated with $S_{ij}$ (m$^2$)
- $r_i$: Closure parameter in the $i$-region associated with $\langle c \rangle_{\gamma} - \langle c_{\omega} \rangle_{\omega}$ ($\cdots$)
- $t$: Time (s)
- $t'$: Non-dimensionalized time ($\cdots$)
- $T$: Period of the oscillations (s)
- $v_i$: Velocity at the microscale in the $i$-region (m s$^{-1}$)