



HAL
open science

Generalized Mixed-Cell Mass Balance Solute Transport Modeling in Pore-Scale Disordered Networks: A New Semi-Analytical Approach

Mohammed Adil Sbai, Toko Kamtchueng, Jean-Louis Rouet

► **To cite this version:**

Mohammed Adil Sbai, Toko Kamtchueng, Jean-Louis Rouet. Generalized Mixed-Cell Mass Balance Solute Transport Modeling in Pore-Scale Disordered Networks: A New Semi-Analytical Approach. Computational Methods in Water Resources (CMWR) 2016, Jun 2016, Toronto, Canada. hal-01273797

HAL Id: hal-01273797

<https://brgm.hal.science/hal-01273797v1>

Submitted on 18 Oct 2016

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Generalized Mixed-Cell Mass Balance Solute Transport Modeling in Pore-Scale Disordered Networks: A New Semi-Analytical Approach

M.A. Sbai^a, T. Kamtchueng^{a,b}, J.-L. Rouet^b

^a BRGM, ISTO UMR 7327, BP 36009, Av. Claude Guillemin, 45060, Orléans Cedex 2, France

^b Université d'Orléans, ISTO UMR 7327, Campus Géosciences, 1A rue de la Férollerie, 45100, Orléans Cedex 2, France

Key words: Mass Transport, Pore Network Modeling, Mixed-Cell Method, Semi-Analytical Solution, Laplace Transform

Introduction

Accurately predicting (non-reactive or reactive) solute transport migration, at multiple scales, in subsurface aquifers is identified among urgent societal and scientific challenges in water resources engineering and environmental pollution [1]. In particular, pore-scale models are essential tools to bridge the gap between the pore and REV scales at which observable macroscopic behavior of solute transport processes become apparent. While challenges do persist in this field, we derive cutting-edge pore scale semi-analytical formulation for solute transport modelling in disordered networks. Continuous concentration profiles along pore throats are calculated analytically, a posteriori, from time-dependent numerically simulated concentrations in neighboring pores. A double Laplace transform method is applied to governing advection-diffusion equations in network elements by enforcing mass flux continuity along their interfaces. We show that these solutions involve a time-dependent convolution product kernels or interpolating functions expressed as convergent exponentially decreasing series of locally embedded pore-throat geometrical and flow properties. Explicit dependence of interpolating kernels on the local Péclet numbers leads to a generalized numerical scheme for accurate simulation of solute transport processes in pore networks. Indeed, widely used numerical schemes in the literature [2-7] are equivalent to the asymptotic (long-time) form of our general scheme for extremely small or high Péclet numbers. Therefore, we demonstrate for the first-time that previously adopted numerical schemes for mass balance in pore networks [2-7] may overlook pore scale dynamics for a full range of intermediate Péclet numbers occurring in subsurface aquifers. These findings are illustrated by analysis of simulated concentration distributions in a benchmark pore network extracted from Berea sandstone three-dimensional pore space image. Our findings [8]

provide additional insights into the understanding of pore-scale solute transport processes to further improve the predictive capability of existing mixed-cell mass balance network models.

References

- [1] C.T. Miller, C.N. Dawson, M.W. Farthing, T.Y. Hou, J. Huang, C.E. Kees, C.T. Kelley, H.P. Langtangen. Numerical simulation of water resources problems: Models, methods, and trends. *Adv. Water Resour.*, **51**, 405-437, (2013).
- [2] R.C. Acharya, S.E.A.T.M. Van der Zee, A. Leijnse. Transport modeling of nonlinearly adsorbing solutes in physically heterogeneous pore networks. *Water Resour. Res.*, **41**, W02002, (2005).
- [3] L. Li, C.A. Peters, M.A. Celia, Upscaling geochemical reaction rates using pore-scale network modeling. *Adv. Water Resour.*, **29**, 1351-1370, (2006).
- [4] D. Kim, C.A. Peters, W.B. Lindquist. Upscaling geochemical reaction rates accompanying acidic CO₂-saturated brine flow in sandstone aquifers. *Water Resour. Res.*, **47**, W01505, doi: 10.1029/2010WR009472, (2010).
- [5] Y. Mehmani, T. Sun, M.T. Balhoff, P. Eichhubl, S.L. Bryant. Multiblock pore-scale modeling and upscaling of reactive transport: Application to carbon sequestration, *TIPM*, **95**, 305-326, (2012).
- [6] A. Raouf, H.M. Nick, S.M. Hassanizadeh, C.J. Spiers. PoreFlow: A complex pore-network model for simulation of reactive transport in variably saturated porous media. *Comput. & Geosci.*, **61**, 160-174, (2013).
- [7] B.Ph. van Milligen, P.D. Bons. Simplified numerical model for clarifying scaling behavior in the intermediate dispersion regime in homogeneous porous media. *Comput. Phys. Comm.*, **185**, 3291-3301, (2014).
- [8] M.A. Sbai, T.Kamtchueng, J.-L. Rouet. Generalised Mixed-Cell Mass Balance Solute Transport Modelling in Pore-Scale Disordered Networks. *Submitted to Adv. Water Resour. for review.*