

## **Groundwater modeling: solute transport simulation**

*A. Dassargues, Hydrogeology & Environmental Geology, Urban & Environmental Engineering, University of Liège, Belgium*

### *Summary*

The first part of the slide show consists of reminders about the basic concepts and equations of saturated solute transport processes. Then, the boundary conditions (BCs) are discussed and the different possibilities are illustrated.

The most common numerical techniques used to solve solute transport are described based on the Finite Difference method. Particular attention is given to advection-dominated problems, as this is the case mostly in aquifers. Specific methods are described, such as Eulerian or grid-based methods with upwind or upstream weighting, TVD methods, Eulerian-Lagrangian methods combining a method of characteristics with traditional FD or FE methods. Peclet and Courant numerical dimensionless numbers help the user to detect the actual numerical conditions, adapt time steps, and to choose which specific method should be adopted. Multi-species reactive transport is a coupled problem that can be simulated sequentially or in parallel. The following long list of references is provided in order to allow the student/researcher to go into more detail on the subject. The references are used and accordingly cited in the associated slide show. Specifically for BCs discussion, a list of provided references from the author and his research team allows finding practical examples of BCs choices in various practical cases.

### *Key words*

Deterministic model, solute transport, saturated conditions, equations, boundary conditions, Finite Difference Method (FDM), numerical Peclet number, numerical Courant number, numerical oscillations, numerical dispersion, upwind methods, upstream methods, total variation diminishing method (TVD), Eulerian-Lagrangian methods, method of characteristic, MOC, HMOC, MMOC, reactive transport modeling.

### *References*

- Batlle-Aguilar, J., Brouyère, S., Dassargues, A., Morasch, B., Hunkeler, D., Hohener, P., Diels, L., Vanbroekhoven, K., Seuntjens, P. and Halen, H., 2009. Benzene dispersion and natural attenuation in an alluvial aquifer with strong interactions with surface water. *Journal of Hydrology* 361: 305-317.
- Bear, J. 1972. *Dynamics of fluids in porous media*. New York: American Elsevier.
- Bear, J. and A. Verruijt. 1987. *Modeling groundwater flow and pollution*. Dordrecht: Reidel Publishing Company.
- Bear, J. and A.H.D. Cheng. 2010. *Modeling groundwater flow and contaminant transport*. Springer.
- Biver P., Hallet V., and Dassargues, A., 1995, Contribution to the simulation of nitrates transport in a double-porosity aquifer, *Proceedings of Solutions'95, XXVI Int. Cong. of IAH*, Edmonton (pages are not numbered but papers are classified by names, see "Dassargues"). <http://hdl.handle.net/2268/2128>
- Brouyère, S., Dassargues, A., and Hallet V., 2004. Migration of contaminants through the unsaturated zone overlying the Hesbaye chalky aquifer in Belgium: a field investigation. *Journal of Contaminant Hydrology* 72: 135-164.
- Brouyère, S., Batlle-Aguilar, J., Goderniaux, P. & Dassargues, A., 2007. A new tracer technique for monitoring groundwater fluxes: The Finite Volume Point Dilution Method. *Journal of Contaminant Hydrology* 95: 121-140.
- Carabin, G. and A. Dassargues. 1999. Modeling groundwater with ocean and river interaction. *Water Resources Research* 35(8): 2347-2358.
- César E, Wildemeersch S., Orban P., Carrière S., Brouyère S. and Dassargues A., 2014. Simulation of spatial and temporal trends in nitrate concentrations at the regional scale in the Upper Dyle basin, Belgium. *Hydrogeology Journal* 22: 1087 – 1100.

- Cheng, R.T., Casulli, V. and S.N. Milford. 1984. Eulerian-Lagrangian solution of the convection-dispersion equation in natural coordinates. *Water Resources Research* 20(7): 944-952.
- Chung, T. 2002. Computational fluid dynamics. Cambridge University Press. Coats, K.H. and B.D. Smith. 1964. Dead-end pore volume and dispersion in porous media. *Soc. Pet. Eng. J.*: 73-84.
- Cox, R.A. and T. Nishikawa. 1991. A new Total Variation Diminishing scheme for the solution of advective-dominant solute transport, *Water Resources Research* 27(10): 2645-2654.
- Dassargues A., 2018. *Hydrogeology: groundwater science and engineering*, 472p. Taylor & Francis CRC press, Boca Raton.
- Dassargues A. 2020. *Hydrogéologie appliquée : science et ingénierie des eaux souterraines*, 512p. Dunod. Paris.
- Daus, A.D. and E.O. Frind. 1985. An alternating direction Galerkin technique for simulation of contaminant transport in complex groundwater systems, *Water Resources Research* 21(5): 653-664.
- Davis, J.A. and D.B. Kent. 1990. Surface complexation modeling in aqueous geochemistry. *Rev. Mineral.* 23: 177-260.
- Delleur, J.W. 1999. *The handbook of groundwater engineering*. Boca Raton: CRC Press.
- Diersch, H-J.G. 2014. *Feflow – Finite element modeling of flow, mass and heat transport in porous and fractured media*. Springer.
- Ewing, R.E., Russell, T.F. and M.F. Wheeler. 1983. Simulation of miscible displacement using mixed methods and a modified method of characteristics. In *SPE Reservoir Simulation Symposium*. Society of Petroleum Engineers, 12241. Dallas (TX).
- Fitts, Ch. R. 2002. *Groundwater science*. Academic Press.
- Freeze, R.A. and J.A. Cherry. 1979. *Groundwater*, New Jersey: Prentice Hall.
- Garder Jr, A.O., Peaceman, D.W. and A.L. Pozzi Jr. 1964. Numerical calculation of multidimensional miscible displacement by the method of characteristics, *Society of Petroleum Engineers Journal* 4(01): 26-36.
- Gerke, H.H. and M.Th. van Genuchten. 1993. A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media. *Water Resources Research* 29(2): 305-319.
- Hadley, P.W. and Ch. Newell. 2014. The new potential for understanding groundwater contaminant transport. *Groundwater* 52(2): 174-186.
- Haerens B., Brouyère S. and Dassargues A., 1999, Detailed calibration of a deterministic transport model on multi-tracer tests: analysis and comparison with semi-analytical solutions, *ModelCARE'99, Pre-published Proceedings*, Eds. Stauffer F., Kinzelbach W. Kovar, K and Hoehn E., vol.1, pp. 319-324. <http://hdl.handle.net/2268/2560>
- Hallet V. & Dassargues A., 1998, Effective porosity values used in calibrated transport simulations in a fissured and slightly karstified chalk aquifer, *Groundwater Quality 1998*, M. Herbert & K. Kovar (Eds.), Tübingen Geowissenschaftliche Arbeiten (TGA), C36, pp. 124-126. <http://hdl.handle.net/2268/2463>
- Hoffmann R., Goderniaux P., Jamin P., Orban Ph., Brouyère S. and A. Dassargues. 2021. Differentiated influence of the double porosity of the chalk on solute and heat transport. In *The Chalk Aquifers of Northern Europe*. Farrell, R. P., Massei, N., Foley, A. E., Howlett, P. R. and West, L. J. (eds), Geological Society, London, Special Publications, 517, <https://doi.org/10.1144/SP517-2020-170>
- Holzbecher, E. 1998. *Modeling density-driven flow in porous media. Principles, Numerics, Software*. Berlin : Springer
- Huysmans, M. & Dassargues, A., 2005. Review of the use of Peclet numbers to determine the relative importance of advection and diffusion in low permeability environments. *Hydrogeology Journal* 13((5-6)): 895-904.
- Huysmans, M. & Dassargues, A., 2005. Stochastic analysis of the effect of heterogeneity and fractures on radionuclide transport in a low permeability clay layer. *Environmental Geology* 48(7): 920-930.
- Huysmans, M. & Dassargues, A., 2006. Stochastic analysis of the effect of spatial variability of diffusion parameters on radionuclide transport in a low permeability clay layer. *Hydrogeology Journal* 14: 1094-1106.
- Huysmans, M., Berckmans, A. and Dassargues, A., 2006. Effect of excavation induced fractures on radionuclide migration through the Boom Clay (Belgium). *Applied Clay Science* 33 (3-4): 207-218.
- Huysmans, M., & Dassargues, A., 2007. Equivalent diffusion coefficient and equivalent diffusion accessible porosity of a stratified porous medium. *Transport in porous media* 66: 421-438.
- Huysmans, M. & Dassargues, A., 2013. The effect of heterogeneity of diffusion parameters on chloride transport in low-permeability argillites. *Environmental Earth Sciences* 68(7): 1835-1848.
- Jamin, P., Dolle, F., Chisala, B., Orban, Ph., Popescu, I.C., Hérivaux, C., Dassargues, A., and Brouyère, S., 2012. Regional flux-based risk assessment approach for multiple contaminated sites on groundwater bodies. *Journal of Contaminant Hydrology* 127(1-4): 65-75.

- Kinzelbach, W. 1992. *Numerische methoden zur modellierung des transports von schadstoffen im grundwasser* (in German). Schriftenreihe GWF Wasser, Abwasser, Bd. 21, -2 Aufl., Munchen: Oldenbourg.
- Konikow, L.F. and J.D. Bredehoeft. 1978. *Computer model of two-dimensional solute transport and dispersion in ground water*. Washington: US Government Printing Office.
- Leonard, B.P. and H.S. Niknafs. 1990. *Cost-effective accurate coarse-grid method for highly convective multidimensional unsteady flows*, In: *Computational Fluid Dynamics Symposium on Aeropropulsion*. NASA Conference Publication 3078.
- Leonard, B.P. and H.S. Niknafs. 1991. *Sharp monotonic resolution of discontinuities without clipping of narrow extrema*, *Computer & Fluids* 19(1): 141-154.
- Molz, F.J., Widdowson, M.A. and L.D. Benefield. 1986. *Simulation of microbial growth dynamics coupled to nutrient and oxygen transport in porous media*, *Water Resources Research* 22(8): 1207-1216.
- Neuman, S.P. 1981. *A Eulerian-Lagrangian numerical scheme for the dispersion-convection equation using conjugate space-time grids*, *Journal of Computational Physics* 41(2): 270-294.
- Neuman, S.P. 1984. *Adaptive Eulerian-Lagrangian finite element method for advection-dispersion*, *International Journal for Numerical Methods in Engineering* 20(2): 321-337.
- Ogata, A. and R.B. Banks. 1961. *A solution of the differential equation of longitudinal dispersion in porous media*. USGS Professional Paper 411-I.
- Orban, P., Brouyère,S., Battle-Aguilar, J., Couturier, J., Goderniaux, P., Leroy, M., Malozewski, P. and Dassargues, A., 2010. *Regional transport modelling for nitrate trend assessment and forecasting in a chalk aquifer*. *Journal of Contaminant Hydrology* 118: 79-93.
- Payne, F.C., Quinnan, A. and S.T. Potter. 2008. *Remediation hydraulics*. Boca Raton: CRC Press/Taylor & Francis.
- Peeters, L., Haerens, B., Van Der Sluys, J. and Dassargues, A., 2004. *Modelling seasonal variations in nitrate and sulphate concentrations in a threatened alluvial aquifer*, *Environmental Geology* 46(6-7): 951-961.
- Pinder, G.F. and M.A. Celia. 2006. *Subsurface hydrology*. Hoboken, New Jersey: Wiley & Sons.
- Price, H.S., Varga, R.S. and J.R. Warren. 1966. *Application of oscillation matrices to diffusion-convection equations*, *Journal of Mathematical Physics* 45: 301-331.
- Rao, P.S.C., Jessup, R.E. and T.M. Addiscot. 1982. *Experimental and theoretical aspects of solute diffusion in spherical and nonspherical aggregates*. *Soil Science* 133(6): 342-349.
- Rausch, R., Schäfer, W., Therrien, R. and Chr. Wagner. 2005. *Solute transport modelling – An introduction to models and solution strategies*. Berlin-Stuttgart: Gebr.Borntraeger Verlagsbuchhandlung Science Publishers.
- Scheidegger, A. 1961. *General theory of dispersion in porous media*. *Journal of Geophysical Research* 66(10): 3273-3278.
- Skopp, J. and A. Warrick. 1974. *A two-phase model for the miscible displacement of the reactive solutes in soils*. *Soil Sc. Soc. Am. Proc.* 38(4): 545-550.
- Zech, A., Attinger, S., Cvetkovic, V., Dagan, G., Dietrich, P., Fiori, A., Rubin, Y. and G. Teutsch. 2015. *Is unique scaling of aquifer macrodispersivity supported by field data ?* *Water Resources Research* 51: 7662-7679.
- Zech, A., Attinger, S., Cvetkovic, V., Dagan, G., Dietrich, P., Fiori, A., Rubin, Y. and G. Teutsch. 2016. *Reply to comment by S. Neuman on 'Is unique scaling of aquifer macrodispersivity supported by field data?'*, *Water Resources Research* 52: 4203-4205.
- Zheng, C. 1993. *Extension of the method of characteristics for simulation of solute transport in three dimensions*, *Ground Water* 31(3): 456-465.
- Zheng, C. and G.D. Bennett. 1995. *Applied contaminant transport modeling: Theory and practice*, New York: John Wiley & Sons.
- Zheng, Ch and P.P. Wang. 1999. *MT3DMS A modular three-dimensional multispecies transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems. Documentation and user's guide. Technical report, Contract Report SERDP-99-1*, Vicksburg MS: U.S. Army Engineer Research and Development Center.