Methods Note:

Upstream dispersion in solute transport models: A simple evaluation and reduction methodology

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We derive 1D analytical solutions to quantify, and provide a simple approach to reduce, upstream dispersion in solute transport models.

Abstract

This article outlines analytical solutions to quantify the length scale associated with "upstream dispersion", the artificial movement of solutes in the opposite direction to groundwater flow, in solute transport models. Upstream dispersion is an unwanted artefact in common applications of the advection-dispersion equation (ADE) in problems involving groundwater flow in the direction of increasing solute concentrations. Simple formulae for estimating the one-dimensional distance of upstream dispersion are provided. These show that under idealized conditions (i.e., steady-state flow and transport, and a homogeneous aquifer), upstream dispersion may be a function of only longitudinal dispersivity. The scale of upstream dispersion in a selection of previously presented situations is approximated to highlight the utility of the presented formulae and the relevance of this ADE anomaly in common transport problems. Additionally, the analytical solution is applied in a hypothetical scenario to guide the modification of dispersion parameters to minimize upstream dispersion.

Introduction

The traditional application of the advection-dispersion equation (ADE) to macroscopically homogeneous aquifers often produces qualitatively dissimilar results to the contaminant transport observed in laboratory experiments and field-scale tests (e.g., Di Donato et al. 2003). One example of unexpected solute transport behavior is caused by upstream dispersion, which occurs when groundwater flows towards a solute source (Konikow 2011). Under these conditions, the concentration and hydraulic gradients are in opposite directions, leading to dispersive mass fluxes

against the direction of flow. Upstream dispersion is an unwanted artefact in simulations of solute transport that are caused by the Fickian dispersion model that underpins the ADE, which assumes that the concentration gradient is the driving force for solute spreading (e.g., Konikow 2011). Mass fluxes in the opposite direction to fluid flow only occur in real-world situations when molecular diffusion is in excess of the advective flux, e.g., as may occur in aquitards (e.g., Barbour et al. 2012; Zhang et al. 2015; Knight et al. 2019).

Upstream dispersion has been noted as an issue in several investigations aimed at quantifying macro-scale solute transport and involving groundwater flow in the direction of increasing solute concentration. Here, the term "macro-dispersion" refers to values of dispersion adopted in real-world problems, where the action of heterogeneity is implicit in field-scale dispersion coefficients, as described by Cvetkovic (2013). Documented examples of problems where upstream dispersion is apparent include: groundwater discharge towards saltwater boundaries (Henry 1964; Wooding et al. 1997), solute transport in aquifers containing structured heterogeneities, including faults and fractures (Robinson et al. 1998; Liu et al. 2004; Sebben and Werner 2016), forced-tracer tests (Chen et al. 1996), and solute exchange between the surface and subsurface domains of hillslope settings (Liggett et al. 2014). Despite its frequent occurrence, no attempt has been made to provide an approach to estimate the scale of upstream dispersion.

This study uses an intentionally simple conceptualization of one-dimensional (1D), steady-state fresh groundwater flow towards a solute source to quantify upstream dispersion under idealized conditions. In this study, we: (1) derive analytical solutions to quantify upstream dispersion for simple conditions; (2) apply these analytical solutions to previously published examples of

47 situations where upstream dispersion is expected to occur; and (3) describe a simple approach to
48 reduce upstream dispersion in solute transport simulations.
49
50 # Materials and Methods
51
52 ## Theory and Analytical Solution Derivation
53
54 The ADE for 1D non-reactive solute transport in a steady groundwater flow field is:

55 $$D_{\mathrm{L}} \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (1)$$

56
57 where C is concentration [ML^{-3}], v is average linear velocity [LT^{-1}], t is time [T], and x is position
58 [L], positive in the direction of groundwater flow. The hydrodynamic dispersion coefficient D_{L}
59 [L^2T^{-1}] includes both molecular diffusion, D_{m} [L^2T^{-1}], and mechanical dispersion, whereby the
60 latter represents the mechanical mixing. That is, $D_{\mathrm{L}} = D_{\mathrm{m}} + \alpha_{\mathrm{L}} v$, where α_{L} is the longitudinal
61 dispersivity [L]. D_{m} is proportional to the aqueous diffusion coefficient, D_{aq} [L^2T^{-1}], and is affected
62 by the porosity and the tortuosity of the porous medium.
63
64 The left side of Equation 1 is related to the solute mass flux gradient, $-\partial J/\partial x$, where J [$MT^{-1}L^{-2}$] is
65 the diffusive solute flux per unit area (i.e., the solute mass flux divided by the cross-sectional area
66 to flow and divided by porosity). Therefore, under steady-state solute conditions ($\partial C/\partial t = 0$), J is
67 a constant obtained by solving the partial differential Equation 1:

68 $$J = vC - e^{\frac{v}{D_{\mathrm{L}}}(x+E)}. \quad (2)$$

Here, J and the integration constant E are found from knowledge of the solute boundary conditions. In our case, the downstream efflux boundary is represented by a Dirichlet boundary conditions (Type 1) of specified solute concentration, C_2, to create the situation of freshwater flow in the direction of increasing concentration. The upstream boundary might commonly be treated as either: (A) a Dirichlet boundary conditions (Type 1) of specified concentration C_1, or (B) a Cauchy boundary condition in which J is specified as J_0. Equations 3 and 4 are easily obtained by applying the boundary condition from Case A to Equation 2, as:

$$J = vC_1 - \frac{v\left(C_2 - C_1\right)}{\left(e^{\frac{vL}{D_L}} - 1\right)}, \tag{3}$$

$$C = C_1 + \left(C_2 - C_1\right)\frac{\left(e^{\frac{vx}{D_L}} - 1\right)}{\left(e^{\frac{vL}{D_L}} - 1\right)}. \tag{4}$$

Applying Case B boundary conditions produces the following solution:

$$C = \left(C_2 - \frac{J_0}{v}\right)e^{\frac{v(x-L)}{D_L}} + \frac{J_0}{v}, \tag{5}$$

where L is length of the model domain [L]. In situations where the conceptualized value of J, given in Equation 3, is the specific mass flux through the boundary, given by vC_1, then the departure from this value is the second term on the right-hand side of Equation 3. The differences in mass flux and solute concentrations between the two boundary condition cases are larger for smaller values of the Péclet number, Pe [−], which is vL/D_L.

The extent of upstream dispersion is defined here as the upstream distance, F [L], to a prescribed solute concentration, given as C_F [−]. Adopting Case A boundary conditions, and with C_1 and C_2 taken as 0 and 1, respectively, leads to:

$$F = L - \frac{D_L}{v} \ln\left(C_F e^{\frac{vL}{D_L}} - C_F + 1 \right). \quad (6)$$

Case B boundary conditions, with J_0 and C_2 taken as 0 and 1, respectively, produces:

$$F = -\frac{D_L}{v} \ln C_F . \quad (7)$$

In cases where $D_m << \alpha_L v$, upstream dispersion is controlled by α_L and L where Case A boundary conditions are imposed, whereas upstream dispersion is a function of only α_L under Case B boundary conditions, according to Equations 6 and 7, respectively. The value of F from Equation 6 increases asymptotically towards that obtained from Equation 7 as L increases. Further simplifications of Equation 7 are possible if the following assumptions are made: α_L is taken as $0.1L$ (Gelhar et al. 1992), notwithstanding other factors and available functions relating α_L to L (e.g., Neuman 1990; Xu and Eckstein 1995; Schulze-Makuch 2005; Zech et al. 2015); $D_m << \alpha_L v$; and for C_F values ranging between 0.01 and 0.1, Equation 6 can be given in a comparative form to Equation 7, as:

$$F \approx -\alpha_L \ln C_F . \quad (8)$$

Numerical Simulations

FEFLOW (Diersch 2014) was used to simulate 2D steady-state solute transport within a uniform flow field to provide a simple test case to apply the analytical solutions (in this case, Equation 6). The model domain was 10 m in the *x*-direction and 5 m in the *y*-direction and was discretized with ~100,000 quadrilateral elements. Groundwater flow towards a region of constant concentration ($C = 1$) was simulated with $v = 0.33$ m/d. Upstream and downstream boundaries were represented with constant concertation ($C = 0$). D_{aq} was set at 8.64×10^{-5} m^2/d, α_L was 0.1 m and the transverse dispersivity (α_T) was 0.025 m. These dispersivity values are within the plasible range for the scale of the problem (i.e., Gelhar et al. 1992; Zech et al. 2015).

Results and Discussion

Assessing Upstream Dispersion Effects in Previous Studies

There are numerous examples in the literature of solute transport problems where groundwater flows in the direction of increasing concentration, and where models have been applied to analyze concentration distributions and/or solute fluxes. For the most part, these involve flow and transport in 2D or 3D, rather than the 1D basis for the previous equations. Nonetheless, the conditions along flow lines are considered to allow for a first-order approximation of upstream dispersion using the 1D equations given above. This allows for testing of whether upstream dispersion is predictable under the simplifying assumptions that led to the previous equations. A selection of cases is presented in Table 1 representing a variety of solute transport situations and scales of analysis.

Only brief descriptions of the cases are provided. The reader is directed to the respective references for further details.

Table 1 Parameter sets used to estimate steady-state upstream dispersion.

Case	v (m/d)	D_{aq} (m^2/d)	α_L (m)	L (m)	C_F (−)	F^* (m)	$F_{(6)}$ (m)	$F_{(7)}$ (m)
Henry (1964)	34.6	1.629	0	2	0.1	0.10	−	0.11
Sebben and Werner (2016)[1]	305	0	0.005	0.583	0.02	0.02	0.023	0.023
Liggett et al. (2014)[2]:								
Very Low D_L	0.1	8.64×10^{-6}	0.1	~8	0.01	0.15[3]	−	0.46
Low D_L	0.1	8.64×10^{-5}	0.1	~8	0.01	0.15[3]	−	0.46
Intermediate D_L	0.1	8.64×10^{-5}	1	~8	0.01	0.31[3]	−	4.6
High D_L	0.1	8.64×10^{-5}	10	~8	0.01	0.80[3]	−	46

F^* is upstream dispersion estimated from solute transport models.

$F_{(6)}$ and $F_{(7)}$ refer to upstream dispersion from Equations 6 and 7, respectively.

[1]Sebben and Werner (2016) results are taken from "Case A1".

[2]Liggett et al. (2014) results are taken from the concave hillslope case "A+Disp".

[3]Transient results, i.e., steady-state conditions were not reached.

The Henry (1964) problem is a commonly applied 2D benchmark case for evaluating density-dependent flow and transport codes. Fresh groundwater enters a 2 m by 1 m coastal aquifer cross section and exits through the upper 0.47 m of the vertical sea boundary, as discernible from flow lines constructed by Henry (1964). The specified concentration boundary conditions representing

the sea induces upstream dispersion, to the degree given as F^* (obtained at the mid-point of the outflow face) in Table 1. Application of Equation 7 provides a close match to the upstream dispersion of the Henry (1964) problem, despite its complex density-dependent conditions.

Sebben and Werner (2016) studied the influence of discrete flow features (e.g., fractures, faults) on the characteristics of steady-state solute plumes in otherwise permeable aquifers. Preferential flow in these features creates conditions where matrix flow occurs in the direction of low-to-high solute concentrations, leading to anomalous solute concentrations in a selection of cases. Sebben and Werner (2016) were unable to justify the anomalous solute concentrations, and hypothesized that "back dispersion" (i.e., upstream dispersion) was the cause. Table 1 provides an estimate of the extent of upstream dispersion encountered in "Case A1" from Sebben and Werner (2016). Both Equations 6 and 7 provide close estimates of the extent of upstream dispersion that was produced in their numerical experiment.

Liggett et al. (2014) studied the transfer of solutes from the surface to the subsurface in 2D hillslope catchments using the numerical modeling code HydroGeoSphere (Therrien et al. 2006) to explore the contributions of event and pre-event water to runoff. Their study investigated various transport mechanisms (i.e., advection only, advection and dispersion, etc.). Here we assess the cases that considered advection and dispersion ("A+Disp" in Liggett et al. (2014)). Their models showed dilution of pre-event water (i.e., due to inflows of event water) in the shallow subsurface that was attributed to upstream dispersion, which also led to significant errors in solute fluxes to the land surface. By scaling from their diagrams of concentration distributions, the extent of upstream dispersion (i.e., F^* in Table 1) was estimated.

Upstream dispersion values obtained from Equation 7, as given in Table 1, are considerably larger than those observed by Liggett et al. (2014). This is attributable to the transient nature of their experiments, in contrast to the steady-state assumption of Equation 7. Given that $F^* < F_{(7)}$ (see Table 1), it is expected that the simulated (and anomalous) dilution of pre-event water in discharge areas of the models from Liggett et al. (2014) would continue to grow if simulation times were extended. The upstream dispersion (F^* in table 1) in the Liggett et al. (2014) study increased as the subsurface α_L increased, as expected from the theory presented herein.

Upstream dispersion has been reduced or eliminated by modifying the downstream boundary condition, in a selection of situations. For example, Liggett et al. (2014) modified the surface-subsurface interface conditions to avoid imposing surface solute concentrations to the upper boundary of the subsurface. The original Henry (1964) problem has also been changed so that concentrations along the sea boundary represent that of discharging groundwater in regions of outflow (Croucher and O'Sullivan 1995).

Konikow (2011) highlights that a better governing equation of solute transport would solve several issues that arise from use of the ADE, including unrealistic upstream dispersion. He cites mass-transfer models (e.g., Haggerty and Gorelick 1995) and continuous time random walk models (e.g., Berkowitz et al. 2006) as steps in the right direction. However, he also notes that these approaches either require additional data, or include parameters that are either non-intuitive, or difficult to measure. Given the control of α_L, we suggest that it is possible to limit the extent of upstream

dispersion by reducing the hydrodynamic dispersion adopted in models in regions where groundwater flows in the direction of increasing solute concentration, i.e., through lowering α_L.

Simple Approach to Minimize Upstream Dispersion

Here, we propose an approach, using the traditional ADE implemented in most models capable of simulating solute transport. Our approach utilizes Equation 6 or 7 to determine the likely upstream dispersion, then places a region of low α_L within this zone. The approach is simple to implement and the scale over which unrealistic upstream dispersion would have occurred can be quantified. An example of a simulation with no low-dispersivity zone is shown in Figure 1a and with the low-dispersivity zone in Figure 1b.

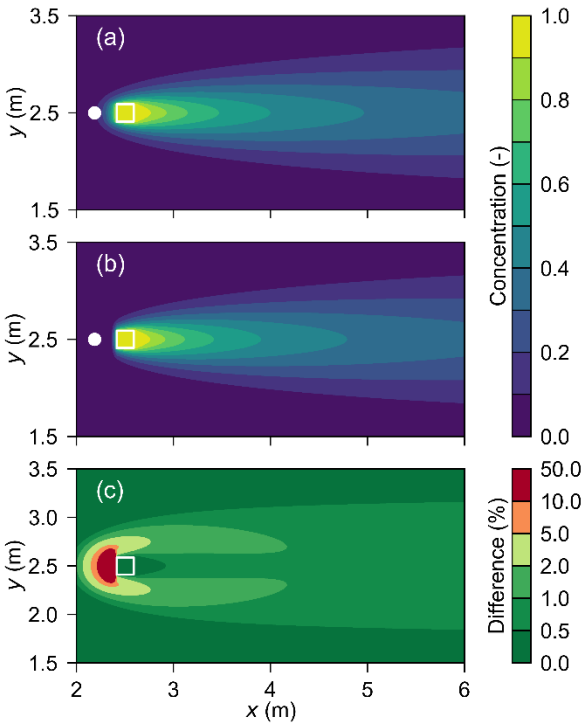

Figure 1. Demonstration of the applicability of Equation 6. White square denotes zone of constant concentration. White circle (Figure 1a, 1b) denotes distance of the 0.1 isochlor as predicted by

Equation 6. (a) Model run where α_L = 0.1 m and α_T = 0.025 m. (b) Model modified to include a zone where α_L = α_T = 0.025 m immediately upstream of the constant concentration zone. (c) Concentration difference (%) between Figure 1a and 1b. Only a subset of the modelling domain is shown, to enhance visual inspection of local-scale phenomena. The model domain was 10 m × 5 m in the *x* and *y* directions, respectively.

Figure 1 shows that unrealestic upstream dispersion can be easly eliminated in numerical simulation by lowering dispersion parameters immediatley upstream of the solute source, producing minimial changes to the solute transport patterns downstream of the region of lowered dispersion that would otherwise have occurred. It is worth noting that the results in Figure 1a and 1b are similar to conceptual diagrams in Konikow (2011). Also, implimenting the change to the model had some influence on the downstream concentrations (Figure 1c).

In this simple application, the lowest possible dispersivity that allows numerically stable results (i.e., $\Delta x/\alpha_L \leq 2$, where Δx is the spatial discretization) was used for four elements upstream of the constant concentration zone, although the results are similar to the use of a single row of reduced-dispersivity elements. This simple approach is intuitive and can be easily implemented in most numerical model codes, even in cases where the mean flow direction varies in time. For example, a zone of lower α_L could be placed around the zone of constant concentration. Reducing the value of α_L close to a solute source is also consistent with its apparent spatial variability (e.g., Gelhar et al. 1992; Zech et al. 2015).

Conclusions

Upstream dispersion, the urealistic movement of solutes in the opposite direction to groundwater flow caused by Fickian dispersion model assumptions in solute transport models, has been identified in a number of previous studies. Yet there has been no previous guidance for solute transport modelers to obtain rapid estimates of its likely steady-state extent. In this study, the one-dimensional advection-dispersion equation for steady-state conditions is solved to produce two rudimentary solutions for the extent of upstream dispersion under either Dirichlet or Cauchy boundary conditions at the upstream boundary. Unsurprisingly, upstream dispersion is shown to be proportional to the dispersivity under common situations. The utility of the new upstream dispersion equations is demonstrated by application to several complex problems in which upstream dispersion is either well-matched or the equations at least provide useful insights into the potential scale of steady-state upstream dispersion effects. We also provide a simple and intuitive approach to reduce unrealistic upstream dispersion, whereby a reduced value of dispersivity is applied to a region immediately upstream of the solute source.

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References

Barbour, S.L., M.J. Hendry, and L.I. Wassenaar. 2012. In situ experiment to determine advective-diffusive controls on solute transport in a clay-rich aquitard. *Journal of Contaminant Hydrology* 131: 79 –88. https://doi.org/10.1016/j.jconhyd.2011.12.002

Berkowitz, B., A. Cortis, M. Dentz, and H. Scher. 2006. Modeling non-Fickian transport in geological formations as a continuous time random walk. *Reviews of Geophysics* 44: RG2003. https://doi.org/10.1029/2005RG000178

Chen, J.-S., C.-W. Liu, C.-S. Chen, and H.-D. Yeh. 1996. A Laplace transform solution for tracer tests in a radially convergent flow field with upstream dispersion. *Journal of Hydrology* 183: 263–275. https://doi.org/10.1016/0022-1694(95)02972-9

Croucher, A.E., and M.J. O'Sullivan. 1995. The Henry problem for saltwater intrusion. *Water Resources Research* 31: 1809–1814. https://doi.org/10.1029/95WR00431

Cvetkovic, V. 2013. How accurate is predictive modeling of groundwater transport? A case study of advection, macrodispersion, and diffusive mass transfer at the Forsmark site (Sweden). *Water Resources Research* 49: 5317–5327. https://doi.org/10.1002/wrcr.20429

Di Donato, G., E. Obi, and M.J. Blunt. 2003. Anomalous transport in heterogeneous media demonstrated by streamline-based simulation. *Geophysical Research Letters* 30: 1608. https://doi.org/10.1029/2003GL017196

Diersch, H.-J. G. 2014. FEFLOW: Finite Element Modeling of Flow, Mass and Heat Transport in Porous and Fractured Media. eBook: Springer.

Gelhar, L.W., C. Welty, and K.R. Rehfeldt. 1992. A critical-review of data on field-scale dispersion in aquifers. *Water Resources Research* 28, no. 7: 1955–1974. https://doi.org/10.1029/92WR00607

Haggerty, R., and S.M. Gorelick. 1995. Multiple-rate mass transfer for modeling diffusion and surface reactions in media with pore-scale heterogeneity. *Water Resources Research* 31, no. 10: 2383–2400. https://doi.org/10.1029/95WR10583

Henry, H.R. 1964. Effects of dispersion on salt encroachment in coastal aquifers. U.S. Geological Survey Water Supply Paper, 1613-C.

Knight, A.C., A.D. Werner, and D.J. Irvine. 2019. Combined geophysical and analytical methods to estimate offshore freshwater extent. *Journal of Hydrology* 576: 529–540. https://doi.org/10.1016/j.jhydrol.2019.06.059.

Konikow, L.F. 2011. The secret to successful solute-transport modeling. *Ground Water* 49: 144–159. https://doi.org/10.1111/j.1745-6584.2010.00764.x

Liggett, J. E., A.D. Werner, B.D. Smerdon, D. Partington, and C.T. Simmons. 2014. Fully integrated modeling of surface-subsurface solute transport and the effect of dispersion in tracer hydrograph separation. *Water Resources Research* 50: 7750–7765. https://doi.org/10.1002/2013WR015040

Liu, G., C. Zheng, and S.M. Gorelick. 2004. Limits of applicability of the advection-dispersion model in aquifers containing connected high-conductivity channels. *Water Resources Research* 40: W08308. https://doi.org/10.1029/2003WR002735

Neuman, S.P. 1990. Universal scaling of hydraulic conductivities and dispersivities in geologic media. *Water Resources Research* 26, no. 8: 1749–1758. https://doi.org/10.1029/WR026i008p01749.

295 Robinson, N.I., J.M. Sharp, and I. Kreisel. 1998. Contaminant transport in sets of parallel finite
296 fractures with fracture skins. *Journal of Contaminant Hydrology* 31: 83–109.
297 https://doi.org/10.1016/S0169-7722(97)00055-7
298 Schulze-Makuch, D. 2005. Longitudinal dispersivity data and implications for scaling behavior.
299 *Ground Water* 43, no. 3: 443–456. https://doi.org/10.1111/j.1745-6584.2005.0051.x
300 Sebben, M.L., and A.D. Werner. 2016. A modeling investigation of solute transport in permeable
301 porous media containing a discrete preferential flow feature. *Advances in Water Resources*
302 94: 307–317. https://doi.org/10.1016/j.advwatres.2016.05.022
303 Therrien, R., R.G. McLaren, E.A. Sudicky, and S.M. Panday. 2006. HydroGeoSphere. Waterloo,
304 Canada: Groundwater Simulations Group, University of Waterloo.
305 Wooding, R.A., S.W. Tyler, and I. White. 1997. Convection in groundwater below an evaporating
306 salt lake: 1. Onset of instability. *Water Resources Research* 33: 1199–1217.
307 https://doi.org/10.1029/96WR03533
308 Xu, M.J., and Y. Eckstein. 1995. Use of weighted least-squares method in evaluation of the
309 relationship between dispersivity and field-scale. *Ground Water* 33, no. 6: 905–908.
310 https://doi.org/10.1111/j.1745-6584.1995.tb00035.x
311 Zech, A., S. Attinger, V. Cvetkovic, G. Dagan, P. Dietrich, A. Fiori, Y. Rubin, and G. Teutsch.
312 2015. Is unique scaling of aquifer macrodispersivity supported by field data? *Water*
313 *Resources Research* 51, no. 9: 7662 –7679. http://doi.org/10.1002/2015WR017220
314 Zhang, Y., C.T. Green, and G.R. Tick. 2015. Peclet number as affected by molecular diffusion
315 controls transient anomalous transport in alluvial aquifer-aquitard complexes. *Journal of*
316 *Contaminant Hydrology* 177−178: 220–238. https://doi.org/10.1016/j.jconhyd.2015.04.001
317