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Studying solute transport using parsimonious groundwater modelling

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1. Abstract

Groundwater modelling is plagued by the increased uncertainty concerning the properties (hydraulic conductivity, porosity, geometry) and the conditions (boundary conditions, initial conditions, stresses) of aquifers. Some studies suggest that the magnitude of this uncertainty does not justify such a level of detailed representation and simulation employed by groundwater models that numerically solve differential equations. Rozos and Koutsoyiannis (2010) suggested that multi-cell models should be considered as an alternative option in cases of increased uncertainty. This study extends that work by including solute transport in a multi-cell model that allows discretization of the flow domain using a low number of cells of flexible geometry. This method was tested in a case study that has analytical solution.

2. Dispersion – diffusion

Molecular diffusion is the solute-spreading caused by the random molecular motion and collisions of the particles themselves.

Kinematic (or mechanical) dispersion is the spreading, or mixing phenomenon, caused by the variability of the complex, microscopic velocities through the pores in the medium (Logah, 2001).

Hydrodynamic dispersion is the spreading (at the macroscopic level) of the solute front during transport resulting from both mechanical dispersion and molecular diffusion (EPA, 2002).

Dispersivity: Is the ratio of the mechanical dispersion coefficient to the average linear groundwater velocity (Fetter, 2001).

Numerical dispersion is a nonphysical effect inherently present in finite-difference time-domain algorithms, which is manifested either as a dependence of wave propagation velocity on frequency (Juntunen and Tsiboukis, 2000) or as oscillations (Hundsdorfer, 2000).

Numerical diffusion (or dissipation) is a nonphysical effect inherently present in the finite-difference schemes based on first order upwind discretization, which is manifested as smearing of concentration profile (Hundsdorfer, 2000).

3. Solute transport in multi-cell model

This study presents an algorithm that can simulate the solute transport advection/diffusion processes in steady state flow using the results of the multi-cell model described in the publication of Rozos and Koutsoyiannis (2010) the output of which are the volume of water V_i inside cell i , and the volume of water $Q_{ij}dt$ exchanged between cells i,j at each time step. These two are necessary to calculate the mass balance of a solute with concentration c_i at cell i . For steady state flow conditions, 1D discretization, flow from left to right, dispersion coefficient D and cross section A the mass balance equation is:

$$\frac{\Delta(c_i V_i)}{\Delta t} = c_{i-1}Q_{i-1/2} - c_i Q_{i+1/2} - DA \frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta x}$$

4. Tackling numerical diffusion

In the previous equation, an upwind scheme is used to estimate the first order space derivative (advection term). This approach, according to Hundsdorfer (2000), suffers from numerical diffusion proportional to the length Δx of discretization cells. This means that the coarser the discretization the larger the error due to numerical diffusion. However, the numerical experiments performed in this study demonstrated that this side effect can be tackled using a lag h in the estimation of this derivative. If the time derivative of the concentration is calculated using forward scheme and $DAX=DA/\Delta x$ then the solute balance equation becomes:

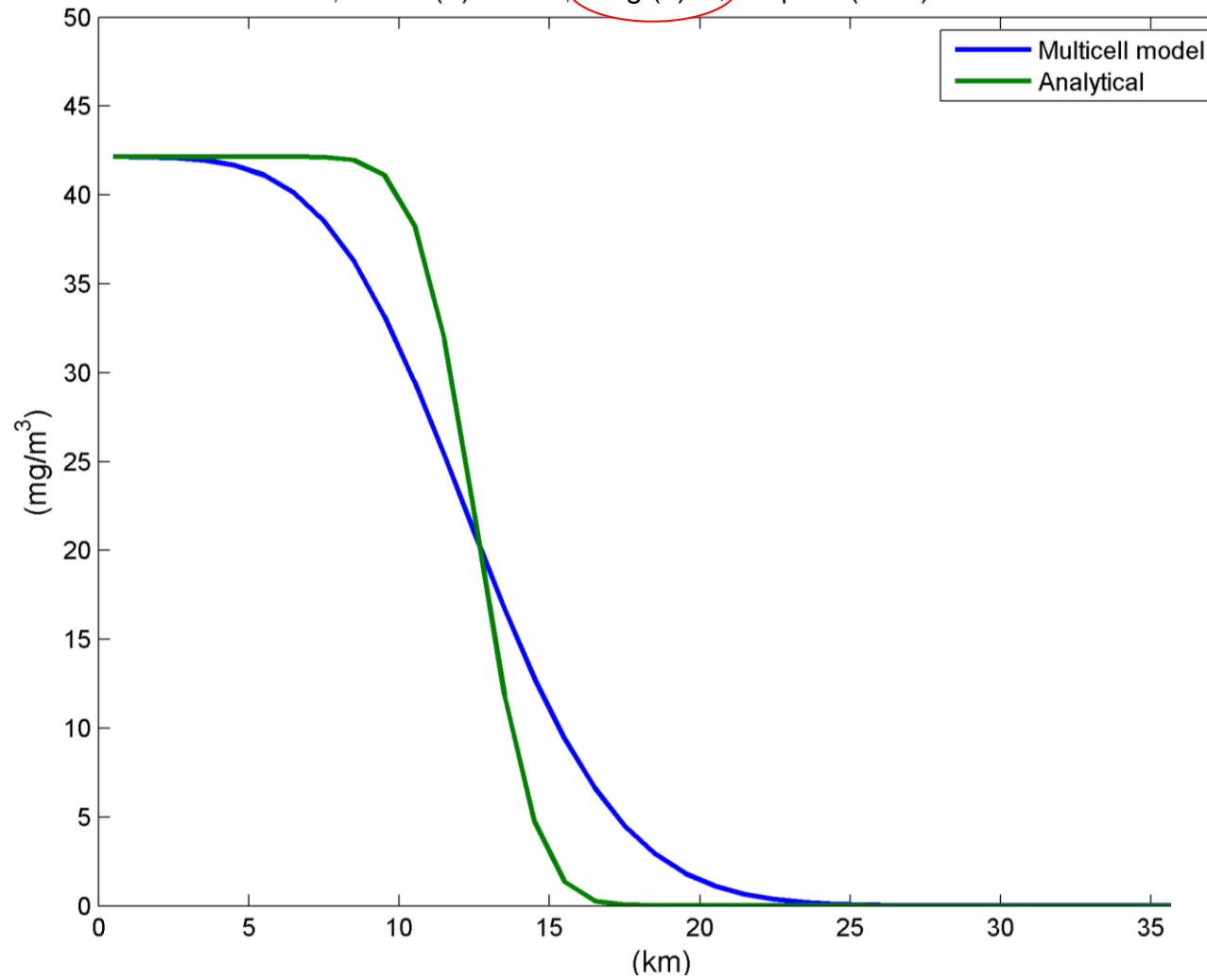
$$c_i^t = c_i^{t-1} + \frac{c_{i-1}^{t-h} Q_{i-1/2} - c_i^{t-h} Q_{i+1/2} - DAX(c_{i-1}^{t-1} - 2c_i^{t-1} + c_{i+1}^{t-1})}{V_i} \Delta t$$

5. Synthetic case studies

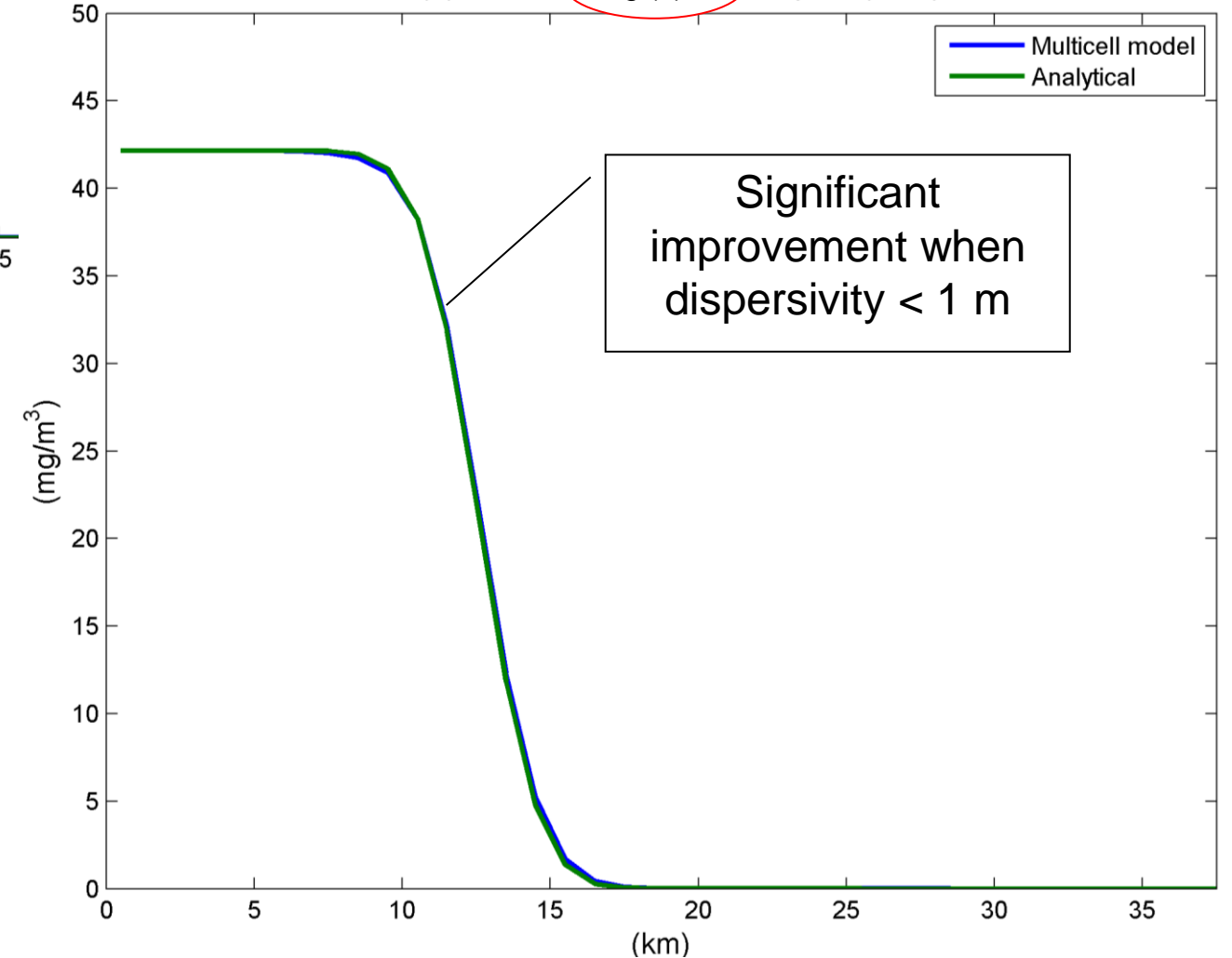
The approach described previously was tested in a hypothetical confined aquifer with length, width and thickness of 38 km, 100 m and 1 km, respectively. The hydraulic boundary conditions were constant head equal to 2190 m at the left end and a series of drains at 100 m at the right end. Two cases of solute boundary conditions were examined, constant injection and pulse injection at the left end. The former was discretized with 38 equally sized cells whereas the latter with 149 equally sized cells. Two dispersivities were assumed for the hypothetical aquifer, 1 m and 10 m. The results of the numerical model were tested against analytical solutions provided by Bear (1979) for the continuous injection in a semi-confined infinite aquifer (equation 7-134) and the pulse injection in a semiconfined infinite aquifer (equation 7-123).

6. Continuous injection, dispersivity 1 m

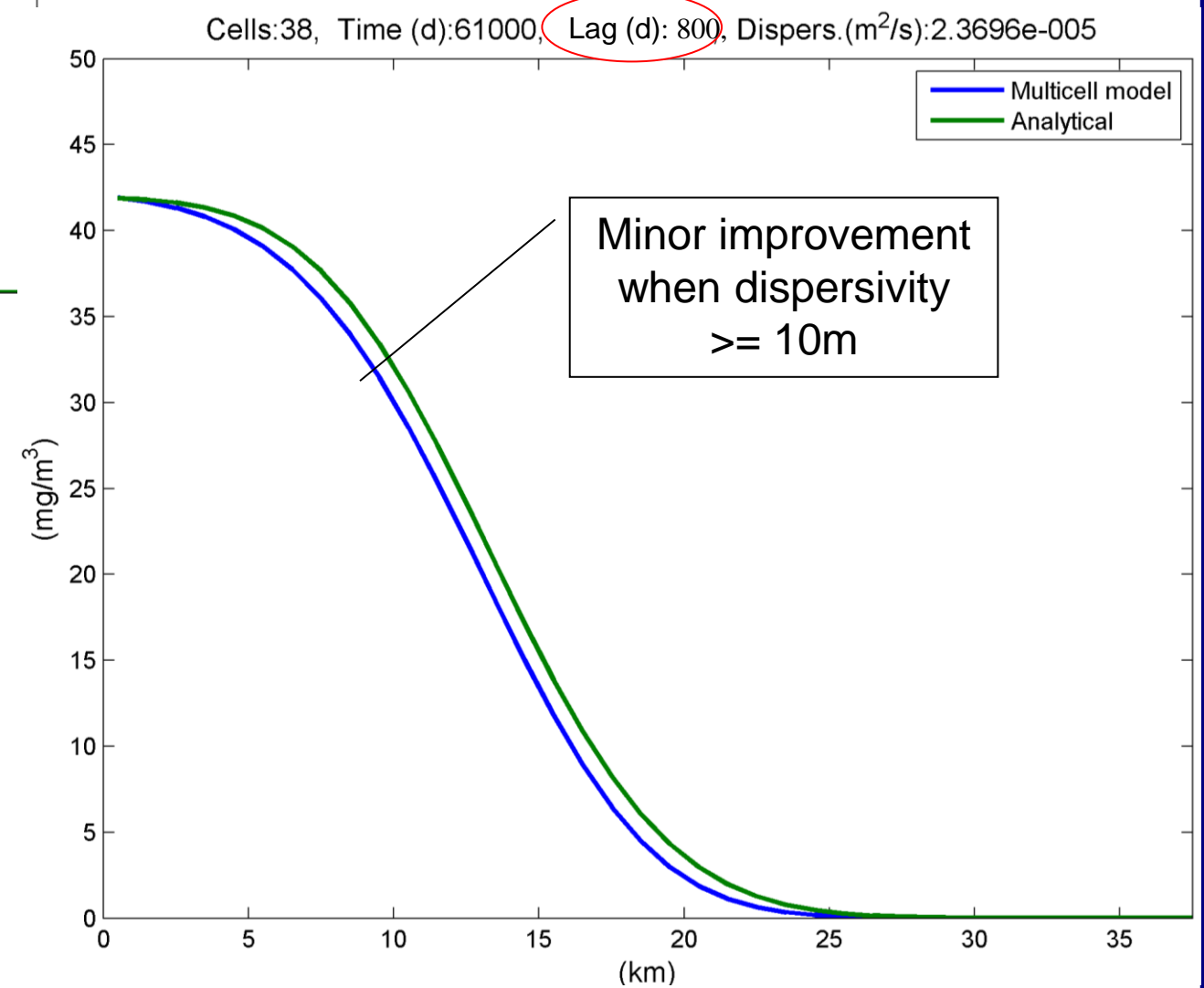
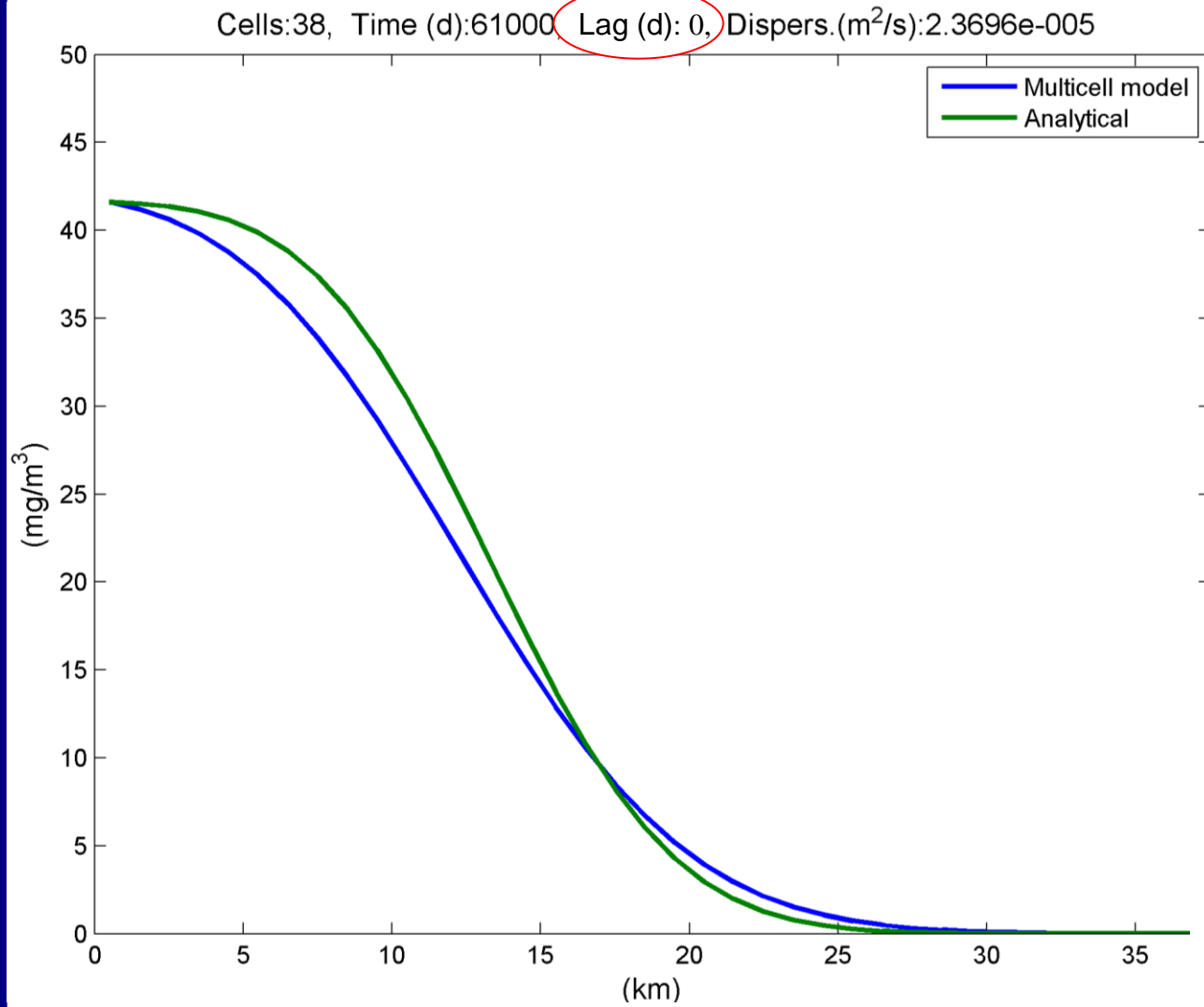
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Cells:38, Time (d):61000, Lag (d): 800, Dispers.(m²/s):2.3696e-006

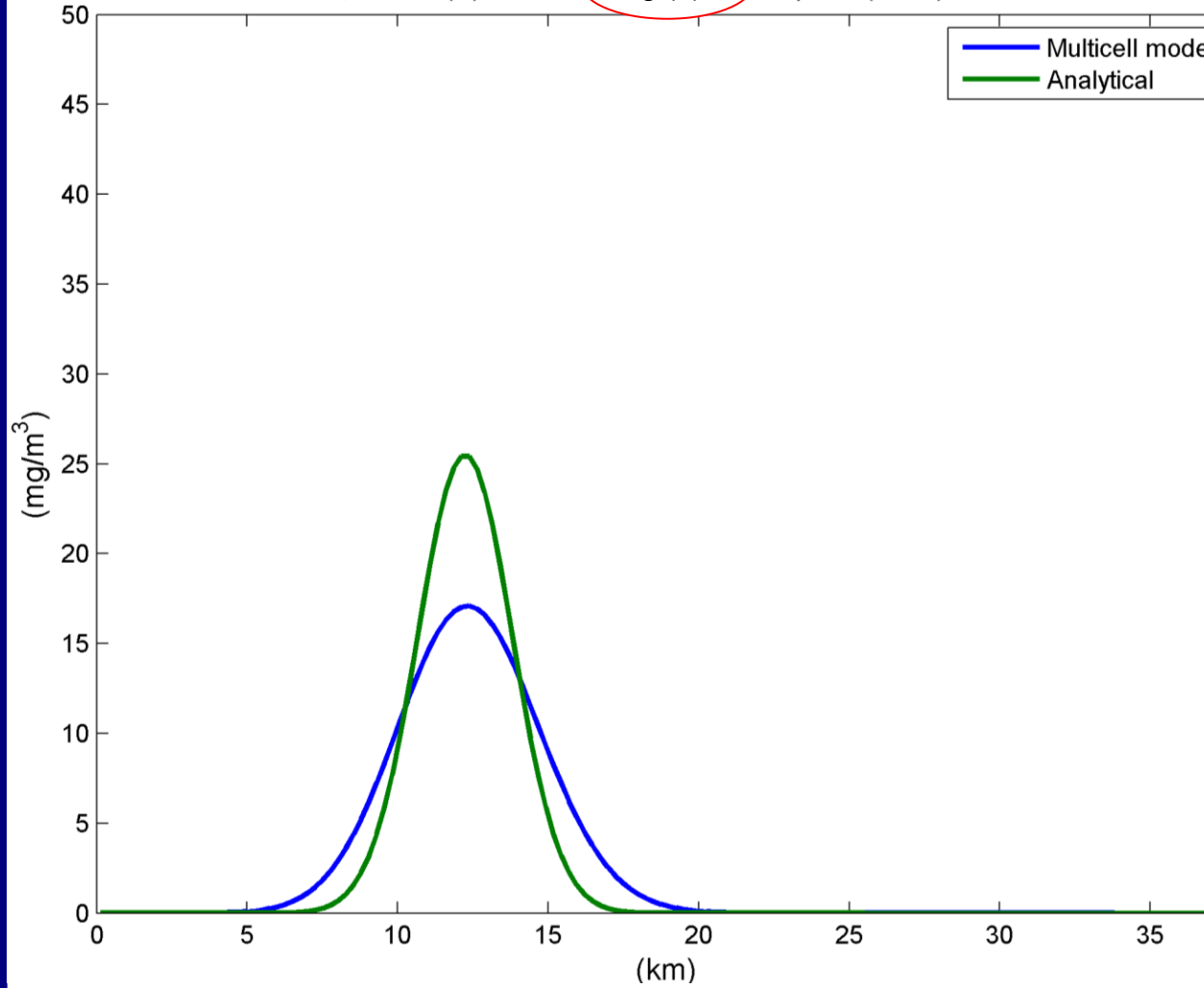


7. Continuous injection, dispersivity 10 m

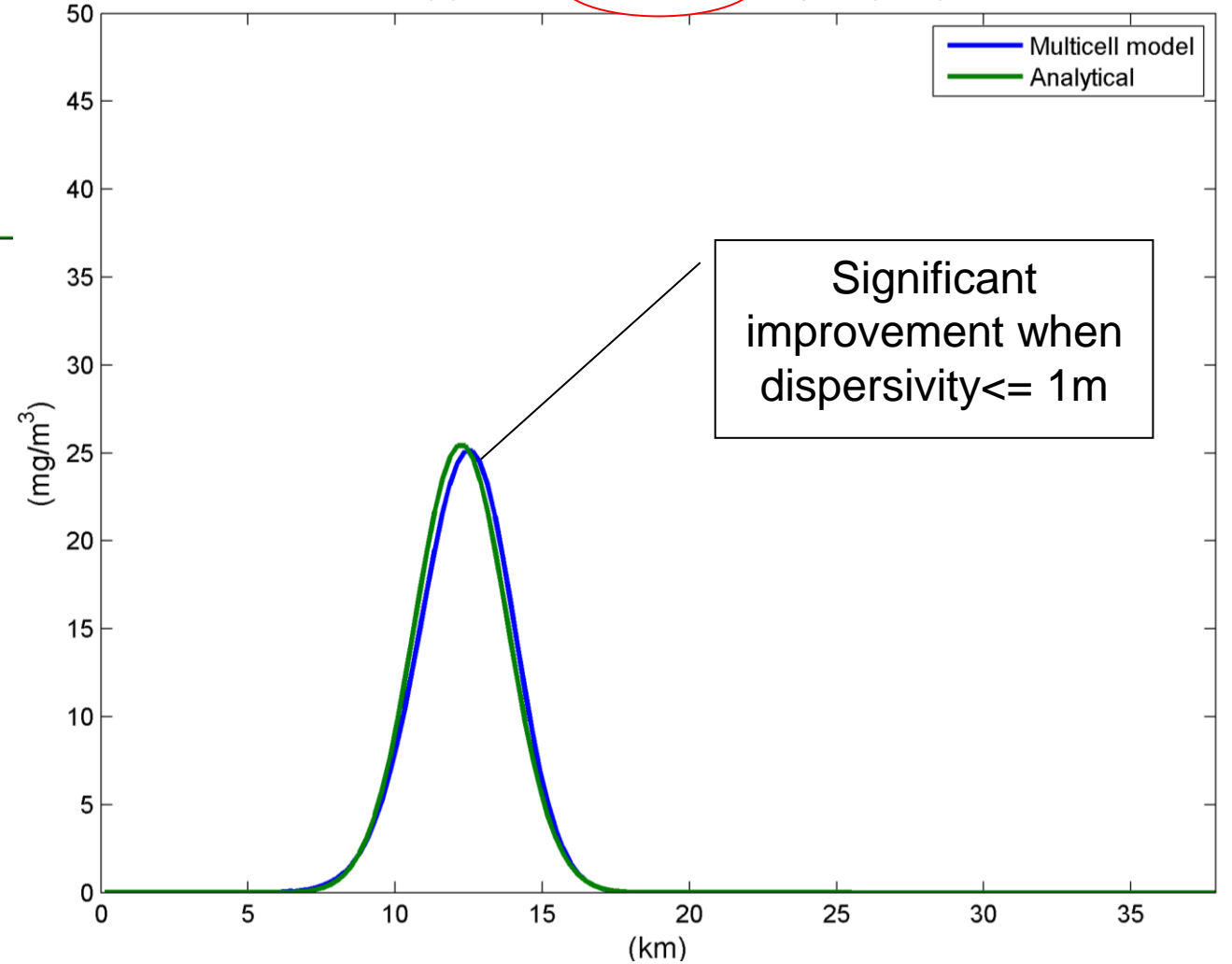


8. Pulse injection, dispersivity 1 m

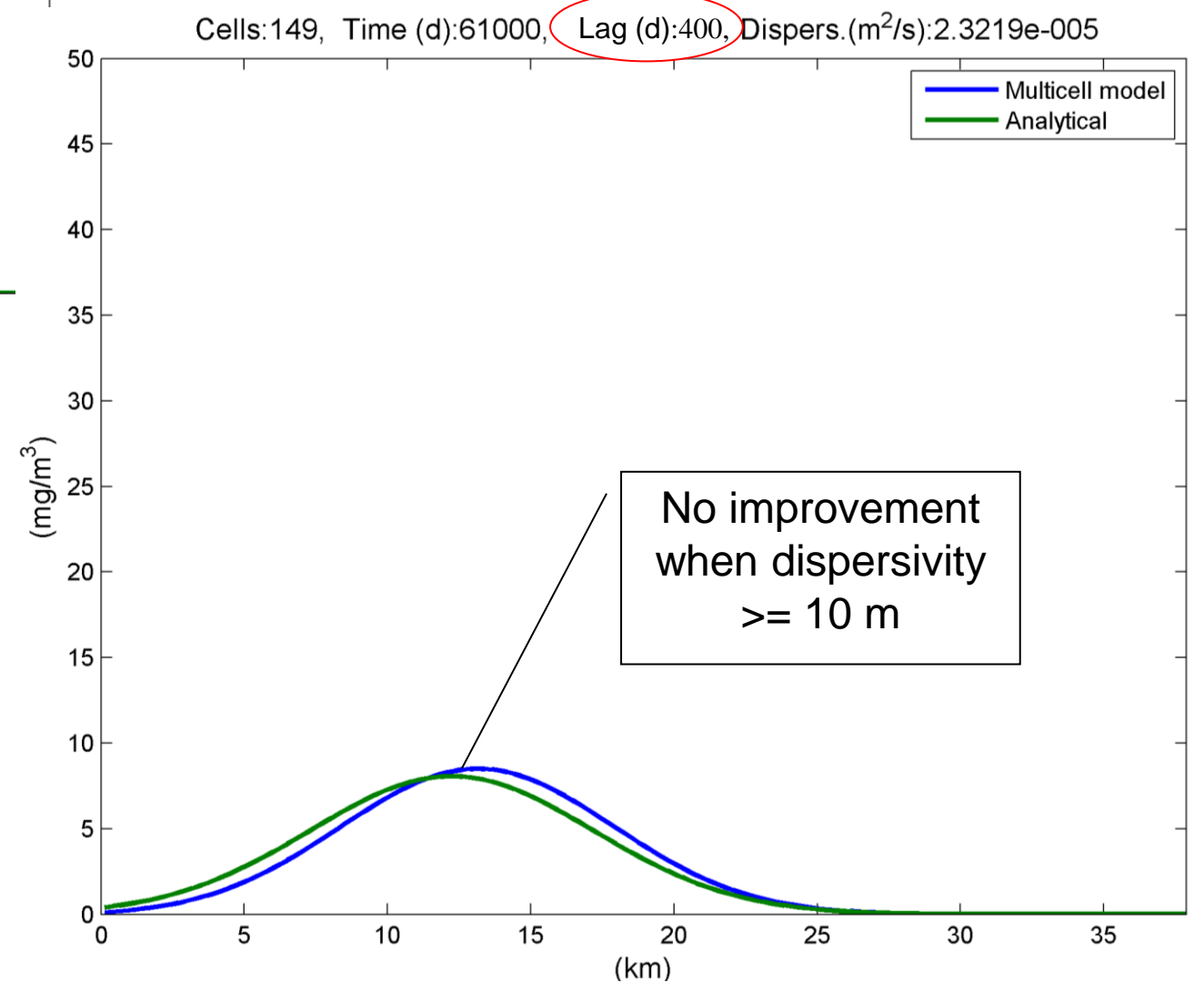
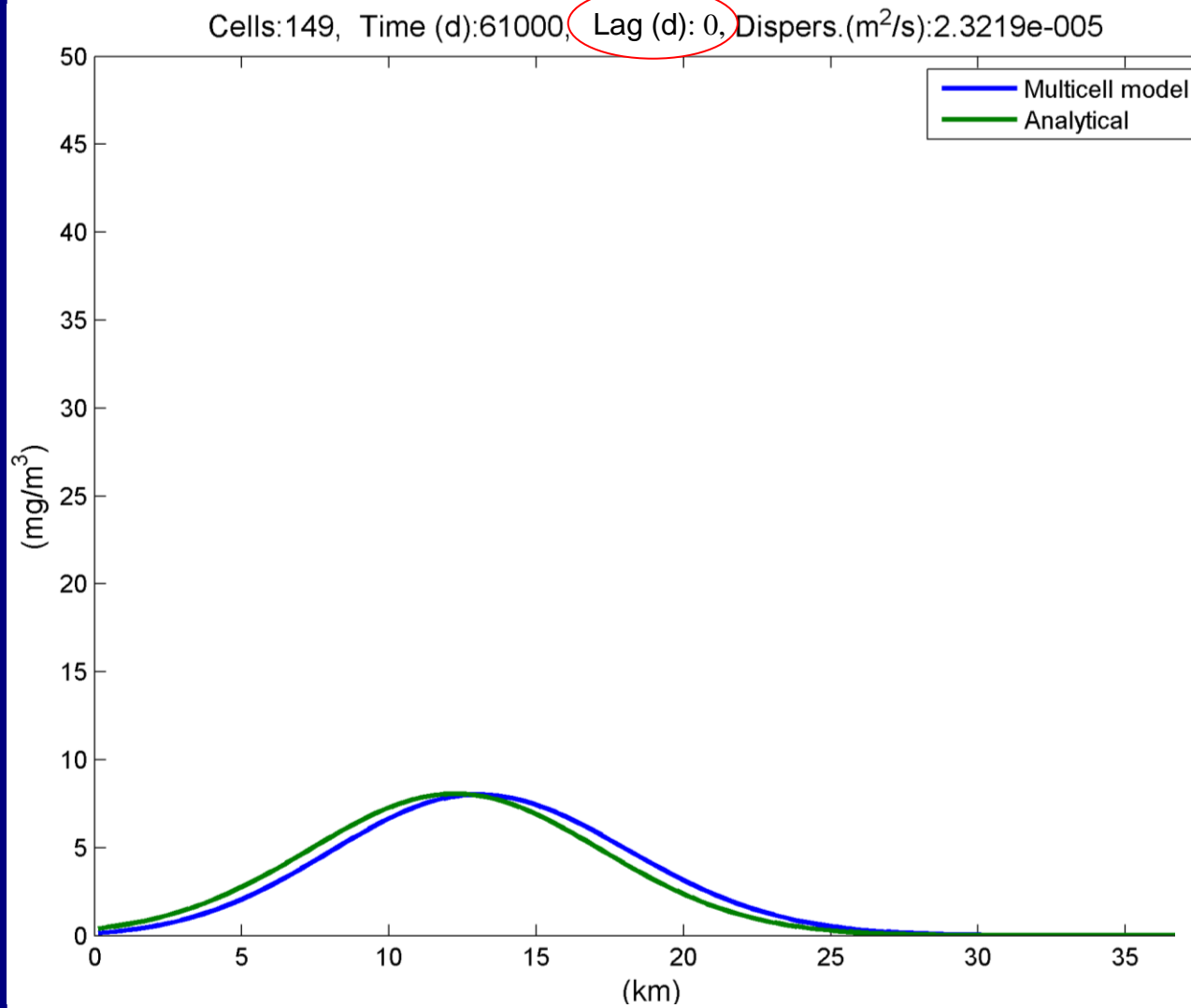
Cells:149, Time (d):61000, Lag (d): 0, Dispers.(m²/s):2.3219e-006



Cells:149, Time (d):61000, Lag (d):400, Dispers.(m²/s):2.3219e-006

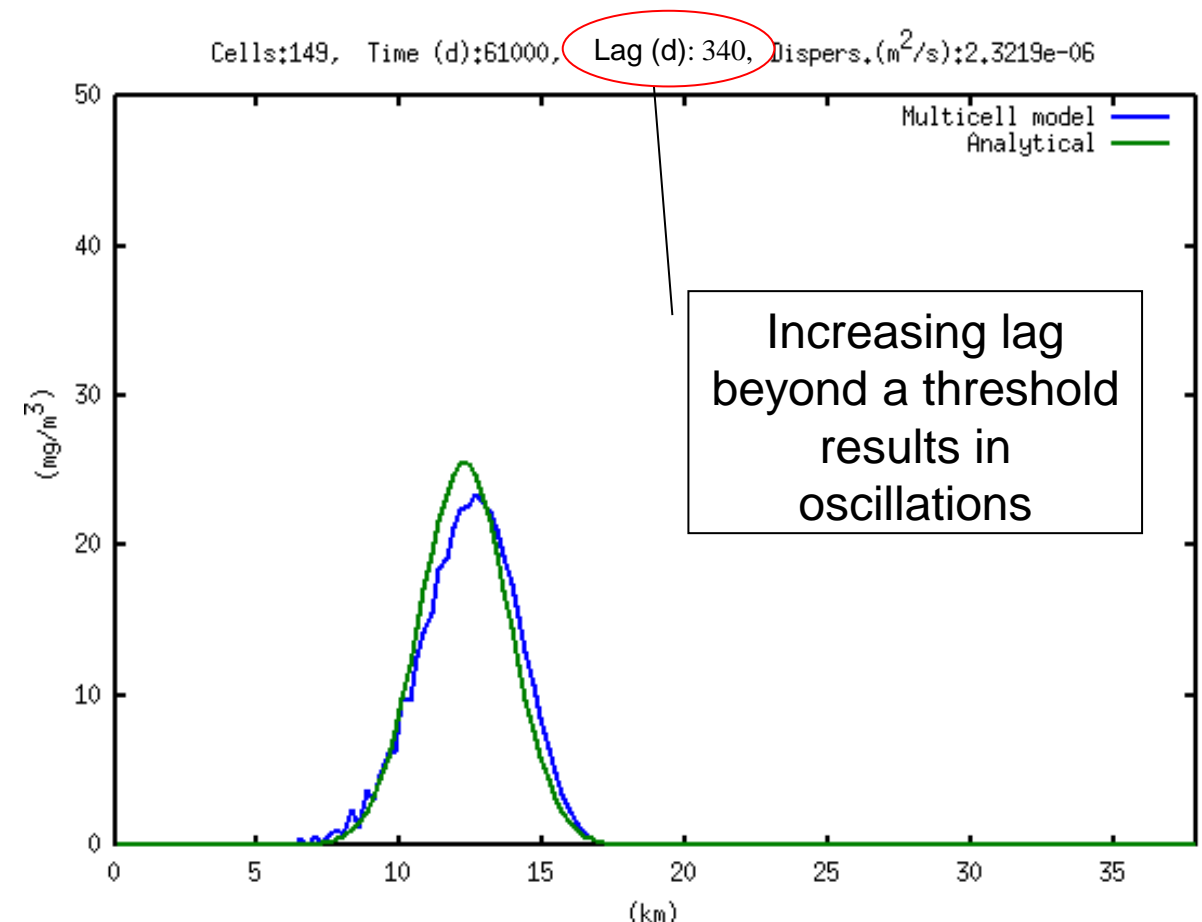
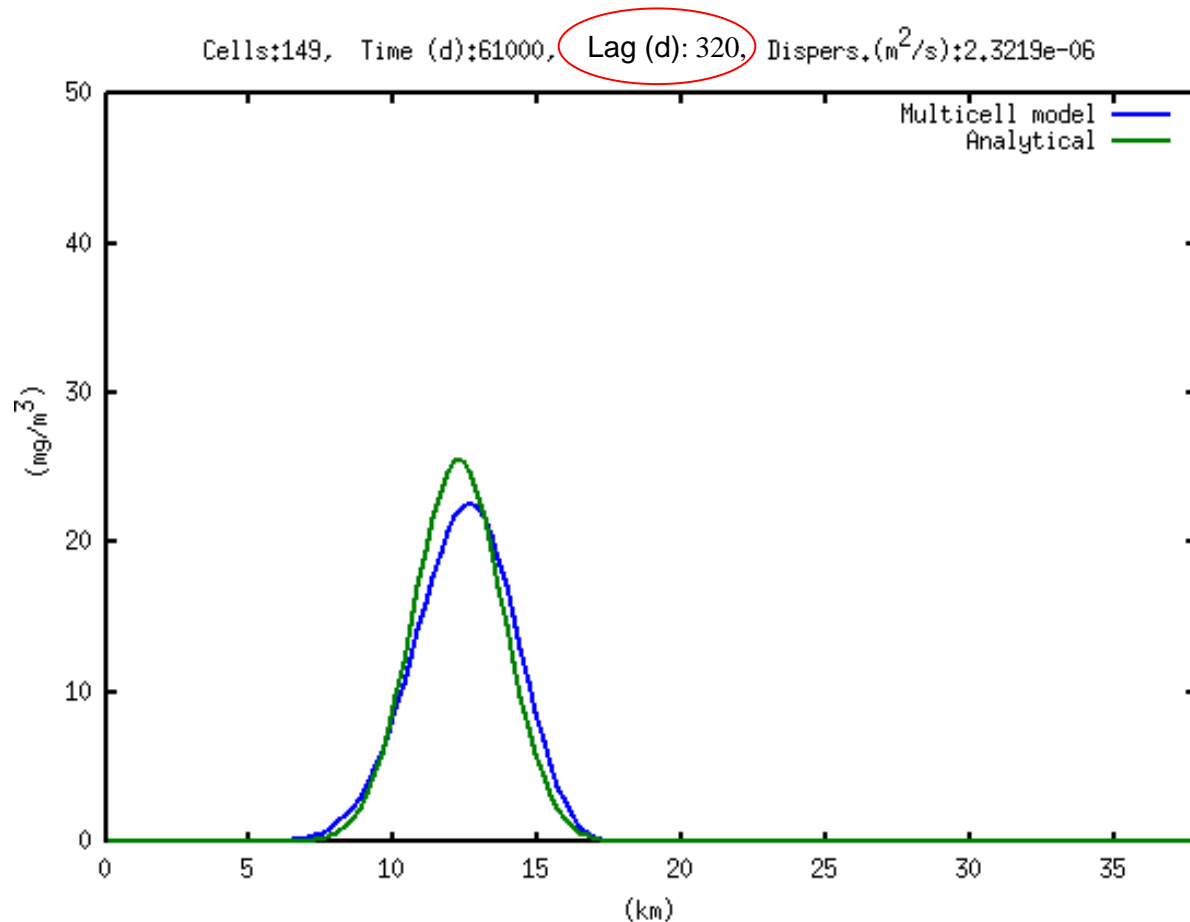


9. Pulse injection, dispersivity 10 m



10. Optimum lag

The numerical diffusion is decreasing monotonically with the lag. To estimate the optimum lag the second order spatial derivative (dispersion) should be estimated with lag, like the first order derivative (advection). Then, the optimum lag is the value that yields oscillation-free results.



11. Conclusions

- Numerical diffusion can be reduced if a time lag is used in the estimation of the first order space-derivative of concentration.
- The error due to numerical diffusion decreases with the dispersivity; so does the usefulness of the method described here.
- The optimum time lag depends on discretization, boundary conditions and dispersivity.
- The optimum time lag can be estimated as the greatest value that yields results without oscillations when space derivatives are lagged (both in advection and dispersion).
- The methodology presented here was tested in a simple 1D case study. However, this methodology is readily applicable in more realistic applications with arbitrarily shaped aquifers.

12. References

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