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Impacts of spatial and temporal recharge on field-scale contaminant transport model calibration

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SUMMARY

This paper investigates the role of spatial and temporal averaging of recharge upon the calibration of trichloroethylene (TCE) contaminant transport parameters for a transient, three-dimensional, variably saturated, physically based, field-scale groundwater flow system in Toms River, New Jersey. Coarse vertical discretizations of unsaturated groundwater systems are prone to numerical difficulties requiring, in some cases, the linearization of the van Genuchten or Brooks Corey equations. A flux-based method for calculating relative permeability was developed and shown to improve numerical stability. To reduce the computational burden of calibration, the simulation time of the transport models was reduced by 95% by decoupling the transport model from the flow model. Multi-start PEST was used to calibrate four models with recharge specified as: constant, spatially varying, temporally varying, and both spatially and temporally varying. For the transient flow model with spatially and temporally varying recharge, the estimated transverse dispersivity coefficients were estimated to be significantly less than those calculated from simulations with spatial and/or temporal averaging of recharge. The calibrated TCE retardation value of 1.58 is within 5% of the laboratory determined value of 1.65. Furthermore, the calibrated TCE retardation values are not as sensitive to the spatial and/or temporal averaging of recharge as compared to transverse dispersivity.

1. Introduction

Modeling the evolution of a contaminant plume requires estimates of transport parameters, contaminant source information, and the definition of the groundwater flow field. Thus, parameter identification and the reconstruction of source release history by calibration (or inverse modeling) of the transport model becomes a critical step in the application of models. Inverse modeling of contaminant transport in groundwater is an inherently difficult process due to the dispersive term in the advection-dispersion equation; it is an irreversible and ill-posed problem, which is unstable and sensitive to errors in data (Skaggs and Kabala, 1994; Woodbury and Ulrych, 1996; Snodgrass and Kitanidis, 1997). One of the first attempts to formulate and solve this inverse problem was initiated by Gorelick et al. (1983) using a linear optimization model. Following this work, a variety of inverse modeling techniques have been proposed, including the estimation of the release history of a known source, identification of the location of sources, and recovery of the historical contaminant distribution. An extensive literature review of commonly used inverse methods has been presented by Atmadja and Bagtzoglou (2001). Zhou et al. (2014) analyzed the evolution and recent trends of the inverse methods in the field of hydrogeology over the last decades.

In general, inverse modeling techniques can be divided into three broad categories based on their mathematical formulations and applications (Liu and Ball, 1999): full estimation methods, parameter estimation methods, and backward tracking. For the cases with no knowledge of a source's temporal history, except for the lower and upper concentration bounds, full estimation methods, which provide a time varying estimate of the contaminant source, are more appropriate and therefore have received a large amount of attention in the past 20 years. Examples of inverse modeling techniques of this category include: Tikhonov regularization (Skaggs and Kabala, 1994; Liu and Ball, 1999), minimum relative entropy (MRE) (Woodbury and Ulrych, 1996; Woodbury et al., 1998), Bayesian geostatistical inversion approach (Snodgrass and Kitanidis, 1997; Michalak and Kitanidis, 2002; Michalak and Kitanidis, 2003; Michalak and Kitanidis, 2004; Butera et al., 2013), quasi-reversibility (QR) (Skaggs and Kabala, 1994; Bagtzoglou and Atmadja, 2003), marching-jury backward beam equation (MJBBE) (Atmadja and Bagtzoglou, 2001; Bagtzoglou and Atmadja, 2003), and progressive genetic algorithm (PGA) (Aral et al., 2001). If prior knowledge of the source model for a

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contaminant is known, it is more efficient and accurate to calibrate the contaminant source term and/or transport parameters by parameter estimation methods. Examples of parameter estimation methods include: lease-squares regression (Gorelick et al., 1983; Sonnenborg and Engesgaard, 1996; Alapati and Kabala, 2000; Sciortino et al., 2000), maximum likelihood estimation (Wagner, 1992), genetic algorithm (Giacobbo et al., 2002; Tsai et al., 2003; Singh and Datta, 2006), tabu search (Zheng and Wang, 1996), and simulated annealing (Zheng and Wang, 1996; Jha and Datta, 2013). In essence, all of the techniques in this category can be classified as optimization approaches ranging from deterministic to stochastic methods. In practical situations, the cases with instantaneous point sources that can be solved by the method of backward tracking are not very common, thereby inhibiting the method's usefulness. However, for certain cases, backward tracking is still an efficient way to obtain information about the prior position of contaminants or travel time of contaminants from an upgradient location (Bagtzoglou et al., 1991; Bagtzoglou et al., 1992; Wilson and Liu, 1994; Neupauer and Wilson, 1999; Neupauer and Wilson, 2001; Neupauer and Wilson, 2002; Neupauer and Wilson, 2003; Neupauer and Wilson, 2004).

Among all the attempts to characterize a contaminant source and/or transport parameters in the past 20 years, many of them are restricted to lumped groundwater flow and transport models with simplified representations of hydrologic and transport processes. For instance, Skaggs and Kabala (1994) employed Tikhonov regularization to reconstruct the nonnegative release history of a plume for a one-dimensional (1-D) contaminant transport problem in a saturated homogeneous aquifer. Woodbury and Ulrych (1996) and Woodbury et al. (1998) applied minimum relative entropy (MRE) to a practical case study with a three-dimensional (3-D) constant velocity and constant dispersivity system at the Gloucester Landfill in Ontario, Canada. Alapati and Kabala (2000) utilized a non-linear least-squares (NLS) method without regularization to determine the parameters in the source release function for a 1-D homogeneous system. The calibration of the transport model is sensitive to the simplifications employed in the development of these lumped models and approximations or simplifications of the hydrologic process could yield non-representative results.

For many field-scale groundwater contaminant problems, the expense of data acquisition combined with the inherent difficulty of obtaining representative values can result in a sparse or incomplete data base. From a modeling perspective, physically-based field-scale groundwater flow and contaminant transport models can be computationally expensive. Furthermore, model calibration or inverse modeling may require many thousands of model evaluations, increasing the computational burden by orders of magnitude. Thus, both the lack of data and high computational requirements have hampered the development of inverse modeling of physically-based, field-scale groundwater flow and contaminant transport models.

An objective of this paper is the development of a computationally efficient approach to calibrate a three-dimensional, variably saturated, physically based, field-scale contaminant transport model with spatially and temporally varying recharge. Among the three categories of the inverse modeling techniques introduced previously, backward tracking is not an ideal approach for this study with continuous non-point pollution and a fast changing flow field. Full estimation approaches are frequently associated with the issue of over parameterization and tend to cause automatic calibration methods to produce nonsensical results (Kitanidis, 1997; Moore and Doherty, 2006). More importantly, due to the lack of a source release history and the high noise level in the data of the field site investigated in this paper, full estimation approaches for this specific case study may not be applicable. As such, a suitable contaminant source model is selected and the parameter estimation method is applied in this study.

To investigate the impact of spatial and/or temporal averaging (upscaling) of recharge on the estimated parameter values, several steps are required. The first step is the development of an efficient computational algorithm for the inclusion of the unsaturated flow zone in the analysis and for the modeling of transient flow and solute transport. Secondly, an estimator and methodology are developed for the calibration of the parameters for a physically-based three-dimensional variably-saturated transient contaminant transport system with appropriate assumptions of the source model. In the final step, an optimization algorithm is selected and used for the model calibrations.

2. Site description and model development history

The study area, the Reich Farm Superfund site, is located in the Pleasant Plains area of Dover Township, Ocean County, New Jersey. The spatial domain for the groundwater model, as shown in Fig. 1, extends eastward from Toms River to Barnegat Bay, and includes the Parkway Wellfield, the Reich Farm Superfund site, and the Dover Township Municipal Landfill (DTML). The spatial model domain covers an area of approximately 139 km^2. Beneath the site lies the unconfined Kirkwood–Cohansey aquifer system, which serves as the principal conduit for lateral groundwater flow in the Reich Farm region. The upper part of this aquifer system is comprised of the Cohansey Sand which extends to a depth of approximately 27 m. The Kirkwood Aquifer is situated below the Cohansey Sand. The average thickness of the Kirkwood–Cohansey aquifer system is approximately 61 m. A clay layer of low hydraulic conductivity underlies the Kirkwood–Cohansey aquifer. The depth of the water table or the unsaturated zone varies spatially and temporally. At the Reich Farm site, the water table depth has been measured to range between approximately 6.7 m and 10.1 m with an average depth of approximately 9.1 m.

During a five month period in 1971, a waste hauler leasing the Reich Farm site disposed of drums containing aromatic hydrocarbons, phenols, halogenated aliphatic hydrocarbons, polymeric resins and unspecified petrochemicals from the manufacture of organic chemicals, plastics and resins. During December of 1971, the owners of the property discovered approximately 5100 drums. Approximately 10% were partially or completely emptied, indicating that part of the wastes were discharged into the soil and groundwater at the site. In 1974, approximately 50 drums buried in trenches were discovered and removed from the site along with approximately 841 m^3 of contaminated soil. Contaminants in the aquifer from the Reich Farm site are non-aqueous phase liquids (NAPLs), including trichloroethylene (TCE), perchloroethylene (PCE) and the styrene-acrylonitrile (SAN) trimer. Only TCE that migrated from the site through the Kirkwood–Cohansey aquifer is modeled in this paper, due to the large number of TCE measurements available.

As part of the preliminary Remedial Investigation of the Reich Farm site, 9 residential wells and 10 Toms River Water Company (TRWC) municipal wells were sampled in 1986. Water samples from two Parkway wells screened in the Cohansey Aquifer contained concentrations of TCE slightly above the New Jersey Maximum Contaminant Level (MCL) of 1 ppb when sampled in May and June of 1986 (Malcolm Pirnie 1990). Further sampling at one residential well and three Parkway wells in November of 1987, indicated that one of the TRWC Parkway wells showed the same concentration of TCE as detected in the previous sample collected in 1986. An air-stripper was installed during 1988 at the Parkway Wellfield to remove volatile organics from contaminated