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Identifying arbitrary parameter zonation using multiple level set functions ☆

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ABSTRACT

In this paper, we extended the analytical level set method [1,2] for identifying a piece-wisely heterogeneous (zonation) binary system to the case with an arbitrary number of materials with unknown material properties. In the developed level set approach, starting from an initial guess, the material interfaces are propagated through iterations such that the residuals between the simulated and observed state variables (hydraulic head) is minimized. We derived an expression for the propagation velocity of the interface between any two materials, which is related to the permeability contrast between the materials on two sides of the interface, the sensitivity of the head to permeability, and the head residual. We also formulated an expression for updating the permeability of all materials, which is consistent with the steepest descent of the objective function. The developed approach has been demonstrated through many examples, ranging from totally synthetic cases to a case where the flow conditions are representative of a groundwater contaminant site at the Los Alamos National Laboratory. These examples indicate that the level set method can successfully identify zonation structures, even if the number of materials in the model domain is not exactly known in advance. Although the evolution of the material zonation depends on the initial guess field, inverse modeling runs starting with different initial guesses fields may converge to the similar final zonation structure. These examples also suggest that identifying interfaces of spatially distributed heterogeneities is more important than estimating their permeability values.

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1. Introduction

Various inverse models have been developed for identifying heterogeneous structures in subsurface environment [3–5]. It is well-known that the inverse problem is typically ill-posed because of limited data available. To avoid the ill-posed problem, one approach is the zonation method [6,7], in which the model domain is divided into a number of zones as a prior, each of which has a uniform parameter value. The zonation method is not only simple but also generally superior to some other methods in case of limited data available [8]. Most of those inverse models focus on identifying the parameter values and determination of the zonation structure is mostly neglected [9]. The main reason is that identifying the zonation structure of an aquifer is much more difficult than estimating the relevant parameter values associated with these zones.

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Any inaccuracy of a priori assumptions on the number of zones and their shapes and locations about the zonation structure may lead to instability in estimating the piece-wise constant parameter field [9].

Recently, a few approaches have been proposed to identify both the zonation structure and the relevant parameter values. The key difference among these approaches is how to parameterize the zonation structure. There are three commonly-used methods to parameterize the structure: clustering analysis, Voronoi tessellation (VT), and the level set method (LSM).

Ayvaz [10] used a fuzzy c-means clustering method to determine the aquifer parameters and zone structures simultaneously. This method starts with one zone and systematically increases the parameter dimension until the best parameter structure is identified, which was determined from three criteria: residual error, parameter uncertainty and structure discrimination. Eppstein and Dougherty [11] developed an approach that estimates transmissivity values and zonation simultaneously for a steady-state flow problem using an iterative k-mean clustering algorithm. The algorithm works by iteratively applying the standard k-means clustering algorithm, where the centroids of clusters are calculated as the arithmetic mean of the transmissivity of the member zones. The number of clusters is increased each iteration until the predefined cluster tolerance is met within all clusters.

In the VT-base approaches, the optimization process determines an appropriate level of parameter structure complexity, and at each level of complexity the zonation is determined from a set of basis points using the Voronoi tessellation, and the parameters to be optimized include the locations (coordinates) of these basis points and conductivity values at these points [12,13]. In [12], Tsai et al. used sequential global-local optimization to minimize the squared error with a global search for the best parameter values and a local search for basis points. Tsai and Yeh [14] combined the Bayesian estimation and the generalized parameterization method, which is capable of creating a mixture of zonation structure and a continuous distribution of conductivity fields. In [15], Tung and Tan identified the number of zones and their hydraulic conductivity values by combining Voronoi tessellation and simulated annealing. Chiu [16] used Voronoi tessellation to represent the material zonation with different number of basis points, and the coordinates and the conductivity values associated with these points were optimized using differential evolution.

The concept of the level set method (LSM) was first introduced by Osher and Sethian [17] and has been proved to be a very powerful tool for solving problems that involve geometric evolution. This method was initially designed for tracking the motion of a front whose velocity depends on the local curvature. The method has been used in several fields, including shape optimization problems [18], image segmentation [19], and inverse problems [1,20,2,21]. One of the advantages of the level set method is that it is much easier to work with a globally defined function than to keep track of the boundaries of regions of interest, which may split into many regions or merge into larger ones. The level set method requires no *a priori* assumptions on shape, size and locations of zones to be sought or correlation structures of these zones.

In the level set based approaches, the zonation is characterized by one or more level set functions (LSFs). These approaches may be classified into two large groups based on how the LSFs are defined. In the first group, the interface evolves explicitly from solving the Hamilton–Jacobi equation (i.e., level set equation) [1,2,22]. The expression for the propagation velocity of the evolving interface is determined from minimizing the objective function, which is related to the discrepancy between the simulated and observed state variables, such as hydraulic head. In the second group, instead of propagating interfaces directly by specifying interface velocity, they evolve implicitly through updating LSFs using a fixed order of polynomial [23], or some basis functions [24–28], or B-splines [29], or LSFs at some selected grid nodes and LSFs at the rest of grid nodes are calculated from interpolation [20,28].

In this study, we extend the analytical approach in [1,2] for binary fields to parameter zonation identification of any arbitrary number of material zones, through mathematically rigorous derivation. In this approach, the propagation velocity of each interface between any two materials is derived from the minimization of an objective function, which measures the differences between the simulated and observed hydraulic heads. A similar expression for the propagation velocity has been given by Cardiff and Kitanidis [22], but it was not clear how the expression was derived. In addition, as an extension of Lu and Robinson [2], in which the permeability values of two materials are fixed, the permeability values of these material zones are also to be estimated. This method can be used to identify, for example, low-permeability layers in a relatively higher permeability porous media (or vice versa), or highly permeable fault zones in the subsurface.

The rest of paper is organized as follows. Section 2 gives the statement of the inverse problem. Section 3 describes the level set representation of materials zones. In Section 4, we derive analytical expressions for updating (1) material zonation through the propagation velocity of material interfaces and (2) permeability values for all materials. The numerical methods and some implementation issues are discussed in Section 5. Section 6 presents several examples to demonstrate the application of the level set method to identify lower permeable zones in both synthetic and real-world flow problems. Conclusions and discussions are presented in Section 7.

2. Problem statement

We consider transient groundwater flow in confined saturated media satisfying the standard governing equation

$$\nabla \cdot [K_s(\mathbf{x})\nabla h(\mathbf{x},t)] + g(\mathbf{x},t) = S_s \frac{\partial h(\mathbf{x},t)}{\partial t}, \;\; \mathbf{x} \in \Omega \tag{1}$$