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Swarm intelligence-based solver for parameter estimation of laboratory through-diffusion transport of contaminants

Tadikonda Venkata Bharat *, Puvvadi V. Sivapullaiah, Mehter M. Allam

Department of Civil Engineering, Indian Institute of Science, Malleswaram, Bangalore, Karnataka 560 012, India

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ABSTRACT

Theoretical approaches are of fundamental importance to predict the potential impact of waste disposal facilities on ground water contamination. Appropriate design parameters are generally estimated by fitting theoretical models to data gathered from field monitoring or laboratory experiments. Transient through-diffusion tests are generally conducted in the laboratory to estimate the mass transport parameters of the proposed barrier material. These parameters are usually estimated either by approximate eye-fitting calibration or by combining the solution of the direct problem with any available gradient-based techniques. In this work, an automated, gradient-free solver is developed to estimate the mass transport parameters of a transient through-diffusion model. The proposed inverse model uses a particle swarm optimization (PSO) algorithm that is based on the social behavior of animals searching for food sources. The finite difference numerical solution of the forward model is integrated with the PSO algorithm to solve the inverse problem of parameter estimation. The working principle of the new solver is demonstrated and mass transport parameters are estimated from laboratory through-diffusion experimental data. An inverse model based on the standard gradient-based technique is formulated to compare with the proposed solver. A detailed comparative study is carried out between conventional methods and the proposed solver. The present automated technique is found to be very efficient and robust. The mass transport parameters are obtained with great precision.

1. Introduction

An accurate estimation of contaminant transport parameters is of critical importance for the performance assessment of landfills. The contaminant transport in landfills is generally approximated as a transient through-diffusion process wherein a finite mass of contaminant is available for transport through the liners of the landfills and finally into ground water systems. In general, laboratory through-diffusion experiments are conducted to estimate mass transport parameters by maintaining conditions similar to those expected in the field, such as using the proposed barrier material and using a leachate as similar as possible to that expected in the facility. The laboratory through-diffusion (also called double-reservoir) experiment represents a well-established technique for the determination of the design transport parameters in a single test. Parameters are generally estimated by matching the theoretical concentration profile with the experimentally observed temporal or spatial variation of the concentration. In general, this is done using packages like Pollute [1], which estimate theoretical solute concentration data for an assumed set of design parameters. Using such packages the unknown fitting parameters are adjusted manually (by eye judgment) to match with the experimental data. These eye-fitting techniques generally give a reliable estimation of parameters, but the decision is based on past experience. Furthermore, those packages are expensive to use. With advanced numerical techniques and recently evolved global search algorithms, an accurate and quick estimation of the mass transport parameters is possible. Once these techniques are tested, automated packages can also be developed.

An inverse technique based on a probabilistic variant of a simplex search was used recently by [2] for parameter estimation from through-diffusion cell experiments. This algorithm was originally developed by Duan et al. [3] for parameter optimization for catchment models. In this model, a one-dimensional solution for the transport equation with the Shuffled Complex Evolution (SCE) search algorithm has been integrated. The simplex search is a gradient-based method and requires computing the derivatives of the objective function with respect to model parameters. In the case of numerical models like the problem addressed in this paper, determination of numerical derivatives is difficult. Moreover, the downhill simplex method and the Levenberg–Marquardt method require choosing initial guesses and the solution depends on these initial guesses.

Particle swarm optimization (PSO), first introduced by Kennedy and Eberhart [4,5], is a population-based stochastic optimization

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* Corresponding author. Tel.: +91 9449151151.
E-mail addresses: tvbharat@gmail.com, bharat@civil.iisc.ernet.in (T.V. Bharat).

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algorithm. It is inspired by the social behavior of animals such as flocking of birds and schooling of fish. Recently, much attention has been drawn to the mechanism of PSO because of its simplicity in implementation and efficiency in tackling complex optimization problems. The PSO approach directly represents each potential solution of the target function as particles. PSO requires only objective function information to determine the solution, thus derivative calculations are not required. PSO methods implement probabilistic transition rules, which allow them to avoid local optima in an effort to move towards a global optimum. PSO appears to be robust to control parameters [6].

As an emerging technology, PSO has received a great deal of attention in many engineering disciplines in recent years [7,8]. Recently, PSO was applied to solve certain geotechnical engineering problems such as: designing multilayer sorptive barrier systems [9,10]; prediction of unconfined compressive strengths of soft soils [11]; fitting sorption isotherms [12]; finding the location of a critical slip surface [13,14]; and in water treatment processes [15]. Even though the PSO is robust, relatively simple to implement and it has many advantages over other evolutionary techniques, it has not received much attention in geotechnical engineering optimization problems compared with other evolutionary algorithms, such as genetic algorithms and simulated annealing. The application of PSO for the inverse problem of parameter estimation in contaminant transport problem has not yet been reported.

With this incentive, in this work a novel automated model is proposed for parameter estimation. A comparative study is carried out to assess the expediency of the proposed approach. The proposed solver is then applied to estimate the design parameters from laboratory experimental data. The estimated parameters are compared with the values obtained by conventional techniques.

2. Contaminant transport model: transient through-diffusion problem

The contaminant transport model consists of the governing equations together with the boundary and initial conditions. This section formulates the mathematical model for the transient through-diffusion case.

2.1. Governing equation

As the transport of contaminants through landfill liners is dominated by the diffusion process (advective velocity is neglected), the transport is treated as Fickian-type. For one-dimensional transport in the x-direction, the mass flux f is given by

$$f = -nD_e\frac{\partial c}{\partial x} \tag{1}$$

in which n is volumetric porosity, D_e is the effective diffusion coefficient and c is the solute concentration in the sample pore water.

Consideration of mass balance results in Fick's second law which gives,

$$-\frac{\partial f}{\partial x} = n\frac{\partial c}{\partial t} + \frac{\partial s}{\partial t} \tag{2}$$

in which s is the sorbed concentration. The degree of sorption, s, in (2) is a function of contaminant concentration in the pore solution, $s = f(c)$. In general, the sorption mechanism is approximated by a linear relationship between the contaminant adsorbed and the concentration in the pore fluid, and therefore,

$$s = \rho K_d c \tag{3}$$

in which ρ is the bulk density of solid; and K_d is the distribution coefficient that is to be estimated along with the diffusion coefficient (D_e) from the experimental observations.

A non-linear Langmuir sorption model is also often used in modeling diffusion through kaolinite soils. In this case, the sorption is related to solute concentration as,

$$s = \frac{s_m bc}{1 + bc} \tag{4}$$

where b is bonding constant between the sorbate and sorbent (l/mg) and s_m is the maximum material sorptivity (mg/g) [16].

Combining Eq. (1) and (2) gives the following transient transport equation for solute through a saturated porous medium

$$nD_e\frac{\partial^2 c}{\partial x^2} = \alpha\frac{\partial c}{\partial t} \tag{5}$$

where α is a dimensionless parameter called the capacity factor which is porosity times the retardation coefficient. For species with linear sorption behavior, α may be defined as

$$\alpha = n + \rho K_d \tag{6}$$

and for the Langmuir isotherm, the capacity factor may be defined as

$$\alpha = n + \rho\left[\frac{s_m b}{(1 + bc)^2}\right] \tag{7}$$

The transport model Eq. (5) is completed with the specification of initial and boundary conditions.

2.2. Initial and boundary conditions

The commonly employed initial conditions in the laboratory diffusion tests [17,2] are

$$c(x = 0, t = 0) = c_0 \tag{8}$$

$$c(x, t = 0) = 0 \tag{9}$$

$$c(x = L, t = 0) = 0 \tag{10}$$

where Eqs. (8)–(10) represent the concentrations in upstream (source), sample pore water and down stream (collector) reservoirs respectively; t is time and x is the distance from the upstream solution–sample interface.

Finite-mass boundary conditions are generally used to represent contaminant sources such as landfills. In landfills the mass of contaminant is finite and the contaminant concentration at the source will decline as contaminant mass is transported into the liner material [16]. Assuming that the concentration variation with time in both source and collector reservoirs is due to diffusion only through the sample, the boundary condition representing the species concentration in the source solution at any time instance t, (*i.e.*, $c(x = 0, t)$) can be written as

$$c(x = 0, t) = c_0 + \frac{nD_e}{H_f}\int_0^t \frac{\partial c}{\partial x}\Big|_{x=0} dt \tag{11}$$

where c_0 is the concentration of the species in the source solution at $t = 0$; n is the total porosity of the sample, which is assumed to be entirely available to the diffusing species; and H_f is the equivalent height of source reservoir, calculated as the volume of source solution divided by the cross-sectional area of the liner sample perpendicular to the direction of diffusion. The boundary condition representing the species concentration in the collector solution ($c(x = L, t)$) is given by:

$$c(x = L, t) = -\frac{nD_e}{H_c}\int_0^t \frac{\partial c}{\partial x}\Big|_{x=L} dt \tag{12}$$

where H_c is the equivalent height of the collector reservoir.