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Robust solver based on modified particle swarm optimization for improved solution of diffusion transport through containment facilities

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ABSTRACT

Accurate estimation of mass transport parameters is necessary for overall design and evaluation processes of the waste disposal facilities. The mass transport parameters, such as effective diffusion coefficient, retardation factor and diffusion accessible porosity, are estimated from observed diffusion data by inverse analysis. Recently, particle swarm optimization (PSO) algorithm has been used to develop inverse model for estimating these parameters that alleviated existing limitations in the inverse analysis. However, PSO solver yields different solutions in successive runs because of the stochastic nature of the algorithm and also because of the presence of multiple optimum solutions. Thus the estimated mean solution from independent runs is significantly different from the best solution. In this paper, two variants of the PSO algorithms are proposed to improve the performance of the inverse analysis. The proposed algorithms use perturbation equation for the *gbest* particle to gain information around *gbest* region on the search space and *catfish* particles in alternative iterations to improve exploration capabilities. Performance comparison of developed solvers on synthetic test data for two different diffusion problems reveals that one of the proposed solvers, CPPSO, significantly improves overall performance with improved best, worst and mean fitness values. The developed solver is further used to estimate transport parameters from 12 sets of experimentally observed diffusion data obtained from three diffusion problems and compared with published values from the literature. The proposed solver is quick, simple and robust on different diffusion problems.

1. Introduction

Chemical and radioactive waste is a major source of soil and groundwater contamination which poses several health issues to the inmates. Engineered containment facilities are thus used to prevent the spread of contamination. Such facilities isolate the waste by minimizing the transport of contaminants. Clay soils serve as barrier material in such containment facilities. Diffusive transport is the dominant and attractive mechanism in such soils due to their low hydraulic conductivity (K). The hydraulic conductivity of the compacted clay soil is typically less than 1×10^{-10} m/s (Barone, Rowe, & Quigley, 1992; Shackelford, 1991). Safe design of waste disposal facilities requires both experimental and theoretical consideration of barrier (soil) – leachate (solute) interaction and diffusion rate fluxes through the barrier material (Rowe, Caers, & Barone, 1988). The effectiveness of compacted clay as barrier material is studied using laboratory diffusion tests. Several laboratory testing procedures and their relative merits were presented elsewhere (Shackelford, 1991). Double-reservoir or transient through-diffusion testing procedure is often employed to estimate diffusion and sorption parameters of the chemical and radioactive species through barrier material in the laboratory (Barone et al., 1992; Du & Hayashi, 2005; Kau, Binning, Hitchcock, & Smith, 1999). The barrier material is connected to source and collector reservoirs in the through-diffusion method as shown in Fig. 1 (Bharat, 2009). The test begins when the solution containing chemical waste of interest is placed in the source reservoir. As the diffusion transport occurs through the soil due to concentration gradient, the concentrations of the specified chemical species decrease with time in source reservoir and increase with time in the collector reservoir. The temporal variation of solute concentration for the assumed input values is shown in Fig. 2. The thorough description of through-diffusion testing procedure was given by Rowe et al. (1988). The observed concentration profiles as a function of time (diffusion data), resulting from diffusion tests are analyzed for mass transport parameters using mathematical models.

The rate of diffusion and retardation of the solute (chemical) in a given barrier material is interpreted and predicted using effective diffusion coefficient, accessible porosity and retardation parameters. These parameters are necessary for overall design and evaluation processes of the waste disposal facilities (Shackelford, 1991).

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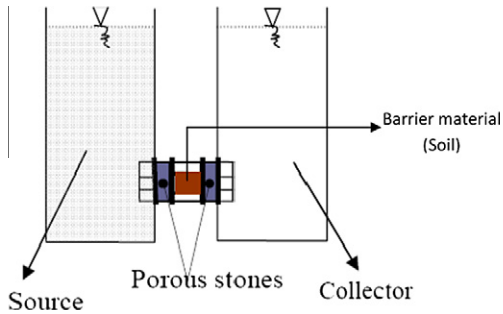

Fig. 1. Schematic diagram of laboratory diffusion test (transient-through diffusion).

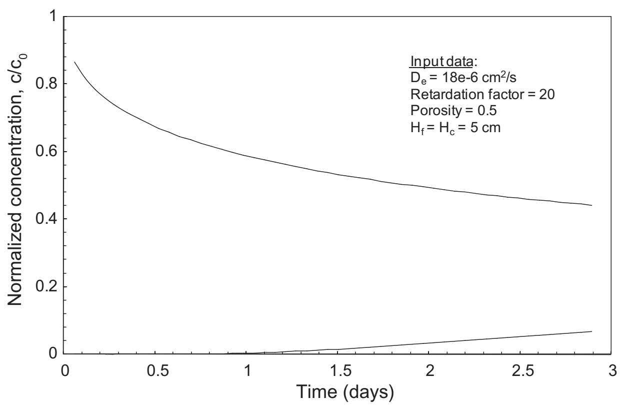

Fig. 2. Diffusion data of temporal concentrations at the source and collector reservoirs from transient through-diffusion tests.

Further these parameters are important in assessing performance of the existing containment facilities and predicting field-scale diffusive fluxes. Thus parameter estimation from the laboratory and field measurements of contaminant concentration is an important component of the overall design and evaluation processes related with waste disposal practice.

Parameter estimation from diffusion data of observed spatial or/and temporal solute concentrations in the barrier material requires inverse analysis. The Fick's diffusion equation along with a suitable sorption mechanism is repeatedly solved with the assumed parameters to match the theoretical concentration profiles to the measured data. The right combination of the parameters yields a best-fit to the measured data. Manual techniques such as Pollute v6 (Rowe & Booker, 1994) are most commonly used in Geotechnical engineering for parameter estimation (Du & Hayashi, 2005). Other commonly used techniques are based on gradient-based optimization methods (Bell, Binning, Kuczera, & Kau, 2002; Pereira, De Souza, Orlande, & Cotta, 1999; Samper et al., 2006). The disadvantage of using these techniques was clearly demonstrated in the earlier paper of Bharat, Sivapullaiah, and Allam (2009a). An inverse model based on particle swarm optimization (PSO) was recently introduced for automated parameter estimation from laboratory diffusion data (Bharat et al., 2009a). This stochastic method based on swarm intelligence technique was simple and provided excellent fitting parameters to the through-diffusion test data. This solver further alleviated the limitations of previously used inverse methods. However, the solver based on particle swarm optimization (PSO) algorithm reportedly has some inherent limitations due to stochastic nature of the algorithm (Bharat, 2009; Bharat, Sivapullaiah, & Allam, 2008). The global methods including PSO do not yield same solution in successive runs even with the same tuning parameters due to their inherent stochastic nature (Formato, 2010) and also due to presence of multiple optimum solutions. It will be shown in this paper that the estimated mean fitness values from independent runs are significantly different from the best solution using the solver based on PSO which can adversely affect the assessment of waste facilities. Hybrid methods that combine other optimization methods with PSO are often used occasionally to alleviate these problems (Bharat & Sharma, 2010). However, such techniques demand additional computation and become complex due to expensive fitness computations. The fitness evaluation is computationally expensive for the present problem as it requires time-marching numerical solutions. Moreover, the PSO based inverse models have not been tested on different diffusion problems that require estimation of different combination of mass transport parameters.

This work presents few modifications to existing PSO algorithm that improve overall performance of the algorithm without the requirement of additional function evaluations. Two variants of the PSO algorithms are proposed based on these modifications. The proposed PSO variants will be integrated with the diffusive transport model for estimating the model parameters. It will be shown that the proposed solvers significantly improve mean fitness solutions on synthetic test data of two different diffusion problems. The developed solver will further be used to estimate transport parameters from 12 sets of experimentally observed diffusion data obtained from three diffusion problems.

2. Theory

Diffusive transport involves movement of contaminants from regions of higher chemical concentration (landfills) to regions of lower concentration such as aquifers or drainage systems. Solute diffusion in soils is much slower than free-solution diffusion because of the presence of tortuous pathways. Additionally, sorption of reactive solutes further decreases the concentration fluxes in the soils. The mass of contaminant transported through a unit area of soil in a unit time is governed by Fick's first law. The governing equation for one dimension case may be written as:

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

where f is the mass flux; ϕ is the diffusion accessible porosity of the soil; D_e is the effective diffusion coefficient; c is the mass concentration of the solute in the liquid phase of the soil; x is the direction of transport and $\partial c/\partial x$ is the concentration gradient. The negative sign arises from the fact that contaminants move from high to low concentration regions and hence the gradient is negative. The effective diffusion of a given chemical species depends on several factors such as clay type, length of the diffusion path, constrictivity, pore-size and pore distribution (Shackelford, 1991). The Fick's second law of diffusion can be written by considering mass balance which is given as:

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

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

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

where ρ is the bulk density of soil solids and K_d is the distribution coefficient that is to be estimated in combination with the effective diffusion coefficient using experimental observations. According to these definitions, the combined diffusion and sorption equation can be written as:

$$D_e \frac{\partial^2 c}{\partial x^2} = R_d \frac{\partial c}{\partial t} \tag{4}$$

where R_d is the retardation factor which is equal to $(1 + \rho K_d/\phi)$. Some work uses a slightly different form of governing equation, when diffusion of radionuclide species through barrier material is used, which is as follows (Garcia-Gutierrez, Cormenzana, Missana, & Mingarro, 2004):

$$D_e \frac{\partial^2 c}{\partial x^2} = \phi \frac{\partial c}{\partial t} \tag{5}$$

where ϕ is treated as unknown (fitting) parameter. The commonly employed initial conditions in the laboratory diffusion tests (Bell et al., 2002) are

$$\begin{aligned} &c(x=0, t=0) = c_0 \\ &c(x, t=0) = 0 \\ &c(x=L, t=0) = 0 \end{aligned} \tag{6}$$

where these equations represent concentrations in source (landfill), sample pore water and downstream (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 barrier material (Rowe et al., 1988). Thus assuming that the concentration variation with time in both source and collector reservoirs are due to diffusion alone, the boundary condition representing the species concentration in the source solution at any time instance t, can be written as:

$$c(x=0, t) = c_0 + \frac{\phi D_e}{H_f} \int_0^t \frac{\partial c}{\partial x}\Big|_{x=0} dt \tag{7}$$

where c_0 is the concentration of the chemical species in the source solution at $t = 0$ 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 soil sample perpendicular to the direction of diffusion. Similarly, the boundary condition representing the species concentration in the collector solution is given by:

$$c(x=L, t) = -\frac{\phi D_e}{H_c} \int_0^t \frac{\partial c}{\partial x}\Big|_{x=L} dt \tag{8}$$

where H_c is the equivalent height of the collector reservoir.

3. Direct analysis

The direct problem involves finding the solute concentration at any spatial location and/or time instant using known mass transport parameters. The governing transport equation and the boundary conditions (2 through 6) are discretized using implicit finite-difference numerical procedure. A grid of mesh points in x–t space is introduced to solve partial differential equations (4) or (5) and (7) and (8) numerically. The finite-difference reference grid with spatial (Δx) and time (Δt) increments is shown in Fig. 3. The indexing is defined by $t = t^n = n\Delta t$ and $x = x_i = i\Delta x$ (where $i = 1, 2, \ldots, M$; $n = 1, 2, \ldots, N$) as shown in reference grid. Finite-difference approximation of c_i^k is calculated at (i, n) grid point as $c(i\Delta x, n\Delta t)$. A constant spatial and temporal grid-spacing of $\Delta x = 1/M$ and $\Delta t = 1/N$ are used. A set of simultaneous equations in the form of tridiagonal matrix are obtained at all grid location in each time-step (Bharat, 2009). These equations in each time-step are solved using Thomas algorithm to determine solute concentration in the next time level. These time-steps are marched until the required theoretical time is achieved. A grid with $M = 1000$ and $N = 1000$ is used in this paper to obtain a good numerical solutions (Bharat, 2009).

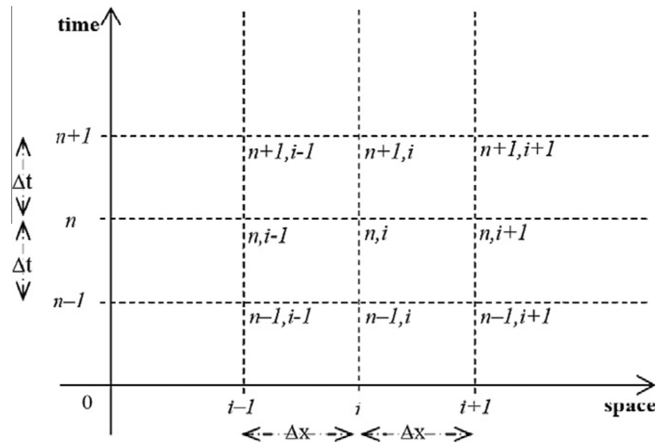

Fig. 3. Finite difference reference grid.

4. Inverse analysis

In practice, temporal and spatial concentrations of chemical contaminants are obtained from laboratory diffusion tests and field containment facilities. The mass transport parameters are estimated from these observations for design and evaluation processes of the waste disposal facilities and also for assessing the performance of existing facilities. The unknown parameters (D_e, R_d, ϕ are estimated by solving the forward problem using different combinations of model parameters by matching the observed diffusion data of contaminant concentration. This inverse analysis is commonly performed using optimization techniques to reduce the number of function evaluations. All the optimization techniques work based on optimizing the model parameters that minimize objective function (error). The objective function determines the fitness or quality of the current solution. Root mean square error (RMSE) is used as an objective function in this paper. The RMSE for transient diffusion problem is formulated, by considering the concentration data from source and outlet reservoirs, as follows:

$$O(D_e, R_d) = \sqrt{\sum_{i=1}^{L} \left\{ \frac{(c_{in,\exp}(t_i) - c_{in,the}(t_i; D_e, R_d))^2 + (c_{out,\exp}(t_i) - c_{out,the}(t_i; D_e, R_d))^2}{2L} \right\}} \tag{9}$$

where L is the number of observational data points. It was earlier shown that gradient-based algorithms are highly inefficient for this problem because the estimated solution is dependent on the initial guess and type of error measure (model adequacy) (Bharat et al., 2009a). Even though the performance of solver based on PSO was satisfactory for diffusion problem (Bharat et al., 2009a), it often wastes huge computational effort by converging to sub-optimal solutions in the parametric space (Bharat et al., 2008). This fitness function (Eq. (9)) is computationally expensive because the reactive diffusion equations need to be solved using time-marching numerical techniques to develop temporal concentrations for several days to years. Thus the developed solver should be able to converge to global solution in small number of iterations. On the other hand, multiple local solutions in the search space arise because of human and instrumental errors in the observed data. Consequently, nature-inspired algorithms do not yield same solution in different runs and converge to sub-optimal solutions. As a result, inverse model based on simple and robust algorithm with good convergence capabilities are required to estimate accurate mass transport parameters. In the following sub-sections, therefore, several variants of the algorithms are proposed to improve performance of the inverse analysis.

4.1. Particle swarm optimization (PSO) algorithm

Particle swarm optimization algorithm has received great attention due to its simplicity compared to any other heuristic algorithms (Coelho, 2010; Kaveh & Laknejadi, 2011). PSO is a population-based optimization method. The foundation of PSO is based on the social behaviors of animals such as flocking of birds and schooling of fishes (Kennedy & Eberhart, 1995). In PSO, each individual (particle) of the population represent a potential solution for the problem. The PSO starts with initializing particles representing set of model parameters on the parametric space. The dimension of the parametric space is equal to the number of model parameters. Each particle has a position and velocity and updates them while moving on the search space in discrete time-steps (iterations). The particles update their positions and velocities according to flying experience of the individuals and flying experience of the best individual in the population to achieve a better position (combination of model parameters) on the search space. Further, each particle has a memory to remember its best position in its flight. Thus, its movement is an aggregated acceleration towards its best previously visited location and towards the best individual of a topological neighborhood. The velocity ($\overrightarrow{v_{ij}}$) and movement ($\overrightarrow{x_{ij}}$) of the i_{th} particle and j_{th} dimension are updated using the equations shown as:

$$\overrightarrow{v_{ij}} = \overrightarrow{v_{ij}} + a_1\gamma_1(\overrightarrow{p_{ij}} - \overrightarrow{x_{ij}}) + a_2\gamma_2(\overrightarrow{p_{gj}} - \overrightarrow{x_{ij}}) \tag{10}$$

and

$$\overrightarrow{x_{ij}} = \overrightarrow{x_{ij}} + \overrightarrow{v_{ij}} \tag{11}$$

where $\overrightarrow{p_{ij}}$ is the history best position of each individual and similarly, $\overrightarrow{p_{gj}}$ represent the global best position of the individual in whole population. The constants a_1 and a_2 represent acceleration constants that accelerate movement of the particles towards individual and global best positions respectively. γ_1 and γ_2 are two independent random numbers that are uniformly distributed between 0 and 1. These random numbers are used to stochastically vary the relative pull of $\overrightarrow{p_{ij}}$ and $\overrightarrow{p_{gj}}$. The second term in the velocity update equation is called the cognitive component which simulates the natural tendency of individuals to return to their history best position. The third term in Eq. (10) is a social component which represents the tendency of individuals to follow the success of other individuals. This iterative process is continued swarm by swarm until a stopping criterion is satisfied. As particles search over time, individuals are drawn towards the success of each other resulting a cluster of particles at global optimum region.

As an emerging technology PSO has received a lot of attention in recent years in many engineering disciplines. The PSO algorithm has been experimentally studied on several benchmark functions and optimization problems. Several experiments on original PSO revealed that the algorithm explodes quickly as the first term in the velocity term (Eq. (10)) increases incessantly (Clerc & Kennedy, 2002). The notable work on improving the performance of the algorithm include, introduction of an inertia factor to control the velocity of the particles (Shi & Eberhart, 1998) and a constriction factor to constrain velocity magnitude (Clerc & Kennedy, 2002). The modified velocity-update equation is given by (Bharat et al., 2009a)

$$\overrightarrow{v_{ij}} = \chi(\omega\overrightarrow{v_{ij}} + \phi_1\gamma_1(\overrightarrow{p_{ij}} - \overrightarrow{x_{ij}}) + \phi_2\gamma_2(\overrightarrow{p_{gj}} - \overrightarrow{x_{ij}})) \tag{12}$$

where χ is the constriction coefficient and ω is the inertia weight that improve the performance of the PSO. The first term in Eq. (12) is the inertia term which does not allow the particles to change its flight direction drastically. This modified algorithm is termed as MPSO in this paper.

4.2. Perturbed particle swarm optimization (PPSO)

The MPSO algorithm and many of its variants suffer from few setbacks during the search process. The major drawback with these algorithms is that they converge to suboptimal solutions when applied to the optimization problems. The reason was due to the use of same movement update equation (Eq. (12)) for *gbest* particle (Bharat et al., 2008). The velocity of the *gbest* particle reduces to simply $\chi\omega\overrightarrow{v_{gj}}$ for *gbest* particle. That means the *gbest* particle simply oscillates with a small value of $\chi\omega\overrightarrow{v_{gj}}$ around current position and attracts all the other particles towards its position. If this position happens to be the suboptimal location and any other particle does not locate the global solution, the swarm converges to this suboptimal solution with a high probability. To alleviate this problem Bharat et al. (2008) suggested perturbed PSO (PPSO) algorithm which uses a perturbion equation for the *gbest* particle. The perturbation equation for *gbest* particle is given by

$$x(i,j) = x(i,j)[1 + \phi_3(\gamma_3 - \gamma_4)] \tag{13}$$

where ϕ_3 is a perturbation constant and $\gamma_3, \gamma_4 \in U(0,1)$. This equation perturbs *gbest* particle randomly in the suboptimal region to find a better solution. This additional randomness to the *gbest* particle enables to acquire considerable knowledge in the *gbest* region in each iteration thus algorithm has a better probability to find global optimum. The advantage of this modification is that the performance of the algorithm improves without any additional fitness computation.

4.3. Proposed PSO algorithm

It will be shown later in this work that the convergence rate of the PPSO algorithm reduces on uncorrupted data obtained by synthetic tests. However, perturbation technique is necessary for noised data to escape from the local solutions. Thus other possible modifications are examined. Several variants of MPSO algorithm have been used for various optimization problems apart from introduction of perturbation to *gbest* particle. These algorithms require additional function evaluations to improve the solution. Consequently these variants are not attractive because the objective function of the present inverse problem is computationally expensive. Thus a simple and inexpensive strategy is introduced into the algorithm along with the perturbation step to improve the exploration capabilities of the swarm. This is achieved in this paper by introducing catfish particles (Chuang, Tsai, & Yang, 2008) into the swarm. The particles are arranged according to the increasing fitness after evaluating the objective function and predefined worst particles (low fit solutions) are then repositioned on the *D*-dimensional search space. These catfish particles explore new feasible regions and guide the whole swarm to promising regions of the search space. This technique further can alleviate premature convergence of the swarm even with small population sizes due to unique combination of perturbation equation for *gbest* particle and exploration capabilities of the catfish particles. This optimization algorithm is referred as CPPSO algorithm in this work. All the inverse models in this work are coded in Fortran 90.

5. Estimation of mass transport parameters

Nature-inspired algorithms such as PSO and other variants have been tested on several benchmark and real-world optimization problems. However, performance of these algorithms varies with the problem and also parametric search space. The developed solvers are validated and demonstrated on several synthetic tests. Further mass transport parameters are estimated from experimentally observed data of various diffusion problems encountered in geotechnical engineering.

5.1. Synthetic tests

The synthetically obtained data is more expedient to obtain optimal set of tuning parameters and also to validate performance of different solvers. Further, it is easy to analyze the behavior of the solvers because the optimum solution is known for this data. The forward solution representing temporal variation of contaminant concentration at the inlet (source) and outlet (collector) reservoirs of the diffusion tests is obtained by solving governing partial differential equations numerically. Two different diffusion problems are considered in this study. The first problem is the most commonly used laboratory diffusion test (Barone et al., 1992). The temporal variation of contaminant concentrations in source and collector reservoirs due to concentration gradient across a homogenous soil sample (containment) are simulated using assumed mass transport parameters, D_e and R_d. The mass transport parameters are assumed to be $D_e = 1.85 \times 10^{-5}$ cm^2/s and $R_d = 22$. The concentrations as a function of time at source and collector reservoirs are developed theoretically in 12 days and are used as input data to back analyze the assumed parameters. The performance of the solvers is further evaluated by adding 20% white noise to the input data.

The second problem is commonly encountered in containment facilities and occasionally used in laboratory for determining mass transport parameters of stratified (layered) soil system (Du & Hayashi, 2005). The sorption parameters are separately determined using batch equilibrium tests to avoid indetermined problem (infinite number of solutions). Thus the unknown parameters are only effective diffusion coefficients of the two different soil layers. The details of the laboratory testing procedure are given elsewhere (Du, Hayashi, & Liu, 2005). The concentration profiles at the source and collector reservoir with time are simulated using assumed values of $D_{e_1} = D_{e_2} = 1.0 \times 10^{-6}$ cm^2/s, where D_{e_1} and D_{e_2} are the effective diffusion coefficients of first and second soil layers. The data of temporal concentrations developed in 30 days is used as input for the developed solvers to determine diffusion coefficients of the two-layers. Similar to the previous case, the performance of the solvers is further evaluated by adding 20% white noise to the input data.

5.2. Experimental description

Several laboratory diffusion tests have been conducted in the past for various diffusion problems. Three different diffusion problems are considered to extract mass transport parameters using the laboratory observed data. The first problem requires estimation of diffusion and retardation coefficients of several volatile organic chemicals in natural clay soils (Barone et al., 1992). The second problem requires the diffusion coefficient and diffusion-accessible porosity of radioactive species, HTO, from the observed diffusion data. Similarly, the third problem involves estimation of diffusion coefficients of ^{36}Cl from observed data in transient through-diffusion tests by inverse analysis. The data of Garcia-Gutierrez et al. (2004) is used to solve the second and third inverse problems. A modified form of the governing equation (Eq. (5)) is used in these cases to enable for the determination of diffusion-accessible porosity (Garcia-Gutierrez et al., 2004). The details of the solute (contaminant) and soil (containment) properties are given in Table 1.

5.3. Parameter setting

All the nature-inspired optimization algorithms have tuning parameters that influence the convergence rate, exploration and exploitation capabilities. These tuning parameters further control overall performance of the algorithms. Several past researchers derived optimum set of parameters after thorough empirical analysis on well-defined benchmark functions (Shi & Eberhart, 1998). Nevertheless, this parameter-set yields poor results on real-world optimization problems (Bharat et al., 2008, 2009a; Bharat, Sivapullaiah, & Allam, 2009b; Bharat, 2008, 2009). The tuning parameters of MPSO, PPSO and CPPSO are determined empirically using several synthetic test data mentioned in Section 5.1.

Same values of acceleration, inertia and constriction coefficients are used for MPSO, PPSO and CPPSO algorithms. The coefficients, $a_1 = 0.3$; $a_2 = \text{rand}()$ and $\chi = 0.79$ provided the best performance. A linearly varying inertia weight is used with the aforementioned optimized parameters. The inertia weight of 0.9 at the beginning of the iteration is linearly decreased to 0.4 at the end of iteration. The perturbation coefficient $\phi_3 = 0.1$ in Eq. (13) provides good convergence for both PPSO and CPPSO algorithms. The CPPSO algorithm requires an additional tuning parameter, namely, number of catfish particles. The five worst-fit particles are considered to be the catfish particles and repositioned on the search space in every alternative iteration for all the diffusion problems considered here. The first four catfish particles are repositioned to extreme points of the search space and fifth particle is repositioned randomly on the search space.

6. Performance on synthetic test data

As it was mentioned before, the fitness function of the present problem is computationally expensive. Thus the performance of the solvers is evaluated using small population sizes and less number of iterations. The performance of the solver is determined using best, mean and worst fitness (RMSE) solutions in 20 independent runs. Further, the solver should be able to estimate best-fit solution alleviating the problems of premature convergence small number of function evaluations.

Performance of the inverse models based on the developed optimization algorithms is tested on synthetic diffusion data. All the algorithms are initialized by generating population of agents randomly on the search space. An initial population of 10 individuals for the first problem and 20 individuals for the second problem are considered. A maximum number of iterations is set to 20 in both problems. The velocity and movement update is initiated with the optimized tuning parameters described in Section 5.3. Two different diffusion problems are considered to determine the performance of the developed solvers. The performance of three different solvers are compared by means of best, worst and mean RMSE values for the two diffusion problems, under the same parameter setting.

The best, worst and mean fitness (RMSE) values of MPSO, PPSO and CPPSO obtained from 20 independent runs for first problem without and with adding 20% noise to the data are given in Tables 2a and 2b, respectively. Best values obtained by the three algorithms for each problem are highlighted as bold. Comparison of MPSO and PPSO show that PPSO achieves better mean fitness only when noise is introduced to the data. However, MPSO outperforms PPSO solver when data is not corrupted. As discussed before, the *gbest* particle perturbs using Eq. (13) around the best feasible position to alleviate premature convergence. This reduced the rate of convergence of the algorithm and thus the particles could not converge to global best position before the maximum number of iterations is achieved. However, perturbation improved the performance of the algorithm when noise is added to the data which is the more likely in the diffusion experiments. The swarming behavior of particles in parametric space in CPPSO algorithm is given in Fig. 3. Performance comparison of CPPSO with MPSO and PPSO algorithms illustrates that CPPSO achieves superior solutions by

Table 1
Details of diffusion test input parameters.

No.	Species	Soil thickness (cm)	$(H_f)_s$, (cm)	$(H_f)_c$, (cm)	Porosity	Dry density (g/cm^3)	No. data points	Unknown parameters	Reference
1	Acetone	1.6	4.6	2.1	0.39	1.68	7	D_e, R_d	Barone et al. (1992)
2	Dioxane	1.7	4.4	2.0	0.39	1.68	7	D_e, R_d	Barone et al. (1992)
3	Aniline	1.8	7.4	1.5	0.39	1.68	7	D_e, R_d	Barone et al. (1992)
4	Chloroform	1.6	7.7	1.5	0.39	1.68	7	D_e, R_d	Barone et al. (1992)
5	Toluene	1.1	7.9	1.5	0.39	1.68	13	D_e, R_d	Barone et al. (1992)
6	HTO	1.0	5.09	5.09	–	1.1	15	D_e, ϕ[a]	Garcia-Gutierrez et al. (2004)
7	HTO	1.0	5.09	5.09	–	1.3	15	D_e, ϕ[a]	Garcia-Gutierrez et al. (2004)
8	HTO	1.0	5.09	5.09	–	1.5	12	D_e, ϕ[a]	Garcia-Gutierrez et al. (2004)
9	HTO	1.0	5.09	5.09	0.222[b]	1.7	17	D_e, ϕ[a]	Garcia-Gutierrez et al. (2004)
10	$^{36}Cl^-$	0.53	5.09	5.09	0.18[a]	1.0	16	D_e	Garcia-Gutierrez et al. (2004)
11	$^{36}Cl^-$	0.53	5.09	5.09	0.105[a]	1.2	16	D_e	Garcia-Gutierrez et al. (2004)
12	$^{36}Cl^-$	0.53	5.09	5.09	0.059[a]	1.4	21	D_e	Garcia-Gutierrez et al. (2004)

[a] Accessible porosity.
[b] Ratio of accessible and effective diffusion coefficients.

Table 2a
Performance of the proposed solvers on uncorrupted synthetic test data for first diffusion problem.

Algorithm	Solution	Optimized values			Mean RMSE values*
		D_e	R_d	RMSE	
MPSO	Best	1.86×10^{-5}	22.34	6.96×10^{-4}	7.552×10^{-3}
	Worst	1.89×10^{-5}	10.94	8.29×10^{-2}	
PPSO	Best	1.86×10^{-5}	22.28	6.64×10^{-4}	8.550×10^{-3}
	Worst	1.54×10^{-5}	45.57	7.70×10^{-2}	
CPPSO	Best	1.85×10^{-5}	22.24	$\mathbf{6.35 \times 10^{-4}}$	$\mathbf{4.190 \times 10^{-3}}$
	Worst	2.30×10^{-5}	20.05	$\mathbf{2.45 \times 10^{-2}}$	

* Mean value obtained from 20 independent runs.

Table 2b
Performance of the proposed solvers on 20% noised synthetic test data for first diffusion problem.

Algorithm	Solution	Optimized values			Mean RMSE values*
		D_e	R_d	RMSE	
MPSO	Best	1.95×10^{-5}	23.01	2.778×10^{-2}	3.551×10^{-2}
	Worst	1.11×10^{-5}	61.42	10.07×10^{-2}	
PPSO	Best	1.95×10^{-5}	22.89	$\mathbf{2.776 \times 10^{-2}}$	3.255×10^{-2}
	Worst	7.49×10^{-6}	46.99	9.993×10^{-2}	
CPPSO	Best	1.93×10^{-5}	22.90	$\mathbf{2.776 \times 10^{-2}}$	$\mathbf{2.833 \times 10^{-2}}$
	Worst	2.19×10^{-5}	25.27	$\mathbf{3.296 \times 10^{-2}}$	

* Mean value obtained from 20 independent runs.

means of best, worst and mean fitness solutions. The mean fitness reduced to half the value when compared with other two solvers. The convergence rate of MPSO, PPSO and CPPSO algorithms are compared in Fig. 4 which shows that CPPSO algorithm is very robust.

Similarly, fitness values obtained by MPSO, PPSO and CPPSO in 20 independent runs while estimating diffusion coefficients of stratified soils are given in Tables 3a and 3b. Tables 3a and 3b provide the results obtained using synthetic data without and with adding white noise to the data respectively. Performance comparison between MPSO and PPSO shows that PPSO outperforms MPSO solver in both corrupted and uncorrupted data. However, the effect of using perturbation equation for *gbest* particle in PPSO algorithm is prominent on noised data as the improvement in the performance is significant. Performance comparison of all the three algorithms shows that CPPSO algorithm outperforms other two solvers. The swarming behaviors of CPPSO particles for the first and second problem are given in Figs. 5 and 6, respectively. The *gbest* particle attracts all the particles towards it and cluster at the global optimum solution. The results clearly indicate that the catfish particles improved the exploration capabilities on the search space while the perturbation equation exploited the good solutions around the *gbest* region. The overall results signify that CPPSO provides promising results for diffusion problems by estimating mean solutions close to best values in different runs.

7. Application to experimental data

The CPPSO algorithm out performed on synthetic tests for all the diffusion problems that are considered in this paper. Further, the estimated values of mean fitness are close to the best fitness in different runs. Thus the developed CPPSO solver is used to determine mass transport parameters of several diffusion data presented in Section 5.2. An initial population of 10 particles is used in all the diffusion data. The parameter setting of the CPPSO tuning parameters is same as used on synthetic tests. The *gbest* solution (fitness), i.e. optimum mass transport parameters, obtained from 10 independent runs is reported in Table 4. Best values obtained by the three algorithms for each problem are highlighted as bold. The *gbest* solution found to be very close to the mean fitness solu-

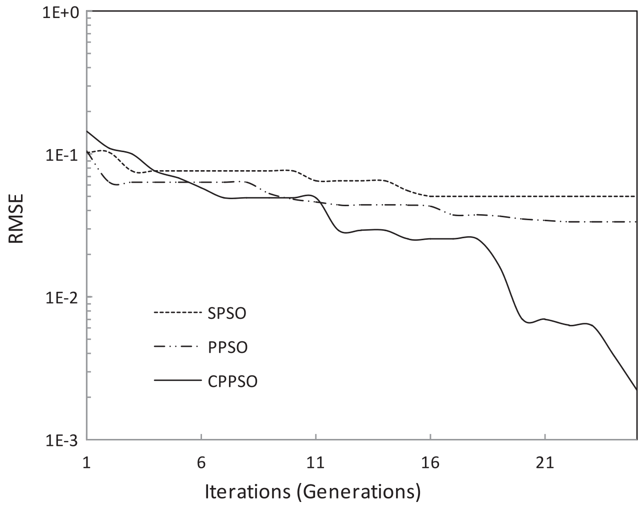

Fig. 4. Performance of different solvers on synthetic test data of first diffusion problem.

tions (not presented here). The published mass transport parameters from the literature (Barone et al., 1992; Garcia-Gutierrez et al., 2004) are also presented in Table 4 for comparison purposes. The published values of parameters for volatile species were obtained by "eye-fitting" technique called Pollute (Rowe & Booker, 1994). On the other hand, transport parameters of radioactive species (HTO and $^{36}Cl^{-}$) were obtained by gradient-based inverse analysis. Comparison of mass transport parameters obtained by predicted and published values shows that the difference in the predicted and published values of retardation factors is significant for the chemical species of Chloroform and Toluene. The proposed solver predicts better estimation of mass parameters with smaller RMSEs. The predicted and published parameters of radioactive species are almost the same. However, the proposed solver is very superior to gradient-based techniques as it does not require initial solution or gradient of the objective function with respect to model parameters. The proposed CPPSO solver is thus capable of predicting mass transport parameters accurately with smaller computational effort. Further, the proposed solver is robust for predicting mass transport parameters from various diffusion problems.

8. Summary and conclusions

In this study, two variants of PSO algorithms, namely, PPSO and CPPSO are presented to improve the performance. The PPSO algorithm uses perturbation equation for *gbest* particle. The CPPSO algorithm uses perturbation equation for *gbest* particle and also *catfish* particles. CPPSO algorithm repositions worst-fit particles (*catfish* particles) into extreme points of the search space and random locations in alternative iterations. Inverse models are developed by integrating the proposed algorithms with forward solution for determining mass transport parameters from diffusion data. The forward solution of reactive transport equations are solved by implicit finite-difference numerical solution. The proposed inverse models are compared with MPSO based solver on synthetic test data. The synthetic test data is generated by corrupting diffusion data obtained from two different diffusion problems. Performance comparison of three models showed that CPPSO solver out-performed the other two solvers on all the tests. Comparison of MPSO and PPSO shows that MPSO solver performs better on the uncorrupted synthetic data obtained from the first diffusion problem. However, PPSO solver out performs for all the other cases. The perturbation equation for the *gbest* particle helped in gaining the information around *gbest* region on the search space especially on the noised data. On the other hand, *catfish* particles improved the exploration capabilities of the algorithm significantly. The CPPSO algorithm which uses these two techniques outperformed the other two solvers on all the tests. The proposed CPPSO solver further applied to estimate mass transport parameters from 12 sets of experimentally observed diffusion data from three diffusion problems. Comparison with published data shows that the proposed solver estimates more accurate parameters and superior than the existing methods. Further, the proposed CPPSO solver quickly converges to global optimum solution using just 200 function evaluations. This is significant for the present problem where fitness function evaluation is computationally expensive. The

Table 3a
Performance of the proposed solvers on uncorrupted synthetic test data for second diffusion problem.

Algorithm	Solution	Optimized values			Mean RMSE values*
		D_{e1} (cm^2/s)	D_{e2} (cm^2/s)	RMSE	
MPSO	Best	1.00×10^{-6}	1.00×10^{-6}	2.944×10^{-4}	7.611×10^{-3}
	Worst	8.65×10^{-7}	7.40×10^{-7}	2.239×10^{-2}	
PPSO	Best	1.01×10^{-6}	1.01×10^{-6}	1.024×10^{-3}	3.639×10^{-3}
	Worst	9.22×10^{-7}	8.34×10^{-7}	1.439×10^{-2}	
CPPSO	Best	1.00×10^{-6}	9.98×10^{-7}	$\mathbf{1.790 \times 10^{-4}}$	$\mathbf{2.791 \times 10^{-3}}$
	Worst	9.23×10^{-7}	9.31×10^{-7}	$\mathbf{8.059 \times 10^{-3}}$	

* Mean value obtained from 20 independent runs.

Table 3b
Performance of the proposed solvers on 20% noised synthetic test data for second diffusion problem.

Algorithm	Solution	Optimized values			Mean RMSE values*
		D_{e1} (cm^2/s)	D_{e2} (cm^2/s)	RMSE	
MPSO	Best	1.16×10^{-6}	1.08×10^{-6}	6.606×10^{-2}	6.748×10^{-2}
	Worst	8.65×10^{-7}	7.40×10^{-7}	7.464×10^{-2}	
PPSO	Best	1.16×10^{-6}	1.03×10^{-6}	6.579×10^{-2}	6.601×10^{-2}
	Worst	1.17×10^{-6}	9.42×10^{-7}	6.662×10^{-2}	
CPPSO	Best	1.17×10^{-6}	1.02×10^{-6}	$\mathbf{6.578 \times 10^{-2}}$	$\mathbf{6.598 \times 10^{-2}}$
	Worst	1.07×10^{-6}	9.15×10^{-7}	$\mathbf{6.656 \times 10^{-2}}$	

* Mean value obtained from 20 independent runs.

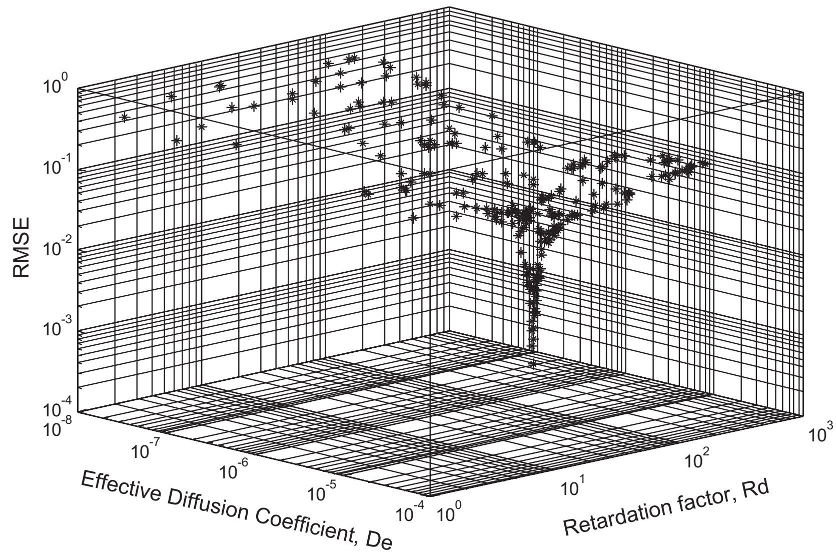

Fig. 5. Convergence of particles in CPPSO algorithm for first diffusion problem.

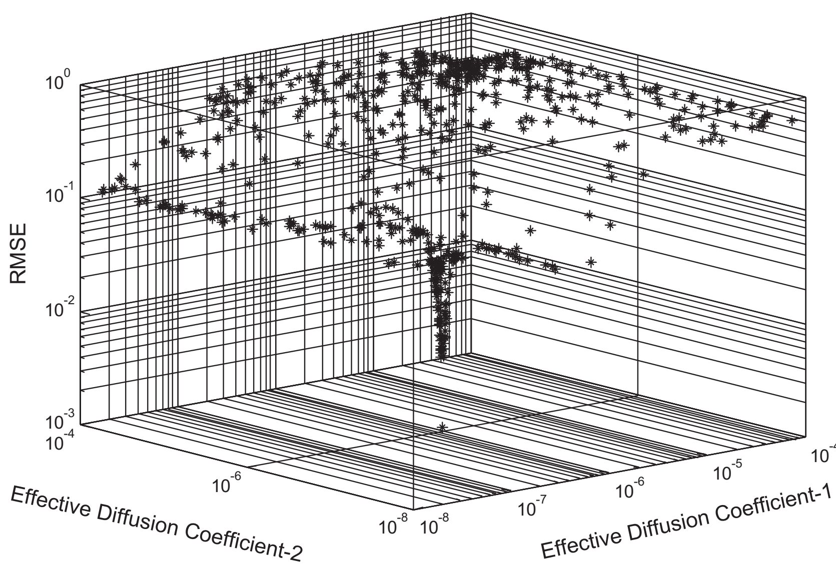

Fig. 6. Convergence of particles in CPPSO algorithm for second diffusion problem.

Table 4
Comparison between predicted model parameters obtained by CPPSO solver with published parameters (from literature).

No.	Species	Predicted parameters			Parameters from literature		
		D_e (cm^2/s)	R_d or ϕ	RMSE	D_e (cm^2/s)	R_d or ϕ	RMSE
1	Acetone	5.55×10^{-6}	1.682	9.66×10^{-3}	5.60×10^{-6}	1.818	1.08×10^{-2}
2	Dioxane	3.84×10^{-6}	1.629	9.72×10^{-3}	4.00×10^{-6}	1.732	1.12×10^{-2}
3	Aniline	7.22×10^{-6}	7.010	2.00×10^{-2}	6.80×10^{-6}	6.600	2.16×10^{-2}
4	Chloroform	1.15×10^{-5}	31.72	2.26×10^{-2}	1.10×10^{-5}	26.85	3.09×10^{-2}
5	Toluene	1.46×10^{-5}	122.2	2.94×10^{-2}	1.38×10^{-5}	113.0	3.17×10^{-2}
6	HTO	1.91×10^{-6}	0.535	1.61×10^{-2}	1.92×10^{-6}	0.582	1.72×10^{-2}
7	HTO	1.33×10^{-6}	0.425	1.21×10^{-2}	1.36×10^{-6}	0.439	1.24×10^{-2}
8	HTO	8.67×10^{-7}	0.414	1.59×10^{-2}	8.80×10^{-7}	0.339	1.63×10^{-2}
9	HTO	5.76×10^{-7}	–	1.66×10^{-2}	5.76×10^{-7}	–	1.66×10^{-2}
10	$^{36}Cl^-$	2.78×10^{-7}	–	1.97×10^{-2}	2.72×10^{-7}	–	1.99×10^{-2}
11	$^{36}Cl^-$	1.12×10^{-7}	–	1.48×10^{-2}	1.08×10^{-7}	–	1.63×10^{-2}
12	$^{36}Cl^-$	3.28×10^{-8}	–	3.24×10^{-2}	2.90×10^{-8}	–	3.54×10^{-2}

proposed inverse model is quick, simple and robust on different diffusion problems. Thus the proposed solver would be of great help for the application to other inverse problems, where fitness function evaluation is highly expensive.

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