Inverse modeling of contaminant transport through soil using natural computation

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ABSTRACT

Several optimization algorithms have been used with varying degree of success to estimate diffusion and retardation coefficients for the design of containment systems. Of these, Particle Swarm Optimization (PSO) algorithms stand out for their simplicity and efficiency; however, PSO algorithms suffer from convergence issues, particularly for the aforementioned inverse problem. Here, a novel algorithm is proposed by combining Big-Bang Big-Crunch algorithm with PSO to overcome convergence issues. The performances of a standard PSO and the proposed algorithms are compared using synthetic data. The proposed algorithm is shown to outperform standard PSO and results in more accurate estimation of parameters from experimental data.

RÉSUMÉ

Plusieurs algorithmes d'optimisation ont été utilisés, avec des degrés variables de succès, pour estimer les coefficients de diffusion et retardement utilisés dans la conception des systèmes de confinement. Parmi ceux-ci, les algorithmes Particle Swarm Optimization (PSO) sont remarquables du fait de leur simplicité et de leur efficacité. Cependant, les algorithmes PSO souffrent de difficultés de convergence, particulièrement pour le problème inverse susmentionné. Un algorithme original est proposé ici en combinant les algorithmes Big-Bang Big-Crunch et PSO pour surmonter les difficultés de convergence. Les performances d'un PSO standard et des algorithmes proposés sont comparées en utilisant des données synthétiques. L'algorithme proposé est montré être plus performant que l'algorithme PSO standard et conduit à des estimations plus précises des paramètres à partir des données expérimentales.

1 INTRODUCTION

Chemical contaminants are the main sources of soil and groundwater pollution. They originate from chemical industries and other contaminated sites. Contamination of the environment poses severe health issues to the inmates. The waste is encapsulated in liner system in the landfills to slowdown the migration of chemical contaminants. Similarly, vertical barrier systems are constructed in the subsurface to arrest the contaminants flow into the subsurface. Thus the importance of contaminant transport studies through barrier system is well recognized worldwide. Such studies help in designing contaminant barrier systems such as landfills and rehabilitation of the contaminated sites. The landfill liner implies any natural or factory manufactured lowpermeable material, to make diffusion as the dominant transport process, used for contaminant confinement applications in landfills. The design of these disposal sites (landfills) and vertical barrier systems requires consideration of the likely contamination of the surrounding ground-water systems in both the short and long term. Thus, accurate estimation of transport parameters through these contaminant barrier systems is of critical importance for the performance assessment of landfills and vertical barrier systems. The contaminant transport in these systems is 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. Generally, laboratory diffusion tests are conducted to

estimate the design parameters of a proposed landfill system or to estimate the performance of an existing landfill system. These laboratory tests are conducted 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. Design parameters are estimated by matching the theoretical concentration profile with the experimentally observed temporal or spatial variation of the concentration. In Geo-environmental engineering, this is commonly done using visual calibration techniques like Pollute (Rowe and Booker, 1998). A few studies also used the gradient-based optimization techniques for solving this inverse problem (Bell et al. 2002). The shortcomings of using the above techniques for contaminant transport problems have been well documented in (Bharat et al. 2008). Recently, the PSO algorithm has been used in geo-environmental engineering for solving inverse problems such as parameter identification (Bharat et al. 2009a) and constructing the past contaminant source history (Bharat et al. 2009b) and also shown the benefits of using PSO based solvers in obtaining good solutions. However, often times PSO, similar to other evolutionary algorithms, converges prematurely to local solutions. Especially in the application to contaminant transport problems, this is a major set-back as this causes not only improper parameter estimation but also a waste of huge computational effort (each fitness calculation involves an expensive time marching numerical computations of partial differential equations).

With this incentive, in this paper a new variant of PSO is presented to improve the efficiency of the algorithm for developing an inverse model for parameter estimation (Bharat and Sharma 2010). The proposed algorithm uses a new point on the search space in each iteration from the Big-Bang Big-Crunch (BB-BC) optimization concept (Erol and Eksin 2006). The modified PSO algorithm uses center of mass of the population using the fitness and locations of all the agents in addition to the fitness of individuals. The detrimental position update formula of global best particle in the standard PSO can be alleviated using this additional information in the search space as the center of mass of the population changes randomly for every generation.

2 CONTAMINANT TRANSPORT PROBLEM

Consider an engineered barrier system with contaminant cells, liner and the leachate collection system. The net change in the mass of solute in the saturated permeable stratum beneath the landfill at any time will be equal to the flux into the permeable stratum from the landfill. The theoretical estimation of contaminant concentration in the landfill requires the solution of the governing transport equations.

2.1 Mathematical Formulation

The concentration at any time instant at the upper boundary can be represented as

$$c(x=0,t) = c_0 + \frac{nD}{H_s} \int_0^\tau \left(\frac{\partial c}{\partial x}\right)|_{x=0} d\tau$$
[1]

where H_s 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, D is the effective diffusion coefficient, c is the concentration of the solute in pore fluid at time t, spatial location X, Π is the soil porosity

and c_0 is the initial contaminant concentration.

Similarly, the concentration at any time instant at the lower boundary can be represented as:

$$c(x = L, t) = -\frac{nD}{H_c} \int_0^t \left(\frac{\partial c}{\partial x}\right)|_{x=L} d\tau$$
[2]

where, H_c is the equivalent height of the collector reservoir.

The one-dimensional governing diffusion equation through soil can be expressed as

$$\frac{\partial c}{\partial t} = \frac{nD}{\alpha} \frac{\partial^2 c}{\partial x^2}$$
[3]

where α is the capacity factor represents the sorption of contaminants on to the surface of the clay particle.

The initial condition in general encountered is

$$c (0 < x < L, t = 0) = 0$$

$$c (x = 0, t = 0) = c_0$$

$$c (x = L, t = 0) = 0$$
[4]

Solute concentration at any spatial location and time instant c(x,t) can be obtained by solving the governing equation [3] along with initial and boundary conditions [4] through [6], simultaneously.

2.2 Numerical Solution

Crank-Nicolson (C-N) numerical solution is used to discretize the governing equation as given below:

$$c_{i}^{n+1} - 0.5DN \left(c_{i+1}^{n+1} - 2c_{i}^{n+1} + c_{i-1}^{n+1} \right) = c_{i}^{n} + 0.5DN \left(c_{i+1}^{n} - 2c_{i}^{n} + c_{i-1}^{n} \right)$$
[5]

Simplifying further by separating the concentration terms of n^{th} and $n + 1^{th}$ time levels,

$$A_i c_{i-1}^{n+1} + B_i c_i^{n+1} + D_i c_{i+1}^{n+1} = K_i$$
[6]

where,

$$A_i = -0.5DN$$
; $B_i = (1 + DN)$; $D_i = -0.5DN$; and
 $K_i = (0.5DN)c_i^n + (1 - DN)c_i^n + (0.5DN)c_{i-1}^n$

Finite difference approximation of the boundaries ([2] and [3]) using fully implicit scheme gives the following equations

$$c_1^{n+1} = \chi_1 c_1^n + \chi_2 c_2^{n+1}$$
[7]

and

$$c_M^{n+1} = \chi_3 c_M^n + \chi_4 c_{M-1}^{n+1}$$
[8]

where
$$\chi_1 = 1 / \left(1 + \frac{nD\Delta t}{H_s\Delta x} \right)$$
, $\chi_2 = \left(\frac{nD\Delta t}{H_s\Delta x} \right) / \left(1 + \frac{nD\Delta t}{H_s\Delta x} \right)$,
 $\chi_3 = 1 / \left(1 + \frac{nD\Delta t}{H_c\Delta x} \right)$ and $\chi_4 = \left(\frac{nD\Delta t}{H_c\Delta x} \right) / \left(1 + \frac{nD\Delta t}{H_c\Delta x} \right)$

Substituting values of c_1^{n+1} and c_M^{n+1} from [7] and [8] into [6], the equation at i = 2 becomes,

$$A_2\left(\chi_1 c_1^n + \chi_2 c_2^{n+1}\right) + B_2 c_2^{n+1} + D_2 c_3^{n+1} = K_2$$
[9]

After simplification it gives,

$$B_2'c_2^{n+1} + D_2c_3^{n+1} = K_2'$$
 [10]

where $B_{2}' = (B_{2} + A_{2}\chi_{2})$ and $K_{2}' = (K_{2} - A_{2}\chi_{1}c_{1}^{n})$

Similarly, at i = M - 1,

$$A_{M-1}c_{M-2}^{n+1} + B_{M-1}c_{M-1}^{n+1} + D_{M-1}\left(\chi_{3}c_{M}^{n} + \chi_{4}c_{M-1}^{n+1}\right) = K_{M-1}$$
[11]

After simplification,

$$A_{M-1}c_{M-2}^{n+1} + B_{M-1}c_{M-1}^{n+1} = K_{M-1}$$
[12]

where $B_{M-1}' = (B_{M-1} + D_{M-1}\chi_4)$ and $K_{M-1}' = (K_{M-1} - D_{M-1}\chi_3c_M^n)$

Thus the matrix form of [12] becomes

$$\begin{pmatrix} B_{2}' & D_{2} & 0 & 0 & \cdots \\ A_{3} & B_{3} & D_{3} & 0 & \cdots \\ 0 & A_{4} & B_{4} & D_{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & A_{M-1} & B_{M-1}' \end{pmatrix} \begin{pmatrix} c_{2}^{n+1} \\ c_{3}^{n+1} \\ \vdots \\ \vdots \\ c_{M-1}^{n+1} \end{pmatrix} = \begin{pmatrix} K_{2}' \\ K_{3} \\ K_{4} \\ \vdots \\ K_{M-1} \end{pmatrix}$$
[13]

To obtain the concentration vector in the $n+1^{th}$ time level,

$$\begin{pmatrix} c_{2}^{n+1} \\ c_{3}^{n+1} \\ \vdots \\ \vdots \\ c_{M-2}^{n+1} \\ c_{M-1}^{n+1} \end{pmatrix} = \begin{pmatrix} B_{2}' & D_{2} & 0 & 0 & \cdots \\ A_{3} & B_{3} & D_{3} & 0 & \cdots \\ 0 & A_{4} & B_{4} & D_{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & A_{M-1} & B_{M-1}^{\prime} \end{pmatrix}^{-1} \begin{pmatrix} K_{2}' \\ K_{3} \\ K_{4} \\ \vdots \\ K_{M-1}^{\prime} \end{pmatrix}$$
[14]

The tridiagonal matrix is solved using Thomas algorithm which uses Gauss elimination technique. The aforementioned forward model estimates the theoretical contaminant concentration c(x,t) when the design transport parameters are known. However, the laboratory contaminants transport experiments and the field monitoring systems in the landfills yield the spatial or temporal concentration of contaminants. The design transport parameters need to be determined from these observations by inverse analysis. In the inverse analysis an objective function is constructed as shown in the equation [15] which helps as a guide to find the best parameters.

$$E_{r} = \sqrt{\sum_{i=1}^{L} \left\{ \frac{\left[C_{in,anal}(t_{i}) - C_{in,num}(t_{i}; D_{e}, \alpha)\right]^{2} + \left[C_{out,anal}(t_{i}) - C_{out,num}(t_{i}; D_{e}, \alpha)\right]^{2} + \frac{\left[C_{out,anal}(t_{i}) - C_{out,num}(t_{i}; D_{e}, \alpha)\right]^{2}}{2n_{L}} \right\}}$$
[15]

where $c_{in,anal}(t_i)$ and $c_{out,anal}(t_i)$ are the contaminant concentrations data obtained from analytical solution and $c_{in,num}(t_i)$ and $c_{out,num}(t_i)$ are the concentrations data obtained by numerical model at given values of t_i , i = 1, 2, ...N, theoretical time.

The forward model (simple explicit numerical procedure) was integrated with standard PSO for the estimation of design parameters in our earlier work (Bharat et al. 2008). However, the success rate of the solver is not striking due to premature convergence of the standard PSO algorithm. The detailed description of PSO algorithm is presented in the next section.

3 PSO ALGORITHMS

3.1 PSO Description

PSO is a class of derivative-free, population-based computational methods which is a recent addition to nature inspired algorithms. The foundation of PSO is based on the social behaviors of animals such as flocking of birds and schooling of fishes (Kennedy and Eberhart 1995). In PSO, each particle of the population is thought of as a collision-free bird and used to represent a potential solution for the problem. In this method each agent representing a potential solution moves in the search space and adaptively updates its velocity and position according to its own flying experience and the flying experience of its neighbors, aiming at a better position for itself. Moreover, each individual has a memory, remembering the best position of the search space it has ever visited. Thus, its movement is an aggregated acceleration towards its best previously visited position and towards the best individual of a topological neighborhood.

PSO starts with the random initialization of a population of individuals in the search space and works on the social behavior of the particles in the swarm. The position of i^{th} particle and j^{th} dimension is represented as $\vec{x}_{ij} = (x_{i1}, x_{i2}, ..., x_{iD})$. The best position of the i_{th} particle in its history that gives the best fitness value is represented as $\vec{p}_{ij} = (p_{i1}, p_{i2}, ..., p_{iD})$. The best particle among all the particles in the whole population and in the entire history is represented by $\vec{p}_{gj} = (p_{g1}, p_{g2}, ..., p_{gD})$. At each iteration step k+1 the position vector of the i^{th}

particle $x_{ij}(k+1)$ is updated by adding an increment vector called velocity $v_{ij}(k+1)$ as shown below

$$\vec{x}_{ij} = \vec{x}_{ij} + \vec{v}_{ij}$$
[16]

The velocity of each individual is updated with the best positions acquired for all individuals over generations, and the best positions acquired by the respective individuals over generations. Updating is executed by the following formula:

$$\vec{v}_{ij} = \chi \left(\vec{\omega v}_{ij} + \phi_1 rand_1 () \left(\vec{p}_{ij} - \vec{x}_{ij} \right) + \phi_2 rand_2 () \left(\vec{p}_{gj} - \vec{x}_{ij} \right) \right)$$
[17]

where χ is called constriction coefficient and ω is the inertia weight introduced by Shi and Eberhart (1998) in order to improve the performance of the particle swarm optimizer. ϕ_1 and ϕ_2 are two positive values called acceleration constants. $rand_1()$ and $rand_2()$ are two independent random numbers that uniformly distribute between 0 and 1 and are used to stochastically vary the relative pull of \vec{p}_{ij} and \vec{p}_{gj} . The personal best position of each particle and the global best position are updated after each generation (iteration). The positions of respective individuals are updated by every generation, and are expressed by the equation [17].

3.2 Shortcomings of Standard PSO and Its Variants

A large number of theoretical studies (Clerk and Kennedy 2002) have shown that the particles positions in standard PSO oscillate in damped sinusoidal waves until they converge to points in between their previous best positions and the global best positions discovered by all particles so far. If some point visited by a particle during this oscillation has better fitness than its previous best position (which is very likely to happen in many fitness landscapes). then particle movement continues, generally converging to the global best position discovered so far. All particles follow the same behavior, quickly converging to a good local optimum of the problem. However, if the global optimum for the problem doesn't lie on a path between original particle positions and such a local optimum, then this convergence behavior prevents effective search for the global optimum. Many of the particles waste computational effort in seeking to move in the same direction (towards the local optimum already discovered), whereas better results may be obtained if various particles explore other possible search directions (Peram et al. 2003).

A number of PSO variants have been proposed to overcome some of the above mentioned problems. The perturbed PSO algorithms are more thriving to overcome premature convergence and successfully applied solve inverse problems (Bharat et al., 2008). However, the performance of these algorithms is highly dependent on the perturbation coefficient which varies from problem to problem (Bharat, 2010). Thus finding an optimum value of perturbation coefficient for a given problem will not be practical in many situations.

3.3 Big-Bang Big-Crunch Algorithm

The Big Bang-Big Crunch (BBBC) optimization method (Erol and Eksin 2006) is built on two main steps: The first step is the Big Bang phase where candidate solutions are randomly distributed over the search space and the next step is the Big Crunch where a contraction procedure calculates a center of mass for the population. The initial Big Bang population is randomly generated over the entire search space just like the other evolutionary search algorithms. All subsequent Big Bang phases are randomly distributed about the center of mass or the best fit individual in a similar fashion. The detailed description of BBBC algorithm is given elsewhere (Erol and Eksin 2006). Though the BBBC algorithm works in the same fashion as any other algorithm does, it lacks good exploration capabilities due to weak position update formula. Thus a hybrid algorithm was proposed which uses the personal best and global best positions of the agents into consideration to update the positions of the agents (Kaveh and Talatahari 2010). However, due to exclusion of velocity term in the hybrid BBBC (HBBBC) algorithm, it doesn't tap the full advantage of original PSO algorithm offers. Thus, a new algorithm is presented which takes into account of centre of mass concept of BBBC algorithm and position update is performed using standard PSO algorithm.

3.4 Proposed Algorithm

The pseudo-code of the proposed PSO algorithm can be summarized as follows:

- Step1: Initialize the population by randomly distributing the agents on the search space
- Step2: Calculate fitness of all agents [15]
- Step3: Update the position of each agent using [16] and [17]
- Step4: Find the center of mass of the whole population using the following equation

$$x_{j}^{k}(c) = \frac{\sum_{i=1}^{N} \frac{1}{fit_{i}} \cdot x_{ij}^{k}}{\sum_{i=1}^{N} \frac{1}{fit_{i}}} \quad j = 1,2$$
[18]

where x_{ij}^{k} is the j^{th} component of the i^{th} solution generated in k^{th} generation and *N* is the population size.

Step5: Compute the fitness of the center of mass point.

Step6: Compare the fitness' of global best agent and center of mass point. Update the global best value using the greedy selection mechanism.

Step7: Return to Step3.

4 INVERSE ANALYSIS

The goal of the present inverse model is to estimate a combination of mass transport parameters that minimizes the error [15] which serves as an objective function between the experimentally measured and theoretically computed concentration data. 4.1 Parameter Setting

In the solvers, the PSO algorithms are based on a population of 25 particles randomly distributed in the solution (parametric) space. The maximum number of generations is set to 200 in each run. Initially, the PSO studies used high values for acceleration coefficients. Although good results have been obtained on standard test functions, it is observed for the present problem that velocities quickly explode to large values, especially for particles far from their global best and personal best positions. Consequently, particles have large position updates, with particles leaving the boundaries of their search space. Thus, best set of PSO variables is found by empirical studies. It is observed that $\varphi_1 = \varphi_2 = 0.5$ is found to give good performance when $\chi = 0.6$ and a linearly varying inertia weight ω from 0.9 to 0.4 from the beginning to end of the search, are used.

4.2 Performance assessment of Different Solvers

To demonstrate and validate the inverse models developed using SPSO, HBBBC and PPSO algorithms, a synthetically generated data is used. The synthetic data of contaminant concentration is obtained by solving the forward problem using an assumed set of mass transport parameters D=1.523×10⁻⁰⁵ and α = 34. This data with and without random noise is given as input to the solvers for finding the true design parameters. The performance of all the developed solvers on synthetic data is tested using 10 independent runs. Table 1 presents the best and the worst values, the tolerance and the success rate obtained for each solver. The result indicates that HBBBC and PPSO models achieve better success rate when compared with SPSO model. Though the performance of HBBBC and PPSO models is the same on synthetic data without noise, the superiority of PPSO model is exhibited when the noise is introduced to the data. Thus, it appears that the performance of the PPSO model is not influenced by the noise in the data which is expected in the experiments. Thus, this model is more reliable in estimating the accurate design parameters.

The movement of the particles for HBBBC and PPSO inverse models is shown in Fig. 1 and 2. In the case of HBBBC model, the particles have quickly converged (in 100 iterations) to near global optimum solution (D= 1.168×10^{-05} and $\alpha = 45.063$) with a success rate of

0.5. However, the PPSO algorithm continues to search till the maximum iterations of 200 and converged to global optimum solution ($D=1.43 \times 10^{-05}$ and $\alpha = 34.805$) with a success rate of 0.7.

4.3 Application to Experimental Data

Laboratory data of (Barone et al. 1992) for transient through-diffusion and sorption of chloroform in clayey soil is used to estimate the design parameters from PPSO model. The best solution (fitting parameters) is estimated from 10 independent runs. The best solution obtained is

 $D = 11.509 \times 10^{-05} \text{ cm}^2/\text{sec}$ and $\alpha = 12.3507$ with $E_r = 0.0213$.

The theoretical profile representing the temporal variation of solute concentration in the source and collector reservoir is obtained for the model parameters estimated by the PPSO model. This is plotted in Fig. 3 along with the experimental data.



Fig. 1. Movement of the particles with HBBBC solver on synthetic data with 5% noise



Fig. 2. Movement of the particles with the proposed solver on synthetic data with 5% noise



Fig. 3. The theoretical concentration data using the optimized parameters from the proposed solver and the input data of experimental observations

Table 1. Performance of different inverse models on synthetic test data

A	Data	т	S	Best solution (D, R)	Worst solution (D, R)
SPSO	Synthetic (without noise)	10 %	0.6	1.4E-05, 36.76 (rmse = 0.0038)	1.1E-05, 42.84 (rmse = 0.01255)
	Synthetic (5% noise)	15 %	0.3	1.3E-05, 37.3 (rmse = 0.0145)	1.2E-06, 141.2 (rmse = 0.0293)
HBBB C	Synthetic (without noise)	10 %	0.8	1.5E-05, 34.0 (rmse = 0.0231)	1.23E-05, 42.8923 (rmse = 0.00891)
	Synthetic (5% noise)	15 %	0.5	1.4E-05, 37.396 (rmse = 0.0143)	8.9E-06, 63.0 (rmse = 0.012)
PPSO	Synthetic (without noise)	10 %	0.8	1.5E-05, 34.0 (rmse = 1.2E-8)	1.2E-05, 41.1 (rmse = 7.7E-3)
	Synthetic (5% noise)	15 %	0.7	1.49E-5, 34.0231 (rmse = 0.001366)	1.1E-05, 45.1 (rmse = 0.003)

5 CONCLUDING REMARKS

In this paper a new inverse model based on particle swarm optimization algorithm is introduced for the parameter estimation of contaminant transport through liner material. A new point is introduced into the SPSO algorithm center of mass of the population. The developed solver thus tested on synthetic data and compared with the solvers based on SPSO and HBBBC. The proposed model outperforms its counterparts on synthetic data with and without the addition of random noise. Further, the model successfully was used to estimate the design parameters with good accuracy from the experimental data. Further work on improving the inverse model to enhance the success rate is in progress.

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