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Short Communication

A modified simulated annealing algorithm for estimating solute transport parameters in streams from tracer experiment data

J.Q. Guo[a], L. Zheng[b,*]

[a]Department of Water Resources Engineering, Chang An University, Xi'an, Shanxi, PR China
[b]Centre for Agricultural Resources Research, IGDB, Chinese Academy of Sciences, Shijiazhuang, Hebei, PR China

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Abstract

It is difficult to estimate solute transport parameters in streams empirically and numerous approaches have been investigated in the past. In the current study, we explored the use of the simulated annealing (SA) algorithm for estimating solute transport parameters in streams from tracer experiment data. For a simple one-dimensional dispersion test case, the standard SA algorithm was very slow to converge. To remedy the problem of slow convergence of the annealing optimization, we proposed three strategies to modify the standard SA algorithm and improve the converging speed. The proposed three strategies are: (1) imposing parameter space constraints; (2) adding a valve value for inner loop break; and (3) including an inner loop memory function. We conducted a numerical experiment to test and demonstrate the effectiveness of the modified SA algorithm for estimating three major solute transport parameters: longitudinal dispersion coefficient, cross-sectional averaged flow velocity, and tracer mass loading. We then discussed the advantages and limitations of the proposed algorithm.

Keywords: Solute transport in stream; Simulated annealing; Dispersion coefficient; Parameter estimation

Software availability

Name of Software:	SAST
Developers:	Jian-Qing Guo and Li Zheng
Contact address:	Department of Water Resources Engineering, Chang An University, Xi'an, Shanxi, P. R. China
Telephone:	+86 311 588 5030
Fax:	+86 311 587 1620
E-mail address:	guojian0248@sohu.com
Availability:	freely available by e-mailing your request to guojian0248@sohu.com or zhengli_usa@yahoo.com

1. Introduction

Important parameters that govern the transport of solute in streams include longitudinal dispersion coefficient D_L, cross-sectional averaged velocity v etc. The most common way for determining these parameters is through conducting tracer experiments and analysing the observed tracer concentration profiles. Methods for estimating transport parameters from tracer data were mostly based on approximating Taylor's analytical solution (1954), and often plagued by the errors introduced by the approximation and numerical integration etc. Singh and Beck (2003) gave a detailed account on the limitations of these methods, and proposed a new routing method that is free from the previously mentioned errors. They then applied Marquardt Method to solve the nonlinear least square problem to obtain optimal parameter estimates. In a separate report, Singh (2003) proposed a new method for the treatment of stagnant zones in

* Corresponding author. Tel./fax: +86 311 587 1620.
E-mail address: zhengli_usa@yahoo.com (L. Zheng).

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streams and also applied similar non-linear regression approach to estimate optimal solute transport parameters. Other recent works on estimating solute transport parameters in streams include Swamee et al. (2000), Deng et al. (2002) and Seo and Baek (2004). Detailed surveys of historical development of this line of research can be found in these works.

When analytical expressions for concentration profiles are available, gradient search based non-linear regression algorithms such as Marquardt Method are commonly used to obtain optimal transport parameter estimates. The applications of these methods, however, require the objective function to be smooth, which may not always be the case for complex objective functions. Further, for the applications where local optimal solutions existed, non-unique solutions could result from different initial parameter values (Li et al., 1999). In the current study, we explored the possibility of using a non-gradient based direct search algorithm, the simulated annealing (SA), for optimal solute transport parameter estimation. Such an exploration to our knowledge has not been attempted before.

Simulated annealing (SA) is a global optimization technique that is not based on gradient search. Instead it was derived from statistical mechanics by mimicking the physical annealing process (i.e., the cooling of molten substances to crystalline lattices of minimum energy). Kirkpatrick et al. (1983) first proposed and demonstrated the use of SA in solving the combinatorial optimization problems. The application of SA was later extended to the optimization of continuous functions (e.g., Bohachevsky et al., 1986). Recently, SA also found applications in problems of groundwater management (e.g., Johnson and Rogers, 2001), agricultural water management (e.g., Kuo et al., 2001), and parameter estimation for solute transport in porous media (Li et al., 1999). In this paper we explored the use of SA for estimating solute transport parameters in streams from tracer experiment data. For a simple one-dimensional transport problem, we found that the standard SA algorithm was very slow to converge. To speedup the SA optimization, we proposed three strategies to modify the standard SA algorithm, including (1) imposing parameter space constraints; (2) adding a valve value for inner loop break; and (3) including an inner loop memory function. We then used a numerical experiment to test and demonstrate the effectiveness of the modified SA algorithm for estimating solute transport parameters in streams.

2. Simulated annealing and its improvement

2.1. Standard simulated annealing algorithm

Inspired by the Monte Carlo method introduced by Metropolis et al. (1953), Kirkpatrick et al. (1983) developed the SA technique for the optimization of combinatorial problem. It makes the analogy between the state of each molecule that determines the energy function and the value of each parameter that affects the objective functions. It then uses the statistical mechanics principle for energy minimization to minimize the objective function and optimize the parameter estimates. Starting with a high temperature, it randomly perturbs the parameter values and calculates the resulting objective function. The new state of objective function after perturbation is then accepted by a probability determined by the Metropolis criterion. The system temperature is then gradually reduced as the random perturbation proceeds, until the objective function reaches its global or nearly global minimum (Kirkpatrick et al., 1983). A typical SA algorithm is described as follows (also see Fig. 1):

Step 1 Specify initial temperature $T_k = T_0$ for $k = 0$; randomly initialize the parameter set estimate $\theta^* = \theta_0$.

Step 2 Under kth temperature, if the inner loop break condition is met, go to step 3; otherwise, for $(j+1)$th perturbation, randomly produce a new parameter set θ_{j+1}, compute the change in objective function $\Delta f = f(\theta^*) - f(\theta_{j+1})$. If $\Delta f \leq 0$, accept $\theta_{j+1}(\theta^* = \theta_j)$; if not, follow the Metropolis criterion to accept θ_{j+1} with a probability of $\min\left(1, e^{-\Delta f/T_k}\right)$ and step 2 continues.

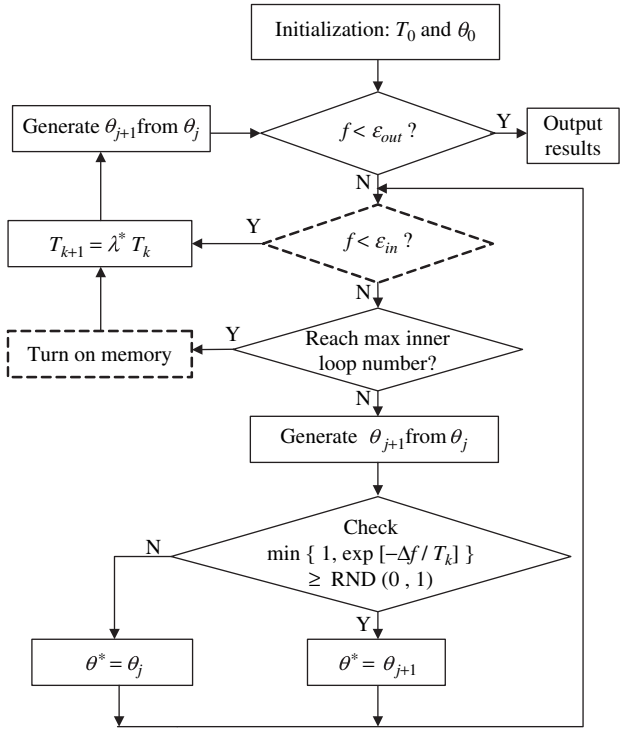

Fig. 1. The flow chart of modified SA algorithm. Boxes with solid lines are original SA algorithm components, and boxes with dashed lines are added new components.