

## Simulated annealing based simulation-optimization approach for identification of unknown contaminant sources in groundwater aquifers

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### ABSTRACT

The exact location and release history of groundwater pollutant sources is often unknown. Identification of unknown release histories is usually carried out by inversion of the equations governing flow and transport over time and space. This is an ill posed problem. Solution of this ill-posed inversion is complicated due to the inherent non-uniqueness of solutions, uncertainties in modeling the flow and transport processes in the aquifer and unavoidable concentration measurement errors. Several methods to solve the ill posed inversion problem have been suggested in past. The simulation-optimization approach using global heuristic search optimization methods has been found to be the most effective with regards to accuracy of solutions. However, these methods are computationally intensive. A linked simulation-optimization based methodology using a variant of simulated annealing (SA) algorithm is linked to the numerical models used to simulate flow (MODFLOW) and transport processes (MT3DMS). The objective function minimizes the difference between observed and simulated contaminant concentration for optimal values of the decision variables representing the unknown source flux magnitude, duration and timing. The developed methodology is tested for an illustrative study area. The SA based source identification methodology is demonstrated to perform more efficiently compared to other methods based on genetic algorithm.

*Keywords:* Source identification; Groundwater pollution; Genetic algorithm; Adaptive simulated annealing

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