

Optimization of Identifying Point Pollution Sources for the Convection-Diffusion-Reaction Equations

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Abstract. In this paper, we consider the optimization problem of identifying the pollution sources of convection-diffusion-reaction equations in a groundwater process. The optimization model is subject to a convection-diffusion-reaction equation with pumping point and pollution point sources. We develop a linked optimization and simulation approach combining with the Differential Evolution (DE) optimization algorithm to identify the pumping and injection rates from the data at the observation points. Numerical experiments are taken with injections of constant rates and time-dependent variable rates at source points. The problem with one pumping point and two pollution source points is also studied. Numerical results show that the proposed method is efficient. The developed optimized identification approach can be extended to high-dimensional and more complex problems.

AMS subject classifications: 35Q93, 65M32

Key words: Convection-diffusion-reaction equation, optimization of identification, pumping point, pollution source point, DE algorithm.

1 Introduction

A rapid increase in industrial activities is accompanied by the release of substantial quantities of pollutants. Environmental pollution has been recognized to be an important and difficult problem that needs to efficiently control the process of industrial releases, etc.

It is no doubt that identifying unknown groundwater sources is a prerequisite for the management and development decision in the water quality, which is also called as the inverse source problem of the groundwater flow. Some methodologies have been proposed for pollution source identifications, such as non-linear least-squares method [1], a geo-statistical approach [17], constrained robust least square approach [20], and so on.

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On the other hand, the aquifer simulation models have been combined with the optimization models to achieve groundwater management objectives for identifying unknown groundwater pollution sources [5,6,14,16]. In these literatures, they embedded the groundwater flow and solute transport equations into the optimization model, and the groundwater flow and solute transport equations need to be solved numerically firstly. While the numerical schemes used in papers [5,6] and [14] were the Galerkin finite element and classical finite difference methods, these methods may bring nonphysical oscillation to convection dominated diffusion problems where the diffusion coefficients are small. Furthermore, the optimization algorithm of paper [5] were MINOS and NPSOL, while paper [14] used MINOS and papers [6] and [16] used Simulated Annealing (SA) and artificial neural network (ANN) respectively. Each of these optimization algorithms has advantages and limitations, authors directly used them and did not compare results there. Our constraint equations in this study are convection diffusion reaction equations, which are different with previous models. We use Differential Evolution algorithm as optimization algorithm and obtain the feasibility of our identification model.

In this paper, we study the optimization of identifying the pollution sources for a groundwater river. A linked simulation-optimization model is proposed, where the convection diffusion reaction equations are computed by the improved/upwind finite difference approach that can avoid nonphysical oscillation of numerical solutions, and the optimization is solved by the constrained Differential Evolution optimization algorithm. The advantage of the methodology is the external linking of the numerical simulation model with the optimization model. We build the objective function aimed at minimizing the weighted sum of squared deviation between observed and simulated concentrations at observation points over time, which also satisfies the constraints of the pumping and injection rates and the concentration restrictions. This process can have the physical explanation: searching the optimal rate, to minimize, in a certain range, the objective function of the simulated concentrations which satisfying the real environment at the same time. We use the constrained Differential Evolution optimization algorithm to solve the optimization problems, which provides the advantages of its global solution solving feature, simplicity, powerful search capability, compact structure, and convergence. Numerical experiments are taken for constant injection rates at one to three source points respectively and for variable rates at one source point. We also consider an example with one pumping point and two pollutant source points. Numerical results show that the developed method is efficient. The method can be extended to high-dimensional and more complex problems.

This paper is organized as follows. In Section 2, we present the mathematical model of the convection diffusion reaction equations with point pollutant sources and pumping wells and give the numerical scheme for solving the convection diffusion reaction equations. In Section 3, we propose a mathematical optimization problem with constraint of numerical solution systems of PDEs. The optimization solving algorithm is described in Section 4. Numerical experiments are presented in Section 5 and some conclusions are addressed in Section 6.