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Estimation of a contaminant source in an estuary with an inverse problem approach

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ABSTRACT

A great challenge today is conciliation of water resources utilization with the expansion of cities and human activities. Considering that the water quality of a given water body is necessarily evaluated through the analysis of some biological, physical and chemical parameters, mathematical and computational models able to describe the behavior of such parameters can be a useful tool, given their ability to generate scenarios and, as a consequence, the possibility to support decisions regarding water resources management. In this work Inverse Problems techniques are applied to estimate the source parameters (location and intensity) of a hypothetical conservative pollutant released in estuarine waters. The case study considered here is the Macaé River estuary, located in the Brazilian southeast coast. The pollutant transport was modeled by the advection–diffusion equation. For the source location estimation were used the Luus–Jaakola (LJ), the particle collision algorithm (PCA) and the ant colony optimization (ACO) methods, and to estimate the source intensity was used the golden section (GS) method. In this study, synthetic sampling data of concentrations with and without noise were used. For the noiseless data, all methods have successfully achieved the objective function target low value in more than 95% of executions. On the other hand, for the data with ±5% of noise level, that happened only in 80% of the runs. Considering the number of different estimated points on the location and also the computational cost, the method LJ-GS showed the best performance. The results of this study demonstrated the feasibility of the inverse problem approach to estimate with satisfactory accuracy the location and intensity of a given pollutant source released in estuarine environments, which can also contribute to possible environmental liabilities identification.

1. Introduction

The quality of a water body is usually evaluated through the analysis of biological, physical and chemical parameters. However, water management involves not only diagnosis but also monitoring and forecasting of future scenarios. For this purpose mathematical and computational models, which can describe the behavior of substances in water bodies, can be useful tools, because, once adequately calibrated, they are able to generate different scenarios, supporting decisions regarding water

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resources management. The water environment considered in this work is an estuary. Estuaries are transitional environments between the continent and the ocean where rivers meet the sea, and thus are subject to river discharge and oceanic variations, resulting in measurable dilution of seawater. The preservation of such environments is justified by the great biological diversity, which exists due to the hydrodynamic characteristics of the prevailing circulation that traps nutrients, algae and other plants, enhancing the productivity of these water bodies [14]. The case study here considered is the estuary of the Macaé River, located at the north coast of the Rio de Janeiro state in Brazil.

The problem tackled in the present work consists on estimating the origin and magnitude of a hypothetical pollutant source whose discharge is diluted in the waters of the estuary. First it implemented the solution of the direct problem, here modeled by the transport equation. This model describes the behavior of a contaminant, involving hydrodynamic parameters, dispersion and a term that represents sources or sinks. Then the direct problem computation model is coupled to computational intelligence methods for parameter estimation (inverse problem) which can express the location and intensity of the pollutant source considered. Thus, the main objective is the estimation of sources through such parameters.

Concerning the determination of parameters related to pollutant sources of transport models follow some works previously developed by other authors. Shen and Kuo [21] used a two-dimensional model of eutrophication laterally integrated to model eight state variables of water quality. In the model, 13 parameters from the source term are estimated, which are functions that describe the time rate of mass growth (or decline) by biochemical reactions and external addition (or removal) of the state variables. Revelli et al. [17] and Revelli and Ridolfi [18] estimated a function used in the modeling of a source term of a one-dimensional pollutants transport problem into channels. In fact, the source term is composed of two functions (one space dependent and another time dependent), being the time dependent function calculated with boundary conditions and concentrations in a given location. Yang and Hamrick [24] estimated open boundary conditions in a three-dimensional transport model of salinity in an estuary. Shen et al. [20] estimated nonpoint sources of fecal coliforms in an estuary. Specifically regarding the estimation of the location of sources or sinks in pollutant transport models, previously developed studies were not found in literature.

2. Direct problem: transport of constituents

The transport of constituents can be described by the advection–diffusion equation [1,3,16]. In the present work, a simplification is considered. The transport equation is vertically integrated, being therefore assumed that the change in concentration is negligible in the vertical direction.

For the discretization of the transport model was applied the finite element method (FEM) for the discretization in space [13,25] and the finite difference method (FDM) for the discretization in time [23]. Finally, we obtain a system of algebraic linear equations (SALE), being solved using the Gauss–Seidel method (GSM) which is convergent when the system has diagonal dominance [6]. A detailed description of the solution of the direct problem is given in Parolin [15], as well as the boundary conditions, the definition of the field of study, geometry, and data from the hydrodynamic model.

The Macaé River estuary, located in the municipality of Macaé in the State of Rio de Janeiro, Brazil, can be viewed in the satellite photo shown in Fig. 1. The study domain, the geometry, the mesh and bathymetry used are shown in Fig. 2.

The spatial and temporal computational mesh was defined after a careful study of consistency and convergence of the numerical method adopted, as described next [15]. A sample transport problem with known analytic solution was considered. Regarding the spatial discretization analysis, three space increments were tested considering a regular mesh ($\Delta x = \Delta y$), with the values of 100 m, 500 m and 1000 m, with a time step of 300 s being kept fixed. For the temporal discretization analysis, five time increments were evaluated, corresponding to 300 s, 600 s, 900 s, 1800 s and 3600 s, with a space step of 500 m being kept fixed. The results were compared with the analytical solution obtained for a specific line of the regular domain, by means of the mean absolute relative error (MARE), considering the highest input contaminant concentration imposed in the problem (10 kg/m^3). For all tests performed the MARE was lower than 10^{-4}. These results are highlighted in Fig. 3, where it is possible to note that, for different instants of time, the analytical solution is always superimposed over the computational solution, supporting, therefore, the choice of the mesh adopted in this study.

In a previous study [15] a sensitivity analysis was performed using the direct problem computational model solution in order to evaluate the possibility of identifying both the location and the intensity of a source in the transport model. A non uniqueness issue was devised, because both parameters are correlated.

3. Parameter estimation

The transport problem of constituents, mathematically represented by the advection–diffusion equation, with the corresponding boundary conditions, hydrodynamic variables and adopted parameters is defined as the direct problem (DP).

The problem of estimating the source of contaminants was formulated as an inverse problem (IP), in which experimental measurements of concentration are assumed known and one is intended to estimate the location and intensity of a source, which are modeled by parameters in the direct transport problem (DP).

As the number of experimental data is usually larger than the number of unknowns, the inverse problem is formulated as a finite dimension optimization problem in which one seeks to minimize the objective function, given by the sum of the squared residues between the calculated and the experimental measured values of the observed variable,

$$SSR = \{\vec{G}_{\text{calc}}(\vec{P}) - \vec{G}_{\text{meas}}\}^T \{\vec{G}_{\text{calc}}(\vec{P}) - \vec{G}_{\text{meas}}\} = \vec{R}^T \vec{R} \quad (1)$$