

Estimation of Water Quality Model Parameters

Taeyun Kim* and Y. P. Sheng**

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Abstract

A modified Gauss-Newton method was utilized to estimate water quality model parameters, which is important in the modeling of water quality transport process. This method served the unknown parameters of three engineering problems exceptionally well. We applied this method to obtain a set of water quality parameters by solving the kinetic equations for dissolved and particulate water quality species during episodic events in the Indian River Lagoon, FL. The method was successful in producing water quality model parameters, and the relative errors between measurements and model predictions are below 46.4% and 39.4% for all dissolved and particulate water quality state variables, respectively. In this study we evaluated a good capability of suggested parameter estimation method by comparing a couple of water quality model simulations: (1) water quality model simulation using model parameters produced by the modified Gauss-Newton method and (2) water quality model simulation employing model parameters obtained by the trial-and-error method. The average relative error and ROC score between observed data and water quality model results using model parameters calculated by the modified Gauss-Newton method are 58.3% and 0.565, respectively. In the case of water quality model simulation using model parameters obtained by the trial-and-error method, the average relative error and ROC score are 60.5% and 0.555, respectively. This suggests that the modified Gauss-Newton method efficiently yields water quality model parameters resulting in better or similar model prediction errors when compared to the trial-and-error method.

Keywords: water quality model, estimation of model parameters, Gauss-Newton Method, water quality state variables

1. Introduction

Estuarine ecosystems have been severely altered or destroyed over the past few decades through direct habitat conversion, introduction of non-native species, and pollution. In recent years, estuarine restoration, protection, and management have become a growing concern of scientists, resource managers, and the public. In order to enable improved understanding of estuarine ecosystems and improve restoration, protection, and management, a useful water quality modeling tool was required. In the past three decades, many studies have focused on creating such a management tool. DiToro *et al.* (1983) developed the Water Quality Analysis Simulation Program (WASP) using the explicit scheme to quantify advective mass transport. HydroQual (1987) developed a water quality model based on the box-model approach. Water quality models, which include transport processes, have been developed and applied to numerous estuaries (e.g., Sheng and Chen, 1992; Baretta *et al.*, 1995; Cerco and Cole, 1995; Park *et al.*, 1995; Poeters *et al.*, 1995). Other water quality models have been developed based on improvement of the above referenced models (Wang and Johnson, 2000; Blackford, 2002; Sheng *et al.*, 2002; Tillman *et al.*, 2004; Zheng *et al.*, 2004; Allen *et al.*, 2007).

In general, water quality models have many kinetic equations

and each equation includes unknown parameters. The determination of the unknown parameters generally requires a great deal of effort because they are dependent on complex physical and biochemical factors, such as geological characteristics of estuaries, temperature, tidal variation, freshwater inflows, point/non point nutrient loads, species of algae, nutrient concentrations at the sediment column, etc. Water quality model parameters are not a common environmental measurement, and thus the values of model parameters are usually selected from a range of feasible values which are acquired from field observation, laboratory experimentation, previous studies, etc. The popular method of parameter selection is the trial-and-error method that adjusts parameters continuously until there is an optimal agreement between predicted nutrient values and measured nutrient data. This method needs a subjective and laborious step in the water quality model calibration process because water quality state variables and model parameters are cross-related to each other. This requires high computational cost and expert practical ability. To overcome these difficulties and obtain reliable water quality model performance, more efficient and robust processes are required.

Many methods are employed to estimate unknown parameters: a marquardt method (Marquardt, 1963), a quasilinearization method (Bellman *et al.*, 1967; Lee, 1968), a Gauss-Newton

*Research Scientist, Pacific Northwest National Laboratory, Seattle, Washington 98109-3598, USA (Corresponding Author, E-mail: Taeyun.Kim@pnl.gov)

**Professor, Coastal & Oceanographic Engineering, University of Florida, Gainesville, FL 32611-6590, USA (E-mail: psheng@coastal.ufl.edu)

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