

Estimation of Water Quality Model Parameters

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Received April 27, 2009/Accepted September 29, 2009

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

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River Water Quality Model P. Reichert, Dietrich Borchardt, Mogens Henze, Wolfgang Rauch, P. Shanahan, Laszlo Somlyódy, Peter A. Vanrolleghem, 2001-08-31 This Scientific and Technical Report STR presents the findings of the IWA Task Group on River Water Quality Modelling RWQM The task group was formed to create a scientific and technical base from which to formulate standardized consistent river water quality models and guidelines for their implementation This STR presents the first outcome in this effort River Water Quality Model No 1 RWQM1 As background to the development of River Water Quality Model No 1 the Task Group completed a critical evaluation of the current state of the practice in water quality modelling A major limitation in model formulation is the continued reliance on BOD as the primary state variable despite the fact BOD does not include all biodegradable matter A related difficulty is the poor representation of benthic flux terms As a result of these limitations it is impossible to close mass balances completely in most existing models These various limitations in current river water quality models impair their predictive ability in situations of marked changes in a river's pollutant load streamflow morphometry or other basic characteristics RWQM 1 is intended to serve as a framework for river water quality models that overcome these deficiencies in traditional water quality models and most particularly the failure to close mass balances between the water column and sediment To these ends the model incorporates fundamental water quality components and processes to characterise carbon oxygen nitrogen and phosphorus C O N and P cycling instead of biochemical oxygen demand as used in traditional models The model is presented in terms of process and components represented via a Petersen stoichiometry matrix the same approach used for the IWA Activated Sludge Models The full RWQM1 includes 24 components and 30 processes The report provides detailed examples on reducing the numbers of components and processes to fit specific water quality problems Thus the model provides a framework for both complicated and simplified models Detailed explanations of the model components process equations stoichiometric parameters and kinetic parameters are provided as are example parameter values and two case studies The STR is intended to launch a participatory process of model development application and refinement RWQM1 provides a framework for this process but the goal of the Task Group is to involve water quality professionals worldwide in the continued work developing a new water quality modelling approach This text will be an invaluable reference for researchers and graduate students specializing in water resources hydrology water quality or environmental modelling in departments of environmental engineering natural resources civil engineering chemical engineering environmental sciences and ecology Water resources engineers water quality engineers and technical specialists in environmental consultancy government agencies or regulated industries will also value this critical assessment of the state of practice in water quality modelling Key Features presents a unique new technical approach to river water quality modelling provides a detailed technical presentation of the RWQM1 water quality process model gives an informative critical evaluation of the state of the practice in water quality modelling and problems

with those practices provides a step by step procedure to develop a water quality model Scientific Technical Report No 12

Risk Analysis of Water Pollution Jacques Ganoulis, 2009-07-14 This new edition of a classic text has now been extensively updated to include the latest developments in risk analysis and water quality assessment and management It takes into account the role of ecological water quality in integrated regional and transboundary water resources management according to the latest UNESCO programmes and the new EU Water Framework Directive This practice oriented textbook is a unique tool for identifying and evaluating local and regional environmental risks from pollution hazards in groundwater river water and coastal seawaters The book explains different risk based probabilistic methodologies and fuzzy logic based approaches and includes various mathematical models for water quality simulation and theories such as the decision analysis the utility theory and the integrated risk based multi criteria assessment and management in order to thoroughly evaluate several case studies from the real world Questions testing the reader's understanding are given at the end of each chapter and a useful appendix provides hints for answering them as well the solutions themselves

Rainfall-Runoff Modelling Keith J. Beven, 2012-01-30 *Rainfall Runoff Modelling The Primer* Second Edition is the follow up of this popular and authoritative text first published in 2001 The book provides both a primer for the novice and detailed descriptions of techniques for more advanced practitioners covering rainfall runoff models and their practical applications This new edition extends these aims to include additional chapters dealing with prediction in ungauged basins predicting residence time distributions predicting the impacts of change and the next generation of hydrological models Giving a comprehensive summary of available techniques based on established practices and recent research the book offers a thorough and accessible overview of the area *Rainfall Runoff Modelling The Primer* Second Edition focuses on predicting hydrographs using models based on data and on representations of hydrological process Dealing with the history of the development of rainfall runoff models uncertainty in model predictions good and bad practice and ending with a look at how to predict future catchment hydrological responses this book provides an essential underpinning of rainfall runoff modelling topics Fully revised and updated version of this highly popular text Suitable for both novices in the area and for more advanced users and developers Written by a leading expert in the field Guide to internet sources for rainfall runoff modelling software

Modelling of Pollutants in Complex Environmental Systems Grady Hanrahan, 2010 Environmental modelling has enjoyed a long tradition but there is a defined need to continually address both the power and the limitations of such models as well as their quantitative assessment This book showcases modern environmental modelling methods the basic theory behind them and their incorporation into complex environmental investigations It highlights advanced computing technologies and how they have led to unprecedented and adaptive modelling simulation and decision support tools to study complex environmental systems and how they can be applied to current environmental concerns This volume is essential reading for researchers in academia industry and government related bodies who have a vested interest in all

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Environmental Fluid Mechanics Hayley H. Shen,Alexander H.D. Cheng,Keh-Han Wang,Michelle H. Teng,Clark C. K. Liu,2002-01-01 Sponsored by the Fluids Committee of the Engineering Mechanics Division of ASCE This report provides environmental engineers with a comprehensive survey of recent developments in the application of fluid mechanics theories to treat environmental problems Chapters cover principles of fluid mechanics as well as contemporary applications to environmental problems involving river lake coastal and groundwater areas Topics include turbulent diffusion mixing of a turbulent jet in crossflow the advected line puff multi phase plumes in uniform stratified and flowing environments turbulent transport processes across natural streams three dimensional hydrodynamic and salinity transport modeling in estuaries fluid flows and reactive chemical transport in variably saturated subsurface media heat and mass transport in porous media parameter identification of environmental systems finite element analysis of stratified lake hydrodynamics water quality modeling in reservoirs and linear systems approach to river water quality analysis In addition to providing valuable information to practitioners this book also serves as a text for an advanced undergraduate or introductory graduate level course

Parameter Estimation and Uncertainty Quantification in Water Resources Modeling Philippe Renard,Frederick Delay,Daniel M. Tartakovsky,Velimir V. Vesselinov,2020-04-22 Numerical models of flow and transport processes are heavily employed in the fields of surface soil and groundwater hydrology They are used to interpret field observations analyze complex and coupled processes or to support decision making related to large societal issues such as the water energy nexus or sustainable water management and food production Parameter estimation and uncertainty quantification are two key features of modern science based predictions When applied to water resources these tasks must cope with many degrees of freedom and large datasets Both are challenging and require novel theoretical and computational approaches to handle complex models with large number of unknown parameters

Environmental Modelling Keith Beven,2018-09-03 Uncertainty in the predictions of science when applied to the environment is an issue of great current relevance in relation to the impacts of climate change protecting against natural and man made disasters pollutant transport and sustainable resource management However it is often ignored both by scientists and decision makers or interpreted as a conflict or disagreement between scientists This is not necessarily the case the scientists might well agree but their predictions would still be uncertain and knowledge of that uncertainty might be important in decision making Environmental Modelling An Uncertain Future introduces students scientists and decision makers to the different concepts and techniques of uncertainty estimation in environmental prediction the philosophical background to different concepts of uncertainty the

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Application of Uncertainty Analysis to Ecological Risks of Pesticides William J. Warren-Hicks,Andy Hart,2010-04-07 While current methods used in ecological risk assessments for pesticides are largely deterministic probabilistic methods that aim to quantify variability and uncertainty in exposure and effects are attracting growing interest from industries and governments Probabilistic methods offer more realistic and meaningful estimates of risk and hence pot

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Identification and System Parameter Estimation ,1985 *Treatise on Water Science* ,2010-09-01

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