Journal of Hydrology 530 (2015) 645–656

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

A reduced-order based CE-QUAL-W2 model for simulation of nitrate concentration in dam reservoirs

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ARTICLE INFO

Article history:
Received 20 June 2015
Received in revised form 30 September 2015
Accepted 1 October 2015
Available online 22 October 2015
This manuscript was handled by Ashok Mishra, Editor-in-Chief, with the assistance of Geoff Syme, Associate Editor

Keywords:
Reduced-order modeling
Karkheh reservoir
Nitrate
CE-QUAL-W2
Proper orthogonal decomposition

SUMMARY

When the number of computational grids increases, water quality simulation complexities arise. Therefore, using a reduced order framework to express the variations of the objective parameter may facilitate the simulation task and also the interpretation of computational results. In this regard, a new reduced-order approach was proposed to link a water quality simulator model (CE-QUAL-W2, W2) with a data reduction technique (proper orthogonal decomposition, POD). The W2 model simulated spatio-temporal variations of nitrate in the Karkheh Reservoir, Iran. Thereafter, the POD model reduced the dimensions of simulated nitrate in the computational grids. The performance of the developed reduced-order model (ROM) results was evaluated through the comparison of the regenerated nitrate data by the model, and the simulated ones by W2. Findings indicated that the first four modes among 1825 computed ones by ROM conserved approximately over 91% of the nitrate variations. It means that the ROM was capable of showing the spatio-temporal variations of nitrate in the reservoir using the first few modes. Finally, confirmation of ROM indicated that the error of order of magnitude was less than 0.001, for nitrate ROM to regenerate nitrate data using 100 basis functions.

1. Introduction

Reservoirs are important water supply systems which play a vital role in providing water for drinking, agricultural, industrial and recreational purposes. Regarding hydrodynamic conditions, reservoirs are relatively steadier than other water bodies such as rivers. Besides, reservoirs can be considered as the ultimate sink for all the pollutants in basins. These facts cause reservoirs to be generally more vulnerable for water quality deterioration as compared to other water bodies. Therefore, proper water quality management in reservoirs requires a high technical expertise. One of the most threatening problems related to water quality in reservoirs is eutrophication. It is the aquatic system response to nutrients abundance, such as nitrogen and phosphorous compounds, through fertilizers or sewage. Eutrophication generally promotes excessive algal growth and dramatically reduces water quality. When algae die and sink to the bottom, their organic matter is decomposed into inorganic form by bacteria. The decomposition process uses up oxygen in deeper water levels which can cause fish and other organisms to die (Liang et al., 2013). Also, eutrophication disrupts normal functioning of the ecosystem, causing a variety of problems such as a decreases water quality for recreation, fishing, hunting, and aesthetic enjoyment. Besides, health problems can occur where eutrophic conditions interfere with drinking water treatment especially in flocculation, filtration and disinfection units (Bartram et al., 1999; Zouabi-Aloui and Gueddari, 2013). Surveys show that 54% of lakes in Asia; 53%; in Europe, 48% in North America; 41% in South America; and 28% in Africa, are eutrophic (ILEC, 1988–1993; Nyenje et al., 2010).

So far, different methods have been proposed to study the eutrophication in aquatic systems. They include simple classification methods (Vollenweider, 1968; Carlson, 1977; Nurnberg, 1996; Dodds et al., 1998) to advanced numerical models based on mass transfer foundations (Kuusisto et al., 1998; Sagehashi et al., 2001; Shukla et al., 2008; Zhang et al., 2008; Deus et al., 2013a; Zouabi-Aloui and Gueddari, 2014). Numerical models can simulate eutrophication in one-dimensional (1D), two-dimensional (2D) and

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http://dx.doi.org/10.1016/j.jhydrol.2015.10.022
0022-1694/

three-dimensional (3D), as required. Numerous investigations have been conducted to model nutrients in reservoirs (Wu et al., 2004; Liu et al., 2006; Mao et al., 2008; He et al., 2011). These studies present important findings about temporal and spatial variations of nutrients in reservoirs. However, when the number of computational grids increases, water quality simulation complexities arise. In other words, managing and processing the spatio-temporal simulated results in a large number of computational grids is very complicated and time consuming due to the huge amount of information generated by numerical calculations during the simulation periods or scenarios.

Representing simulated results by a few state vectors can therefore be an appealing method in this field. Thus, developing a new methodology that represents dominant variations of the system is very important. In fact, providing a reduced-order model (ROM) to condense the simulated results, while maintaining the reliability of findings, is the main objective of this research. For this purpose, connecting simulation models with data reduction techniques is interested. Literature showed that CE-QUAL-W2 (W2), a laterally averaged 2D water quality and hydrodynamic model (Cole and Buchak, 1995) had appropriate performance for water quality modeling in water bodies, especially in reservoirs (Huang and Liu, 2008, 2010; Liu et al., 2009; Dai et al., 2012; Huang, 2014; Chang et al., 2015). Besides, a powerful method of data reduction to obtain a low-dimensional approximate description of high-dimensional processes is proper orthogonal decomposition (POD) (Liang et al., 2002; Smith et al., 2005). Data analysis using POD is conducted to extract a set of basis functions from experimental data or from numerical simulations. These functions are optimal, in the sense that fewer POD modes are required to account for the same amount of "signal energy", compared to any other orthogonal basis. Thus, the POD basis functions are a minimal set of output signals that can be used to identify the dominant energy of the system (Holmes et al., 1996, 1997). POD has been extensively used in fluid mechanics to study turbulent flows and to reduce the degrees-of-freedom of the numerical models (Utturkar et al., 2005; Perrin et al., 2007; Béghein et al., 2014), in the reduction of complex viscous transonic aerodynamic fields inside turbomachinery (Epureanu et al., 2001), and for dynamic studies of structural vibrations (Quaranta et al., 2004; Georgiou, 2005).

In this research, with respect to effects of nitrate on eutrophication problem, this parameter has been simulated in the Karkheh Reservoir located at the Southwest of Iran. Also, reduced-order modeling using POD method is conducted to extract a set of basis functions from numerical simulations by W2 model. Finally, obtained results of ROM have been compared with those of simulator model W2.

2. Study area and data

Karkheh Reservoir, located in the western part of Iran at 32°06′N and 48°08′E and shown in Fig. 1, has been selected to evaluate the models' performance for nitrate simulation. This Reservoir is a multi-purpose dam designed to irrigate agricultural lands, produce hydro-electricity, supply potable water, and prevent downstream floods. The reservoir has a capacity of 5.9 billion cubic meters with an average and maximum depths of 61.8 m and 117 m, respectively. The average annual rainfall, temperature, evaporation, and relative humidity of the Karkheh River Basin are 288 mm, 26 °C, 324 mm, and 67%, respectively. Karkheh Basin is shared between Iran and Iraq, from which 5 million hectares belong to Iran. About 55.5% of this area is located in mountainous region and the rest comprises of plains and mountainsides. Mountainous regions of this basin are mostly concentrated in the middle and eastern parts, while plains are commonly located in the northern and southern parts.

In recent years, the Karkheh Reservoir has faced water quality degradation due to an increase in agricultural and industrial activities in its watershed. One of the most common water quality problems in the reservoir is an increasing trend of algae growth. Based on the available field data and evidence reported by the operators, the reservoir is considered susceptible to nutrient enrichment, because it has been subjected to increased loads from watershed upstream (Afshar and Saadatpour, 2009).

Input data required for simulation of hydrodynamics and nitrate–nitrite parameter using W2 model include bathymetry, daily inflow and outflow quantities, inflow temperatures, water quality parameters (e.g., nitrite, nitrate, ammonia, total nitrogen, phosphate, total phosphorous, chlorophyll-a, dissolved oxygen, total dissolved solids, and total suspended solids) and daily meteorological data (e.g., precipitation, water temperature, air and dew

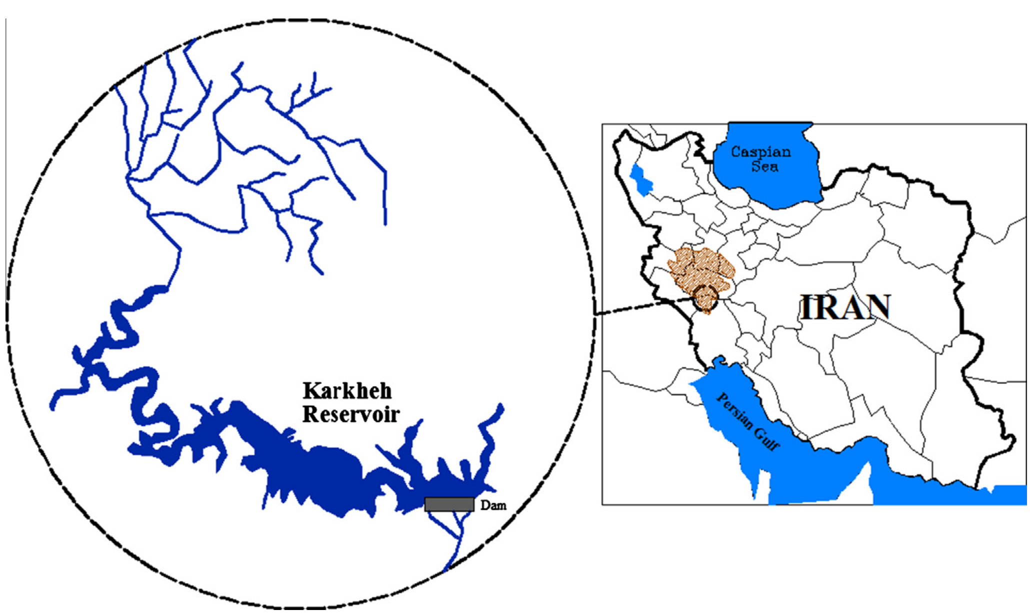

Fig. 1. Location of study area in the west of Iran.