Auto-calibration of a one-dimensional hydrodynamic-ecological model (DYRESM 4.0-CAEDYM 3.1) using a Monte Carlo approach: simulations of hypoxic events in a polymictic lake

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Abstract. Automated calibration of complex deterministic water quality models with a large number of biogeochemical parameters can reduce time-consuming iterative simulations involving empirical judgements of model fit. We undertook auto-calibration of the one-dimensional hydrodynamic-ecological lake model DYRESM-CAEDYM, using a Monte Carlo Sampling (MCS) method, in order to test the applicability of this procedure for shallow, polymictic Lake Rotorua (New Zealand). The calibration procedure involved independently minimising the root-mean-square-error (*RMSE*), maximizing the Pearson correlation coefficient (*r*) and Nash-Sutcliffe efficient coefficient (*Nr*) for comparisons of model state variables against measured data. An assigned number of parameter permutations was used for 10,000 simulation iterations. The 'optimal' temperature calibration produced a *RMSE* of 0.54 °C, *Nr*-value of 0.99 and *r*-value of 0.98 through the whole water column based on comparisons with 540 observed water temperatures collected between 13 July 2007–13 January 2009. The modeled bottom dissolved oxygen concentration (20.5 m below surface) was compared with 467 available observations. The calculated *RMSE* of the simulations compared with the measurements was 1.78 mg L^{-1}, the *Nr*-value was 0.75 and the *r*-value was 0.87. The autocalibrated model was further tested for an independent data set by simulating bottom-water hypoxia events for the period 15 January 2009 to 8 June 2011 (875 days). This verification produced an accurate simulation of five hypoxic events corresponding to DO < 2 mg L^{-1} during summer of 2009–2011. The *RMSE* was 2.07 mg L^{-1}, *Nr*-value 0.62 and *r*-value of 0.81, based on the available data set of 738 days. The auto-calibration software of DYRESM-CAEDYM developed here is substantially less time-consuming and more efficient in parameter optimisation than traditional manual calibration which has been the standard tool practiced for similar complex water quality models.

Key words: Auto-calibration, Monte Carlo sampling, DYRESM-CAEDYM, hypoxia, water quality model

Introduction

Water quality models provide an important framework for scientific assessment to support water quality management decision making (Stow et al., 2007, Schmolke et al., 2010) and test the future climatic impacts on aquatic ecosystems (Elliott, 2012; Tang et al., 2015). They can help in understanding processes operating at a wide variety of temporal and spatial scales, such as the mechanisms contributing to algal blooms, resuspension of sediments, and climate impacts on water quality (Asaeda et al., 2001; Robson & Hamilton, 2004, Chung et al., 2009; Pierson et al., 2013). Process-based water quality models use process representations of the major physical and biogeochemical processes in order to simulate observed data and to forecast changes that may occur under scenarios with changed forcings, for example, altered hydrology or climate (Cox, 2003, Whitehead et al., 2009). There have been many applications of coupled hydrodynamic-ecological models for assessments of surface water quality, including DYRESM-CAEDYM (Han et al., 2000; Asaeda et al, 2001; Copetti et al., 2006; Tanentzap et al., 2008, Takkouk & Casamitjana, 2016), ELCOM-CAEDYM (Vilhena et al., 2010; Chung et al., 2014; Mosley et al., 2015), EFDC (Li et al., 2013a; Alarcon et al., 2014), QUAL2Kw (Pelletier et al., 2006; Kannel et al., 2007a; Marsili-Libelli & Giusti, 2008), PCLake (Hu et al., 2016) and SWAT (Santhi et al., 2001; van Griensven et al., 2002; Jayakrishnan et al., 2005; Heathman et al., 2008). Each of these models requires extensive calibration in order to simulate relevant water quality state variables.

Before the application of any environmental model, it is necessary to conduct parameter sensitivity analysis, calibration and validation before the model can be used as a tool or to set up prognoses for a specific case area (Jorgensen, 1995; Refsgaard et al., 2007). Much of the uncertainty relating to model predictions can be traced back to the assigned values of model parameters and the initial and boundary forcing data. In most model applications, parameters may be arbitrarily chosen within selected ranges, or manually adjusted using laboratory experimental data (Robson & Hamilton, 2004), small-scale field results (Burger et al., 2008, Zhang et al., 2009), modeller experience or reference to values in the literature (Copetti et al., 2006; Kannel et al., 2007b), or mathematical optimization methods (Jackson et al., 2000; Kim & Sheng, 2010; Li et al., 2013b; Liang et al., 2015). The traditional calibration procedure of a stepwise iterative manual adjustment of parameters by the model user is labour intensive and the success of the calibration is strongly dependent on the experience, skill and knowledge of the modeller. The increasing complexity of many water quality models has made manual calibration a significantly more difficult task. Numerous development efforts are on the way to ease the model burden (e.g. adjustment of massive parameters and management of a vast amount of data in heterogeneous computing environments) and offer model development platforms that allow scientists to focus on their science (Fekete et al., 2009). Auto-calibration, which takes advantage of the speed of modern computers while being more objective and potentially increasing the accuracy of model simulations, is an alternative approach (Vrugt et al., 2003, Wu et al., 2014). It can overcome some of the shortcomings of trial-and-error calibration, as noted in a number of case studies (Gan & Biftu, 1996; Solomatine et al., 1999; Madsen, 2000; van Griensven & Bauwens, 2003; Green & van Griensven, 2008; Liu, 2009).

Auto-calibration usually involves automated adjustment of model parameter values in order to find those values that minimize the error between model outputs and observations, represented in terms of single- or multi-objective functions or statistics. The normalized objective functions, with a range from 0–1 (0 being the best and 1 the worst) are minimized by searching for parameter space combinations that give objective functions as close as possible to zero (van Griensven & Bauwens, 2003). This method has been widely used in watershed-runoff simulations (Krajewski, et al., 1991; Madsen, 2000; van Griensven & Bauwens, 2003; Green & van Griensven, 2008) but less frequently for models with many state variables such as water quality or ecosystem models (Rose et al., 2007). An auto-calibration procedure involves a sampling algorithm (e.g., random Monte-Carlo sampling, Latin Hypercube sampling etc.) to define a parameter value from within its defined range, which is based on experimental, field and/or literature values. A search algorithm, which evaluates the objective function, is then typically used to identify optimal parameter values, based on a number of model iterations. This auto-calibration approach can save the modeller time by effectively calibrating models which may have large numbers of parameters. There are numerous approaches to search algorithms that aim to evaluate a parameter space and minimize model error. These include, for example, set coverage techniques, random search methods such as Monte Carlo sampling, probability distribution search algorithms such as Bayesian Monte Carlo (Arhonditsis et al., 2006) or Markov Chain Monte Carlo (MCMC) techniques, multiple local search methods (multi-start) using clustering, simulated annealing, trajectory techniques and tunnelling approaches (Solomatine, 1998; Solomatine et al., 1999).

In complex models with many parameters, there are potentially many "sets" of parameter values that can be manipulated in concert to yield similar model performance (Stow et al., 2007). In environmental systems this problem is known as "equifinality" (Beven & Binley, 1992; Beven, 1993; Beven & Freer, 2001, Beven, 2006, Vrugt et al., 2009a, 2009b; Beven 2009). This phenomenon has been exploited to define a range of model responses, rather than a single solution (Madsen, 2000). With traditional multi-objective optimization, it is well known that a lower value for one optimization function may correspond to an increase of one or more other optimization functions (van Griensven & Bauwens, 2003). As a result, Beven & Binley (1992) advocated a generalised likelihood uncertainty estimation (GLUE) procedure in which model input parameters are randomly selected. This Monte Carlo simulation approach has been increasingly used to obtain parameter values in hydrological models (Seppelt & Voinov, 2002; Refsgaard et al., 2007). Monte Carlo selection of parameters can be readily incorporated into a modelling framework (Hession et al., 1996; van der Perk & Bierkens, 1997; Kannel et al., 2007a) but a large number of simulations and extensive computer storage may be required in order to reliably estimate the probability distribution of model output variables (Refsgaard et al., 2007).

A Monte Carlo simulation method has previously been built into the water quality model QUAL2E for the purpose of assisting with parameter selection (Ng & Perera, 2003) but there have been few other examples of the application of auto-calibration in lake or reservoir water quality models. Because many of these models have a large number of state variables and the algorithms tend to be empirical, based

on biogeochemical rates, there are often a larger number of parameters, especially compared with rainfall-runoff models. Our objective was therefore to use a Monte Carlo approach to develop an auto-calibration procedure for the one-dimensional water quality model DYRESM-CAEDYM, a lake ecosystem model that has been applied to simulate water quality in a large number of lakes and reservoirs (e.g., Hamilton, 1999; Antenucci et al., 2003; Trolle et al., 2008a, 2008b; Cui et al., 2016). We set out to test the performance of this technique using an example of concentrations of dissolved oxygen in bottom waters of a large lake which, because of its eutrophic status and polymictic nature, undergoes large variations in dissolved oxygen that have important ecosystem-wide effects (Burger et al., 2008).

2. Methods

2.1 DYRESM-CAEDYM

DYRESM-CAEDYM was developed at the Centre for Water Research (CWR), University of Western Australia. It couples the one-dimensional hydrodynamic model DYRESM with an aquatic ecology model CAEDYM, thus allowing investigation into the relationships between physical, biological and chemical variables in waterbodies over seasonal and inter-annual timescales. DYRESM divides a lake or reservoir into a series of horizontally-homogeneous Lagrangian layers. The number of layers is determined largely by the resolution required to adequately represent the vertical density gradient. Layer sizes are reduced where the vertical density gradient is greatest. Layers can also expand or contract in response to inflows or outflows, and mixing is accomplished by amalgamation of adjacent layers (Hamilton & Schladow, 1995). CAEDYM comprises subroutines for phytoplankton production and loss, nutrient cycling and dissolved oxygen dynamics (Hamilton & Schladow, 1997). It can simulate up to seven phytoplankton groups, dissolved oxygen (DO), and nutrient concentrations using a series of partial differential equations that include different biogeochemical rate constants (Robson & Hamilton, 2004). The bottom sediment is characterised in the model as a permanent sink for particulate matter that settles out of the water column, with releases of dissolved nutrients from the sediments prescribed from overlying water column properties (Burger et al., 2008). Makler-Pick et al. (2011) has developed a sensitivity analysis approach for this coupled model but there are few reports about automatic calibration software for this model. More detailed information about DYRESM-CAEDYM is given in Hamilton & Schladow (1997), Romero et al. (2004) and applications (Trolle et al., 2008a, 2008b; Gal et al., 2014; Cui et al., 2016).

2.2 Dissolved oxygen module

In CAEDYM, the algorithms that affect DO relate to air-water fluxes, sediment oxygen demand (SOD), microbial uptake during organic matter mineralization and nitrification, oxygen production and respiration by primary producers (e.g., phytoplankton), and respiration by other optional biotic components (Hipsey et al., 2007). The air-water DO flux is calculated using the model of Wanninkhof (1992) and the flux equation of Riley & Skirrow (1974). SOD is represented by a function that varies the rate with overlying water temperature and DO concentration. Removal of DO is by microbial

activity, including mineralisation of organic matter and nitrification, as well as phytoplankton respiration. Fig. 1 shows a schematic for the DO flux paths in CAEDYM.

Insert Fig. 1 here

2.3 Data collection

A water quality and meteorological monitoring buoy was installed in Lake Rotorua, New Zealand, near the deep central part (38°04′32.7″S, 176°16′01.88″E) in July 2007. Lake Rotorua is a shallow, eutrophic lake with area 80 km^2 and mean depth 10.8 m. The buoy transmits in near real-time data collected at 15-minute intervals for a range of variables encompassing meteorology (wind speed and direction, air temperature, relative humidity, barometric pressure, precipitation) and water quality (surface and bottom DO concentration and percentage saturation, surface chlorophyll fluorescence, and water temperature at 2 m intervals over the 21 m water depth where the buoy is located). The data are telemetered to an on-line database by GRPS modem. Short-wave solar radiation was measured at a weather station near the lake edge. All sensors were calibrated regularly for quality assurance. The quarter-hourly data were aggregated to hourly and daily time-steps prior to analysis, in order to smooth some of the unexplained instantaneous anomalies that can sometimes occur with in situ optical instrumentation. In addition, total phosphorus and total nitrogen concentrations were measured monthly at two depths (1 meter and 19 meters below surface) near the lake buoy station.

2.4 Auto-calibration procedure for DYRESM-CAEDYM

The auto-calibration model was implemented by following a number of steps. First, the modeller chooses a fixed simulation period when all the data required by the model were collected (i.e. the initial water quality data at the beginning of simulation, inflows, outflows and meteorological data during the whole period). The time step was set to be 3600 seconds for the numerical integration in all simulations. Then all physical and biogeochemical parameters were fixed in their respective input files. When the model output was not sensitive to the parameter judged by experience or when fixed parameter values could be used (e.g., stoichiometric parameters), the minimum and maximum value were set to be equal and the parameter calibration was deemed unnecessary. A random search module was then run for all remaining parameters to produce files with combinations of parameters which could then be used to generate independent runs of the DYRESM hydrodynamic module. Simulations of water temperature extracted from the output file (DYsim.nc) were then compared with temperatures measured at corresponding depths and times. A physical parameter set was then chosen automatically based on minimising the *RMSE* in comparisons between simulations and observations (Tab. 1). An alternative approach is to enter the physical parameters manually as many of these parameters can be fixed on the basis of their theoretically constrained values. We used a total of 10,000 iterations to choose the best-fit of the physical parameter set. The DYRESM-CAEDYM model was then run with the selected physical parameters and a set of water quality parameters chosen from the MCS procedure with the same number of iterations. The root mean square error (*RMSE*) was estimated for comparisons of simulations and observations for the variables chlorophyll *a* and DO. The combined *RMSE* is the

sum of *RMSEs* for chlorophyll *a* and DO with each *RMSE* multiplied by an arbitrarily chosen weighing factor varying from 0 to 1. The four DYRESM-CAEDYM parameter files (par, bio, chm and sed) were chosen which minimised the combined *RMSE* of these variables with corresponding weighing factors between the model simulations and measured values.

2.5 Statistical evaluation methods for the auto-calibrated model

The accuracy of the auto-calibrated model was tested by *RMSE*, Nash-Sutcliffe efficient coefficient (*Nr*) and Pearson correlation coefficient (*r*) as follows:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(S_i - O_i)^2}$$

$$N_r = 1 - \frac{\sum_{i=1}^{N}(S_i - O_i)^2}{\sum_{i=1}^{N}(O_i - \overline{O_i})^2}$$

$$r = \frac{\sum_{i=1}^{N}(O_i - \overline{O_i})(S_i - \overline{S_i})}{\sqrt{\sum_{i=1}^{N}(O_i - \overline{O_i})^2 (S_i - \overline{S_i})^2}}$$

where O_i is the measured value, S_i is the simulated value, $\overline{O_i}$ is the average of measured values, $\overline{S_i}$ is the average of simulated values and N is the total number of observations. N_r is known as the modelling efficiency and can be negative or positive. A positive value indicates that the simulations describe the trend of measurements better than the mean of observations and a negative value shows the opposite. The maximum value of N_r is 1.0, which means the model fits the observed values exactly. The subscript *i* for *O* and *S* represents the serial number of observations and simulations which are used for the statistical analysis. The objective of the auto-calibration procedure was to minimize the *RMSE* values and maximize N_r and *r*-values. One of these three parameters or a combined value of them can be chosen for obtaining the serial number of the iteration that produces the 'best' simulation.

We used the period 13 Jul. 2007–13 Jan. 2009 (551 days) for model calibration, and validated the calibrated model using data from the period 15 Jan. 2009–8 Jun. 2011 (875 days)

3. Results

3.1 Physical parameter set selection

Tab. 1 shows the set of physical parameters that minimised the *RMSE* for temperature over the 10,000 model runs. A comparison of simulated and observed water temperature is shown in Fig. 2.

Insert Tab. 1 here

Insert Fig. 2 here

The water temperature simulations agreed well with observed values at all 11 observed depths (0.5 m to 20.5 m at intervals of 2 m), and captured dynamic nature of lake mixing, which in Lake Rotorua is characterised by occasional periods of stratification in which there are vertical temperature gradients interspersed with little or no temperature gradient when the lake is vertically mixed (Read et al., 2011). The Pearson correlation coefficient (r) between model output and measured temperature over all depths exceeded 0.98 with a *RMSE* of < 0.71 °C (Tab. 2). The *RMSE* was lowest at a depth of 6.5 m (0.44 °C) of all of the observed depths, and the r value was also greatest and N_r closest to 1.0 at this depth. The accuracy of simulations of bottom water temperature were not generally as accurate (in terms of *RMSE*, r and N_r statistics) as for surface water temperature, but the ability of the model to capture the timing, frequency and duration of stratification events (Fig. 2) was considered acceptable as a basis to carry out simulations of water quality by coupling DYRESM with CAEDYM.

Insert Tab. 2 here

3.2 Hypoxia simulation

3.2.1 Auto-calibration

In CAEDYM, the most sensitive parameters in the DO simulation are the sediment oxygen demand and half saturation constant for DO consumption, DO production through phytoplankton photosynthesis, and DO consumption through respiration of phytoplankton, mineralisation of organic matter, nitrification and denitrification. These processes are represented schematically in the CAEDYM configuration shown in Fig. 1. From a total of 10,000 simulations of the DYRESM-CAEDYM model with different input parameters it was possible to identify the parameter data set with the minimum value of *RMSE* to obtain the best match to observed values of DO. The values of the optimized parameters are shown in Tab. 3 and the hypoxia simulation results, represented by concentrations of DO, are shown in Fig. 3.

Insert Tab. 3 here

Insert Fig. 3 here

During the simulation period, there were five separate DO depletion events (DO < 4 mg L^{-1}) observed in the bottom waters. The first occurred during 7 Sep–1 Oct 2007 with minimum DO of 3.95 mg L^{-1} (simulation 2.46 mg L^{-1}) on 24 Sep (Julian day 267). The second and third events were observed in summer 2008, specifically 7 Jan 2008–10 Feb 2008 and 17 Mar–3 Apr 2008. The lowest DO (observation 0.21 mg L^{-1} and simulation 0.36 mg L^{-1}) for the second event occurred on 18 Jan 2008 and for the third event on 31 Mar 2008 (0.19 mg L^{-1} and simulation 0.89 mg L^{-1}). The fourth and fifth events were recorded in summer of 2009 with a minimum value of 0.72 mg L^{-1} (simulation 0.84 mg L^{-1}) on 10 Dec 2008 and 0.5 mg L^{-1} (simulation 1.6 mg L^{-1}) on 11 Jan 2009. All five bottom DO depletion

events were captured with the DYRESM-CAEDYM model simulations, although the simulated trough (minima) of the first event was slightly below the observed values while all the other troughs exceeded the observations. Statistical tests to relate simulated and observed values over the entire simulation period gave a *RMSE* of 1.78 mg L^{-1}, *r* of 0.87 and N_r of 0.75 (*N*=467). The simulations well reflected the variation pattern of time-serial measurements with slightly oscillated gap in winter and early autumn of 2008 (Julian day from 170 to 309). There was a small DO depletion event during 18 September 2008 (Julian day 262)–3 October 2008 (Julian day 277), which was not captured by the model with the average value of DO (11.90 mg L^{-1}) higher than the average observation value (8.40 mg L^{-1}) by 3.5 mg L^{-1}.

3.2.2 Model validation

The recorded bottom DO data from 15 January 2009 to 8 June 2011 (875 days) were used for model validation with the selected parameter set from the auto-calibration process. The model captured all five hypoxic events with DO < 2 mg L^{-1} measured during 31 January 2009–21 February 2010, 12 February–25 March 2010, 2–24 December 2010, 9–17 January 2011 and 16 February –1 March 2011, with a *RMSE* of 2.07 mg L^{-1}, *Nr*-value of 0.62 and *r*-value of 0.81 (*N*=738, Fig. 4). There was only one hypoxic event induced by intense stratification in each summer of 2009 and 2010, while three events were observed in the summer of 2011. In all cases, DO concentrations were < 0.7 mg L^{-1} during these events. The pattern of variation during these events was well reproduced by the model with the auto-calibration parameter set although there were still minor differences between the absolute values for simulations and observations.

4. Discussion

The DO capacity of water is greatly affected by temperature but the distribution of DO in the water column is also strongly influenced by water column stratification, which in Lake Rotorua is controlled by variations in water density as water heats and cools. Therefore, to be able to simulate accurately the DO concentrations, it is necessary to choose a model of lake physical processes which accurately simulates water temperature dynamics, as shown with DYRESM model simulations in this study. The temperature profiles were well reproduced by the model although there was water loss reflected by water level decrease in the model by almost half meter in the January and February of 2008. The water loss probably resulted from the inflows/outflows boundary conditions which were induced by a catchment model.

Compared to the previous model parameter values reported by Burger et al. (2008), the value for water albedo yielded by the auto-calibration was somewhat higher (0.084 compared to 0.07 in Burger et al., 2008), but water surface emissivity (0.94 in this work and 0.96 reported by Burger et al. (2008)) was very similar. Thus our auto-calibration procedure results in slightly less total solar energy received by the lake. Albedo at the water surface is one of the key parameters affecting the water heat budget in DYRESM. Nunez (1972) found that on a daily basis, albedo ranged between 0.07 in early July to 0.11 in mid–November for Lake Ontario, North America, and that surface waves increase the value of

direct-beam albedo, particularly at higher solar zenith angles. Albedo varies according to latitude and season, so some physical parameters may continue to require some flexibility in their values as long as there is not a complete process representation for them. There are five parameters related to vertical mixing in DYRESM: critical wind speed, potential energy mixing efficiency, shear production efficiency, wind stirring efficiency and the vertical mixing coefficient. Their values, as selected by auto-calibration were 6.5 m s^{-1}, 0.29, 0.084, 0.29 and 305.5, while they were given by Burger et al. (2008) as 4.0 m s^{-1}, 0.25, 0.08, 0.6 and 400 based on trial-and-error calibration within the parameter limits (Yeates and Imberger, 2003). Statistical tests showed that *RMSE* values between simulated and observed water temperatures for the upper mixed layer (0.48 ºC, 0–9 m) and the bottom layer (0.61 ºC, 19.0 m) using our auto-calibration approach were smaller than those reported by Burger et al. (2008) (0.97 ºC for the surface-mixed layer and 0.88 ºC for the bottom waters for a calibration period, and 0.86 ºC and 0.67 ºC, respectively, for the validation period). Therefore, auto-calibration of DYRESM water temperature appears to be a useful tool to improve simulation accuracy for Lake Rotorua and potentially for other lakes.

Simulated bottom DO represented observations well in the calibration process, as it correctly captured the occurrence of five DO depletion events for bottom waters. One of the most sensitive parameters for DO simulations in bottom waters is sediment oxygen demand (SOD, g m^{-2} d^{-1}). It varies as a function of the overlying water temperature and dissolved oxygen levels in CAEDYM but, as noted by Burger et al. (2008), it does not account for variations contributed by the dynamic nature of sediment composition (e.g. increased organic deposition following algal blooms). The SOD selected by auto-calibration was 8.08 g m^{-2} d^{-1} in this study, which is greater than values selected for modelling a eutrophic estuary in Western Australia (6.0 g m^{-2} d^{-1}; Robson and Hamilton, 2004), Tolo Harbour in Hong Kong (0.4–1.3 g m^{-2} d^{-1}, Hu et al., 2001), shallow eutrophic Lake Alsdorf in Germany (1.5 g m^{-2} d^{-1}, Strauss & Ratte, 2002) and Lake Onondaga in New York (1.68 g m^{-2} d^{-1}, Gelda et al., 1995), but in the range of 0.34–9.02 g m^{-2} d^{-1} measured in the five southwestern lakes of USA by Veenstra and Nolen (1991). Sources of SOD may be divided into three basic categories: 1) microbial oxygen demand (bacteria, protozoa); 2) macrofaunal oxygen demand (primarily tubificid oligochaetes and insect larvae); and 3) chemical oxygen demand by inorganic oxidation of reduced chemical compounds (Finkelstein & McCall, 1981). Due to these varied influences, SOD can vary widely over time and space, both within and between lakes. For example, SOD in Lake Rotorua has been measured at values from 0.3 g m^{-2} d^{-1} (site 2, Aug 2003) to 4.0 g m^{-2} d^{-1} (site 3, Nov 2003, Burger et al., 2008). A value of 2.8 g m^{-2} d^{-1} was used for DO simulations with DYRESM-CAEDYM by Burger et al. (2008). In five southwestern U.S. lakes (Broken Bow, Texoma, Birch, Pine Creek, and Pat Mayse) SOD ranged from 0.34 to 9.02 g m^{-2} d^{-1}, after correction for temperature (Veenstra & Nolen, 1991). This parameter is mostly dependent on sediment components (i.e. organic matter, bacterial activity, and benthic fauna) and the overlying water environment (water temperature, underwater light and vertical mixing), which will vary over seasons and locations in a specific lake.

Monte Carlo methods are generally preferred and more widely used for parameter estimation in environmental models than first-order variance propagation (Hession et al., 1996). Monte Carlo-based approaches continue to evolve and include Bayesian Monte Carlo (BMC, Dilks et al., 1992; Bergin & Milford, 2000), Markov Chain Monte Carlo (MCMC, Gelfand & Smith, 1990; Gelfand et al., 1990; Zobitz et al., 2011) and GLUE techniques (Beven & Binley, 1992; Vrugt et al., 2009a, 2009b). Among these methods, the Monte Carlo sampling is a general approach and assumes no structure associated with model error. It often serves as a screening approach to identify plausible regions of model parameter values (Stow et al., 2007). The BMC is based on MCS but with assumptions about model error structure to delimit plausible parameter regions (Stow et al., 2007). The main problem with this technique is that it does not converge toward the most probable region of the posterior distribution and can be extremely inefficient, rarely sampling from the most probable region (Qian et al., 2003). This problem is likely to be exacerbated when there are wide parameter ranges designated to include all possible values but this may miss the important region of the posterior distribution in the Monte Carlo sample (Qian et al, 2003). GLUE is similar to BMC but permits a broader range of functions that define the model error structure (Stow et al., 2007). MCMC is specifically designed to sample from the posterior distribution in order to eliminate these problems and is regarded as one of the most efficient approaches for parameter sampling (Stow et al., 2007). It has been integrated into some auto-calibration tools such as the shuffled complex evolution (SCE-UA, Duan et al., 1992; 1993), the shuffled complex evolution metropolis algorithm (SCEM-UA, Vrugt et al., 2003) and WinBUGS (Gilks et al., 1994). This method requires an appropriate algorithm dependent on the model form and a choice of distributional structure appropriate to represent the stochastic terms (Stow et al., 2007). A poor choice of the proposed distribution of parameters will result in slow convergence of the Markov Chain (Vrugt et al., 2003).

Random Monte Carlo simulation, as adopted in our study, has the advantage of being easily incorporated into model code and programming, and can also include adequate consideration of "equifinality" of water quality models with large sets of parameters, without the need for the user to make assumptions regarding parameter distributions (as a simple uniform parameter distribution within the defined range is used). However, the success of parameter value selection is closely related to the user-defined upper and lower ranges of key parameters, and the number of iterations performed. The number of simulations should be sufficiently large to reliably estimate the probability distribution of the output variables. Although a lot of hard disk space is required for saving stochastically produced parameter files, this is a progressively lesser concern due to the increased availability and reduced cost of storage space. An approach for reducing required hard drive space is to conduct a comparison between model outputs and measurements in terms of pre-defined statistical parameters for error evaluation after each model run, then sort all the iteration errors and save the parameter files with which the errors between simulations and observations are smaller than an arbitrarily-chosen threshold value of error. Sensitivity analysis might be an alternative option for reduction of required space for parameter file storage and to achieve an increase in model run-time speeds, since only the most sensitive parameters will be considered to change in the model auto-calibration process.

Auto-calibration tools have been widely used in watershed-runoff models but have had limited application to water quality models. This paper has detailed our prototype for an auto-calibration tool for the widely used DYRESM-CAEDYM model. The success of its application is strongly dependent on prior knowledge about parameter value ranges, the number of iterations performed which is closely related to the computer's performance capability and the accuracy of observations, but it has great potential to reduce the repetitive model iterations that are required using traditional trial-and-error calibration. Sub-modules for analysis of parameter sensitivity and model uncertainty could be included in further developments of the auto-calibration approach in order to decide the most appropriate model parameters (on a case-by-case basis) to be used during calibration and thereby increase performance and reduce computation consumption.

5. Conclusions

1. MCS is an effective method for calibration of a dynamic water quality model with a massive number of parameters and equifinality to find an optimized parameter set in a complex environmental system although it requires robust hardware.

2. For most of model users, the auto-calibration software of DYRESM-CAEDYM developed in this paper is substantially less time-consuming and more efficient in parameter optimisation than conventional manual calibration procedure which has been the standard tool practiced for similar complex water quality models.

Code and/or data availability

The code for the automatic calibration of DYRESM-CAEDYM is available at the supplements. The DYRESM-CAEDYM model is available from (http://www.hydronumerics.com.au/software/aquatic-ecosystem-model-3d).

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Table captions

Tab. 1 Selected physical parameters used in DYRESM based on autocalibration from 10,000 iterations.

Tab. 2 Statistical results (*RMSE, Nr* and *r* value) between simulations and observations of water temperature at different depths from 0.5 m to 20.5 m at intervals of 2 m. The sample number is 436 for the bottom layer (depth 20.5 m) and 510 for all other layers.

Tab. 3 Values of key parameters for DO production and consumption in DYRESM-CAEDYM, chosen through auto-calibration.

Tab. 1 Autocalibration-chosen physical parameters used in DYRESM with 10,000 iterations.

Parameter	Value
Bulk aerodynamic momentum transport coefficient	0.00135
Albedo of water	0.084
Emissivity of water surface	0.94
Critical wind speed (m s^{-1})	6.5
Shear production efficiency	0.084
Potential energy mixing efficiency	0.29
Wind stirring efficiency	0.29
Effective surface area coefficient	1.27 x 10^{7}
BBL dissipation coefficient	0.0
Vertical mixing coefficient	305.5

Tab. 2 Statistical results (*RMSE, Nr* and *r* value) between simulations and observations of water temperature at different depths from 0.5 m to 20.5 m at intervals of 2 m. The sample number is 436 for the bottom layer (depth 20.5 m) and 510 for all other layers.

Depth (m)	RMSE	*Nr*	r
0.5	0.529	0.985	0.994
2.5	0.462	0.989	0.995
4.5	0.510	0.986	0.995
6.5	0.435	0.990	0.995
8.5	0.471	0.988	0.995
10.5	0.555	0.983	0.994
12.5	0.610	0.979	0.992
14.5	0.529	0.983	0.992
16.5	0.553	0.981	0.991
18.5	0.606	0.977	0.989
20.5	0.703	0.966	0.984

Tab. 3 Values of key parameters related to DO production and consumption in DYRESM-CAEDYM, chosen through auto-calibration.

Parameter	Value
Static sediment oxygen demand (SOD, g m^{-2} d^{-1})	8.08
Half-saturation constant for sediment DO flux (mg O L^{-1})	3.38
Denitrification rate coefficient (day^{-1})	0.588
Nitrification rate coefficient (day^{-1})	0.0144
Maximum potential growth rate of cyanobacteria (day^{-1})	0.588
Maximum potential growth rate of diatoms (day^{-1})	1.194
Respiration, mortality and excretion parameter for cyanobacteria (day^{-1})	0.0788
Respiration mortality and excretion parameter for diatoms (day^{-1})	0.138

Figure captions

Fig. 1 Schematic of dissolved oxygen dynamics in CAEDYM.

Fig. 2 Comparison of observed (top) and simulated (bottom) water column temperature based on daily data from 13 Jul. 2007–13 Jan. 2009.

Fig. 3 Model auto-calibration with comparison of daily bottom DO between simulations (grey dots) and observations (black dots) for depth of 20.5 m from 13 Jul. 2007–13 Jan. 2009 (551 days). The X-axis represents time in the format of mm/dd/yy and the Y-axis represents DO concentrations (unit: mg L^{-1}).

Fig. 4 Model verification with comparison of daily bottom DO between simulations (grey dots) and observations (black dots) at depth of 20.5 m from 15 Jan. 2009–8 Jun. 2011 (875 days). The X-axis represents time in the format of mm/dd/yy and the Y-axis represents DO concentrations (unit: mg L^{-1}).

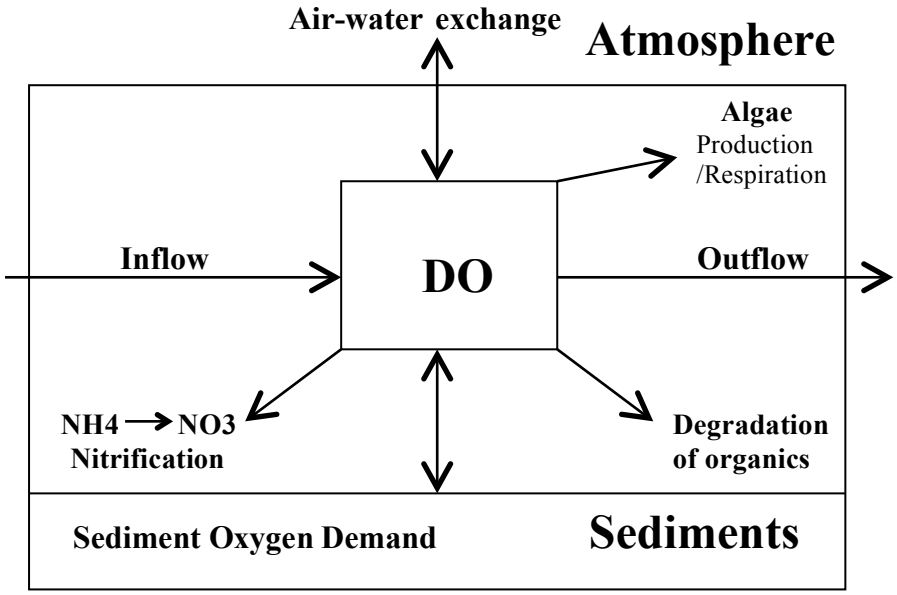
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Fig. 1

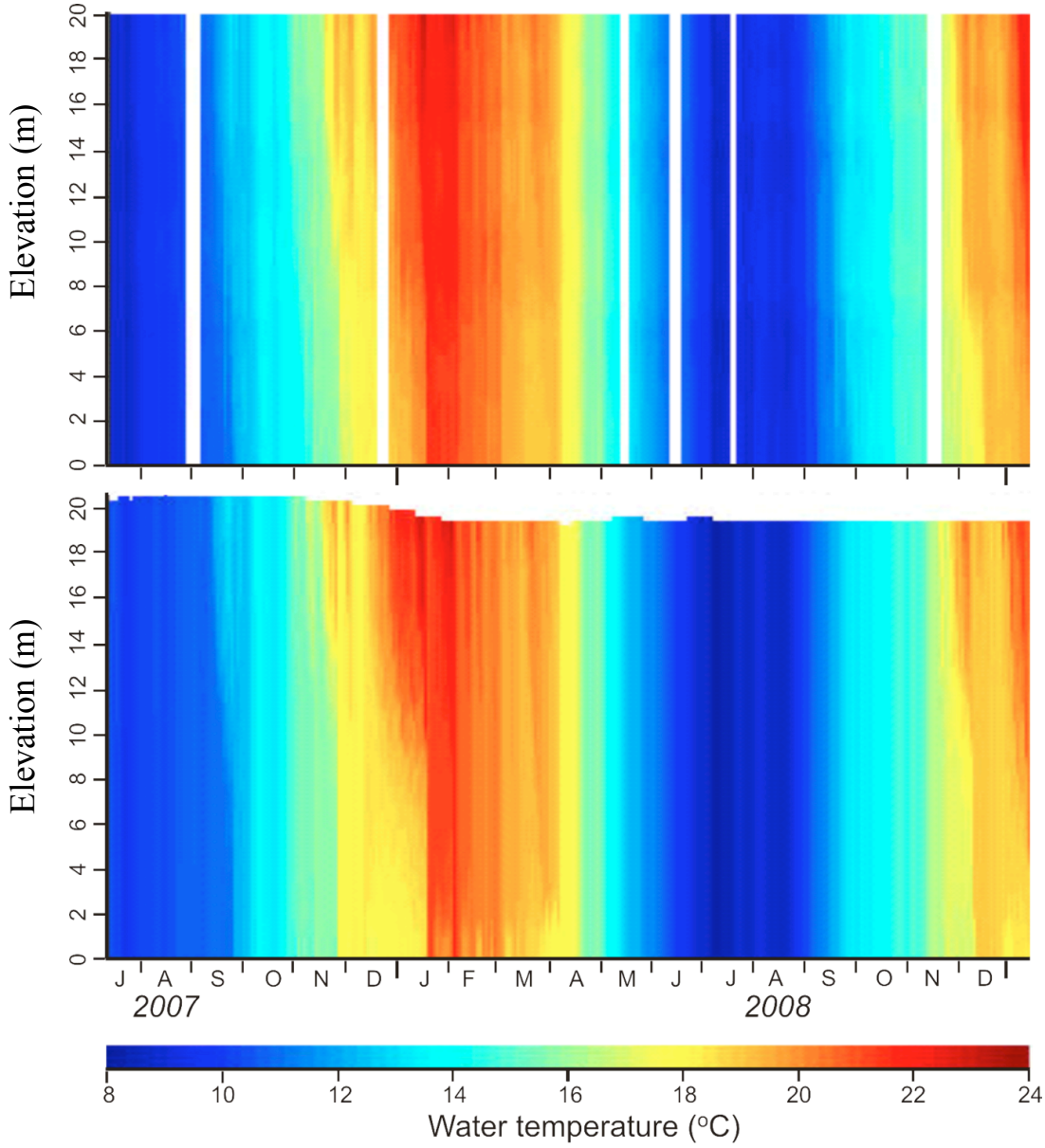
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Fig. 2

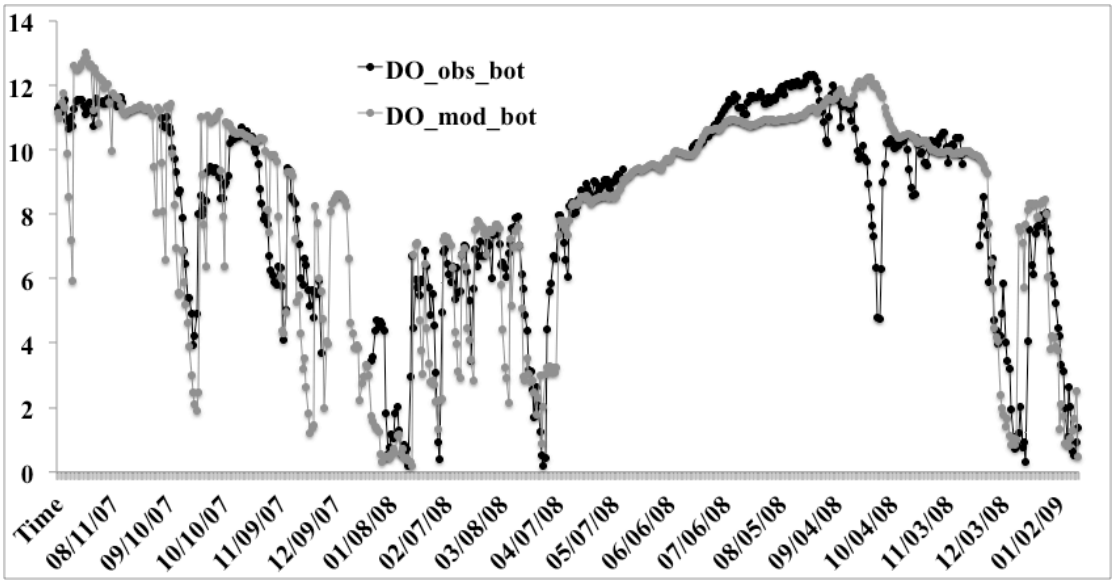
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Fig. 3

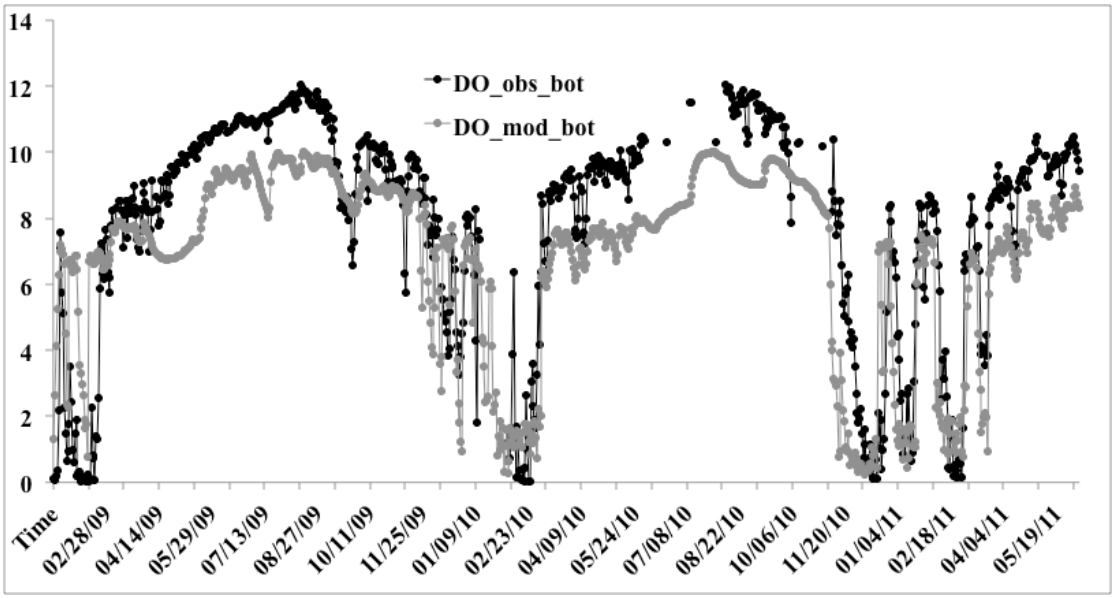
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Fig. 4