Review 1

This paper uses a Monte Carlo Sampling (MCS) method to auto-calibrate a hydrodynamic ecological model. This is perhaps the first application of MCS method for auto-calibration a hydrodynamic lake ecosystem model, and thus, the study is providing new concepts/methods. The paper is well organized, and the methods are valid, as backed up by their use in the calibration of other types of models. The results are discussed in an appropriate and balanced way, the discussion comparison to the Burger et al (2008) paper is very useful for putting this method in context. The method presented definitely has the potential to lead to significant scientific results. For example, if future use of hydrodynamic ecological models are able to incorporate these methods, the researchers can spend more time doing the science instead of tedious trial-and-error calibration. A very valuable part of the paper will be the code for auto-calibration, so that other researchers may modify to fit their own needs and application. There are a few areas that need more explanation (see "specific comments" below) in addition to some typing errors (see "technical corrections" below).

Specific Comments

5:21 how was it determined that the model output was not sensitive to the parameter? Please describe with at least a little more detail in the text. What is the threshold you used for if a parameter is sensitive or not?

Response (now 5:25-5:27)

Thanks for the nice comments.

There are many parameters which are not necessary to change in the calibration. For example, the density of suspended solid particles is normally set to be 2.65×10^3 *kg/m*^{3} *for all the types of sediment with difference size. So we might set "2.65E+03 2.65E+03" in the sediment parameter file and the same with diameters of POM1 and POM2 particles in the chemical parameter file. Also the same way will be used for many other similar parameters. The model users can decide which parameter needs to be changed during calibration by their experience or set the value range for every parameter if they are not able to judge. All the stoichiometric parameters will have fixed value so they have the same minimum and maximum values.*

Change in the text:

"judged by experience" has been added at the end of "When the model output was not sensitive to the parameter" at 5:27 in the text.

5: 27 "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."

Why do you provide the alternative approach here? This statement sounds more appropriate for the introduction or discussion. Are you saying the auto-calibration isn't really necessary for the physical parameters? Please explain more, or move to intro/discussion.

Response (now 5:35-5:36):

Sorry for the confusion and thanks for the excellent comments.

In the DYRESM-CAEDYM model, there are physical (par), biological (bio), chemical (chm) and sediment (sed) parameter files. It is actually very easy to calibrate the physical parameters for a experienced model user and the model outputs are still very good even all the physical parameters are set to be the default value from the sample files previously downloaded from CWR website. So it is not necessary to calibrate the physical parameters if the model user can easily get their suitable value based on comparison of observed and modeled temperatures. There is a switch for each parameter file (i.e. par, bio, chm and sed) in the configure file to tell the model to calibrate the parameters in this file or not. For a beginner, I would suggest all the four files be included for calibration. This description is part of auto-calibration procedure so I would keep it at the same place.

No change in the text.

5:35 What were the weighing factors? What where they based on? (then possibly in Discussion: Would your results change if the weighing factors were different?)

Response (now 6:1):

*For each variable, a RMSE value can be calculated based on the simulations and observations from the equation at "**2.5 Statistical evaluation methods for the auto-calibrated model**". The combined RMSE is the sum of each variable-specific RMSE multiplied by a weighing factor from 0 to 1. So if the model users might choose "0" as the weighing factor for a variable if they don't want to calibrate parameters for this variable or choose a comparatively smaller weighing factor (e.g. 0.2) if they think this variable is less important than the other ones. Otherwise they might choose "1" for all the variables if they are equally important.*

Change in the text (5:39 – 6:2)

"The root mean square error (RMSE) was estimated for comparisons of simulations and observations for the variables chlorophyll a and DO." has been changed to "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."

5:22 Table 3 has a stoichiometric parameter (Stoichiometric ratio of C to O2 for respiration); yet on line 5:21-23 you state: "When the model output was not sensitive to the parameter 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." Can you explain why you calibrated this particular stoichiometric parameter in your method? Or, be more clear about for which parameters calibration is not necessary. Can you provide a table of all parameters (including ones that were not auto-calibrated) in the supplementary document? Useful columns would be: parameter name and unit, parameter value, indication of if the parameter was auto-calibrated or not, if parameter was not auto-calibrated provide a very brief description of why parameter was not auto-calibrated (e.g. deemed not sensitive in sensitivity analysis, fixed parameter based on literature/theory/etc.)

Response (now 5:27):

Thanks for the nice comments. All the stoichiometric parameters shouldn't be calibrated but they still need to set a minimum and maximum values (the same value) because the software has to read the two values for each parameter. In this case study, we set up a very small range (2.6 - 2.7) for stoichiometric ratio of C to O_2 for respiration to check if the model outputs are sensitive to this parameter. We have found the model results were the same with the stoichiometric value of 2.66667 and MCS-generated value 2.69 in this paper. So the stoichiometric value should be used for DYRESM-CAEDYM and we have deleted the revelent information in Table 3. As required by the anonymous reviewer, the parameters which were calibrated in this case study was shown in the supplement table. There are still some parameters which were not calibrated but can be calibrated with a minimum value and a maximum value to be set up because I though they might be constant (e.g. diameter and density of different type of sediments).

11:5 Change "massive parameters" to "a massive number of parameters" and maybe replace "massive" with a more quantifiable measure? Also: change "dynamic water quality model" to either "a dynamic water quality model" or "dynamic water quality models." Also: add "calibration of" to ". . .effective method for [calibration of] dynamic water. . ."

Response (now 11:14):

Thanks for the nice comments. "massive parameters" has been replaced by "a massive number of parameters" at 11:14. It is difficult to quantify the exact number of all the parameters which need to be calibrated for me because different model user might have different opinion on how many parameters need to be calibrated. So the exact number might depend on the experience of model user. CAEDYM model has 4 parameter files (par,

chm, bio, sed) including more than 300 parameters. So I would use "a massive number of parameters" in the text.

"dynamic water quality model" has been changed to "calibration of a dynamic water quality model" at 11:14.

11:9 Did you quantify the "time-consuming" part of this conclusion? Perhaps be a bit more descriptive in the extent to which you know it is in fact

Technical Corrections

Equation 1 and 2 have an undefined Q variable.

Figure 2 needs a color ramp scale/legend

Figure 1 is referred to in text as "Figure 1" whereas Figure 2 is referred to in text as "Fig. 2" –should be consistent in abbreviating or not with in text figure references.

Response (now 11:18):

Thanks for the nice comments.

We were not quantify the "time-consuming" part of the conclusion" since we didn't take any comparison. However, it might be actually more time-consuming for most of model users to calibrate so many parameters using conventional method than using this auto-calibration software. However, some experts might manually calibrate the parameters with less time than this software running time. So we added "For most of the model users" at the beginning of this conclusion at 11:17.

The variable O_i *has been defined below the equations.*

Color scale has been added to fig.2.

All the "figure" has been referred to "fig." in the text.

Review 2

As someone who has used coupled hydrodynamic - ecosystem water quality models (including previous versions of DYRESM and CAEDYM) to provide science information for assisting lake managers in making decisions, I welcome this contribution by Luo et al. Aside from potentially making calibration of complex water quality models more efficient, it makes calibration less subjective , which ultimately adds to the credibility of model results . This paper describes a tool that is shown to be efficient and effective, producing convincing results in a well - documented case study. I found the paper to be clearly written, concise and well - focused, with good descriptions of technical aspects the optimization technique and associated statistics, and of the lake processes associated with the case study.

I found the literature review in the introduction to be comprehensive and helpful, in its coverage of both water quality models and optimization methods used for model calibration, and in its description of the strengths and weaknesses of the various optimization methods . I thought the authors satisfactorily explained the reasons for their choice of MCS as an appropriate method for their DYRESM - CAEDYM applications. I agree with the authors' observation that, compared with rainfall - runoff models, there are very few examples in the literature that describe optimization methods for calibration of complex water models that contain large number s of parameters and state variables for empirical algorithms based on biogeochemical rates – hence the need for studies like the one presented here.

I felt that the restriction of the optimization application to simulation of dissolved oxygen and prediction of hypoxic events was sensible in this prototype stage of development for an auto - calibration tool. In practice, however, phytoplankton productivity and biomass, chlorophyll - *a* concentrations, and nitrogen and phosphorus dynamics are often the ultimate focus of interest in water quality modelling. These latter processes and variables are accounted for in the present work in terms of the parameters listed in Table 3, but only as they affect oxygen concentrations, not measures of chlorophyll, nitrogen or phosphorus.

I wonder if the authors would care to comment (or speculate) briefly on the possible future development and applications of their auto - calibration approach to cases where it is important not only to model oxygen dynamics reliably, but also to predict one or more other measures of chlorophyll, nitrogen and /or phosphorus concentration. For example, how many other parameters would this bring into the auto - calibration process? Is there a number beyond which the procedure would not perform satisfactorily? How could the approach be extended if there were more than one variable (oxygen or temperature in the present work) of major concern in a given optimization run? Would the user have to be content with choosing the single most important variable to optimize on? Would a stepwise approach, such as described here for first optimizing temperature prediction, then oxygen dynamics, be appropriate? I realize that this is complicated by the fact that many of the same parameters that affect oxygen prediction also affect chlorophyll, nitrogen and phosphorus concentrations. This is in contrast to the application presented in the paper where the two sets of parameters (one set for temperature, another for oxygen) are independent of each other. Perhaps an iterative strategy could be used? Or does that defeat the purpose of auto - calibration in terms of reducing time - consuming iterative procedures?

I felt that the authors' comment at the bottom of page 10 regarding the value of their approach, as qualified by the need for experience, knowledge and expertise with the water quality model; the lake processes concerned; and the accuracy of the field data available for calibration – provided a fair assessment of both the contribution and

limitation of their work: " The success of its [the auto - calibration ' s] 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. "

Response:

Thanks a lot for the very valuable comments. Our answers are briefly listed below:

This auto-calibration software can be used for all the water quality variables included in the CAEDYM model (e.g. TP, TN, NO3, NH4, PO4, CHLA). The only thing needs to do for that is set up all the variable information in the configure file, for example, the number of variables, variable names, the observation length of variables, and the weighting factor for each variable. The statistical assessment parameter (e.g. RMSE) will be the sum of RMSE multiplied by the weighting factor for each variable. In this paper, we just presented a DO case study to show the procedure for how the software works.

There is a switch (1 or 0) for calibrating the physical (par), chemical (chm), biological (bio) and sediment (sed) process or not. The model user can choose which file parameters need to be calibrated or not or he/she can choose all the files for calibration with switch 1 for each file.

It is true that the success of this software's 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. The parameter value ranges can be mostly found from related literatures. The more iterations, the more possibility to find the "optimized" parameter set. The same with the accuracy of observations.

Specific comments (mostly relating to questions of clarification)

Page 5, Auto - calibration procedure for DYRESM - CAEDYM: I think the authors might consider adding some further explanation to this section to clarify some of the details of their auto - calibration procedure. Questions that arose in my mind as I read this section included:

· CAEDYM parameters not included in the optimization – How many other parameters were there? How were their values chosen? Were any changes made to these values as the calibration proceeded?

Response:

Actually all the parameters can be potentially calibrated but some parameters are not necessary. For example, the stoichiometric parameters, the density, size and critical shear

stress of different types of sediment, some non-sensitive parameters. So if the mode user doesn't know which parameter is sensitive or not, I would recommend this parameter be included in calibration. If a parameter is not included in the calibration, the minimum and maximum values should be the same value and this value can be obtained from relevant literatures or observations or experiments.

All the parameters calibrated in this case study were listed in the attached table required by the reviewer 1.

· Random search module – Could the authors supply a little more detail about how the random search model worked? For example, was each parameter chosen independently of the others? Were any particular probability distributions assumed when generating random values? (It seems that this question is answered later on page 10 [see comment below for page 5, lines 23 - 25] but it might be helpful to include this here.)

Response:

Thanks for the comments. Answers below.

Was each parameter chosen independently of the others?

Yes, a random number for each parameter is independent.

Were any particular probability distributions assumed when generating random values?

No. Just random number.

· Line 25: Would it help to refer to Table 1 here, to identify the parameters and values used?

Response (now 5:32):

Thanks for the comments. Tab. 1 is refered at 5:34

· Lines 34 - 36: Could the authors consider supplying a little more explanation or detail about how " A single parameter file was chosen which minimised the combined RMSE of these variables with different weighing factors between the model simulations and measured values. "

Response (now 5:40-6:2):

Thanks for comments. We have made explained the "combined RMSE" before this sentence (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. see 6:2). "A single parameter file was chose…" has been changed to "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." (6:2 – 6:4).

Model validation: **Was any check made on model performance for temperature simulation for the validation runs (as it apparently was in Burger et al. 2008) ? Or was this done only for DO? It might be good to clarify this at some stage, perhaps in section 3.2.2 , or perhaps earlier, e.g. in section 3.1 (Physical parameter selection set) .**

Response:

Thanks for comments. We did not check the model performance for temperature simulation for the validation runs but we did that for the calibration. The DYRESM model has been previously successfully applied to water temperature simulations. In this paper, its performance in the calibration process was also good and moreover we focused on the software development and application with a case study of hypoxic event. That's way we didn't check its performance for temperature simulation in the validation.

Discussion section:

· Consider including some further discussion of how the timing of hypoxic events related to strength of stratification.

Response:

Thanks a lot for the nice comments. It looks very scientifically interesting to provide substantial information about how the timing of hypoxic events related to strength of stratification. There will be a lot of work to do, for example, how to define the hypoxic events, how to decide the timing of hypoxic events, and how to quantitatively calculated the strength of stratification (e.g. lake number). These parameters are strongly dependent on hydrodynamics and meteorological conditions. We wouldn't include this work in this paper since we are just addressing the principles of the auto-calibration for DYRESM-CAEDYM with a case study of hypoxic events in this paper, but would be very happy to work on another paper about that.

· Do the authors have any explanation for the under - prediction of DO concentration by the model in the validation run when measured DO concentrations were above 8 mg L^{-1} ?

Response:

I presume that the problem might be from the model itself. I talked to Professor David Hamilton about this problem before and he had no idea either. However, we could fix the problem by setting the "Photo-respiration phytoplankton DO loss" as negative value in the "chm" file although this is not the reality.

I have applied DYRESM-CAEDYM to a Chinese reservoir (Lake Qiandao) and got the same problem with under prediction of DO concentration. So I am still thinking about where the problem is possibly from.

Technical corrections

Page 2, line s 11 - 12 and line 25 : There are two Li et al. 2013 publications listed in the References; perhaps the authors can assign designations for 2013a and 2013b .

Response:

Thanks for the nice comments.

We have added "a" to the first reference paper and "b" the second one. We have also correspondingly changed the citation at 2:14 and 2:28.

Page 2, line 25: Consider replacing " This traditional calibration procedure … " , with " The traditional calibration procedure … " ; in lines 21 - 24 the authors list a number of procedures, and it is not clear which one " This " refers to.

Response:

"This" has been changed to "The" at 2:28

Page 3, line 8: " evaluate " – should be " evaluates " .

Response:

Done at 3:12. Thanks for the comments.

Page 5, line14: Can the authors specify the values of the two depths at which samples were collected ?

Response (5:19):

One is 1 meter below surface and the other one is 19 meters below surface. We have added "(1 meter and 19 meters below surface)" after "two depths" in the text.

Page 5, lines 23 - 25: Consider specifying here the type of probability distribution used for the random search module; text on page 10, lines 17 - 21, indicates the this was a uniform distribution, and no further distributions were used, but it would be helpful to also provide this information earlier on when the auto - calibration procedure is being described.

Response:

Thanks for the comments. 5:23-5:25 is now probably 5:29-5:31 referring to "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." Which has been changed according to previous comments. The random module produces random number without any consideration on probability distribution.

Text 10:17-10:21 (now 10:25-10:29) is "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)." ***Here we just say the Random Monte Carlo simulation has the advantage of being easily incorporated into model code and programming and DOES NOT NEED TO CONSIDER PARAMETER DISTRIBUTIONS.***

Page 6, Equations 1 and 2: Should Q_i be O_i ?

Response:

Changes have been made in the text.

Page 7, Table 2: Table 2 is to be inserted after line 5, but Table2 does not appear to be referred to anywhere in the text. Possibly it could be referred to at the end of the first sentence in line 4, in which the variation in model performance with depth is discussed.

Response:

Thanks a lot for letting me know this mistake. Tab. 2 has been inserted to the end of 7:7-7:8 (see below).

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).

Page 7, line 26, value for simulation minimum DO concentration: The text specifies that the minimum DO concentration from the simulation was 2.46 mg L^{-1}, but in Fig. 3 the minimum appears to be less than this, around 2.0 mg L - 1 for the event being described. However, the time scale of Figures 3 and 4 is not so easy to follow – see comment below under " Figures 3 and 4 ".

Response (now 7:34 – 7:35):

In the text, it is "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)". That means the minimum observed DO in this hypoxic event was 3.95 mg L^{-1} and the corresponding modeled DO was 2.46 mg L^{-1} on 24 Sep. It was not talking about the modeled minimum DO.

Page 7, line 30: Value for minimum measured DO concentration – it appears from Fig. 3 that minimum measured DO concentration for the fourth and fifth hypoxic events was less than the value 0.72 mg L^{-1} specified in the text.

Response (now 7:39):

Thanks for the valuable comments. The bottom DO started to decrease from 3 Dec. 2008 and the lowest DO concentration (0.72 mg L^{-1}) was found on 10 Dec 2008. On the next day, the bottom DO increased until 13 Dec. 2008 and began to decrease on 14 Dec. 2008. The minimum value (0.32 mg L^{-1}) was found 16 Dec. 2008 and then the observed DO increased dramatically from 0.32 mg L^{-1} to 7.5 mg L^{-1} in two days. However, the simulations followed the similar pattern but were much higher than the observations. The simulated DO was 7.7 mg L^{-1} on 16 Dec. 2008 while the observed value was 0.32 mg L^{-1}. So we thought the problem was probably from the meteorological conditions driving DYRESM-CAEDYM during 13 – 16 Dec 2008 but there is no any other available meteorological data. So we excluded this period from the fourth hypoxic event time because we really didn't know why there was huge difference between the observations and simulations at that time. So the fourth hypoxic event was from 3-10 Dec. 2008. In the fifth event, the lowest DO was 0.5 mg L^{-1} on 11 Jan 2009 after my double check.

Page 8, lines 20 - 21: Consider specifying the months that " spring " refers to. Also, the water level decrease mentioned in the text does not seem to be shown in the bottom panel of Fig. 2, where the top of the figure seems to have been cut off – the top is straight and horizontal, and in the scale for elevation the tick for 18m has been labelled as 20m.

Response (now 8:30):

Thanks for the comments. "Spring" has been changed to "January and February". We have replaced the figure with the originally produced figures, which looks clearer . The

figure caption has been changed to "Comparison of observed (top) and simulated (bottom) water column temperature based on daily data from 13 Jul. 2007–13 Jan. 2009."

Page 9, lines 9 - 10: Are the five DO depletion events that are referred to for the calibration? Or for the validation? Or both?

Response (now 9:16):

Thanks for the comments and sorry for the confusion. In the text, "in the calibration process" has been added to the end of "Simulated bottom DO represented observations well" at 9:16.

Page 9, line15: Consider replacing " in the upper ranges of values … " with " greater than values … " .

Response (now 9:22):

Done at 9:22.

Page 9, line 25: Should " Burger et al. 2007 " be " Burger et al. 2008 " ?

Response (now 9:32):

Yes it is "2008". Done at 9:32

Figure 2: Time scale labels are missing. See also comment above (page 8, lines 20 - 21) – the top of the bottom panel showing simulation results seems to have been cut off (the top is straight and horizontal), and in the scale for elevation it appears that the tick for 18m h as been labelled as 20m.

Response:

I replaced the figure by the original picture produced by Modeller 2.0 which looks clearer. I would be very happy if this clearer figure doesn't meet the journal standard.

Figures 3 and 4, Time scale: I recommend that time scales explicitly showing the date in a day , month an d year format (e.g. 13 Jul 07 for 2007194) be provided in addition, or instead of, the YYYYDDD format (presumably the format used by DYRESM) shown. This would make it easier for the reader to relate the description in the text, which refers mostly to conventional dates and only occasionally to day numbers. It also makes it easier for the reader to recognize seasonal influences. I also suggest that the authors consider adding a legend to the plots showing the difference between lines

used for simulated and measured DO concentrations; this difference is included in the figure caption, but a legend would help make the plot more self - contained.

Response:

The format has been changed according to the comments. Now it is at "mm/dd/yy" format which will be easier to know the season information. Legend has been added to the plottings.

Reference section: Check alphabetical order for citations in the References (e.g., Alarcon precedes Antenucci; Copetti follows Chung; Cui follows Cox).

Response:

The reference order has been adjusted.

Page 12, line18, upper case B for Bombardelli

Response (12:22):

Done at Line 12:22.

Page 14, lines 30 - 34: should there be 2013a and 2013b for the two Li et al. references? (Also noted above in comment for page 2, lines 11 - 12, 25 .)

Response:

"a" and "b" have added to the two references and the citation has also been changed in the text.

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).

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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.

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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 then chosen which minimised the combined *RMSE* of these two variables with corresponding weighing factors.

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.

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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.

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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.

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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).

Acknowledgements

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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.

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已删除: Table 1 Selected physical parameters used in DYRESM based on autocalibration from 10,000 iterations. , ... [1]

Tab. 1 Selected physical parameters used in DYRESM based on autocalibration from 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

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已删除: Autocalibration-chosen physical parameters used in DYRESM with 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.

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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 for 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

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Figure captions

Fig. 1 Schematic of dissolved oxygen dynamics in CAEDYM.

Fig. 2 Comparison of observed (A) and simulated (B) 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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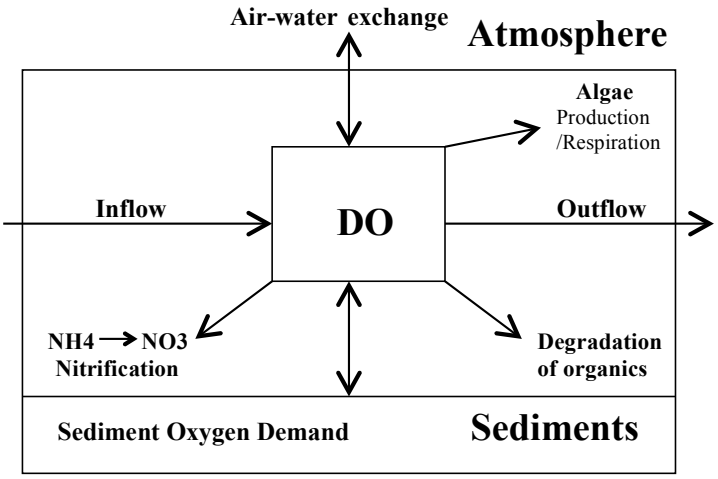
已删除: Fig. 3 Model auto-calibration with comparison of daily bottom DO between simulations (grey dots) and observations (black dots) for depth of 20.5 m from 13 Jul. 2007–13 Jan. 2009 (551 days). ... [3]


Air-water exchange
Atmosphere
Algae
Production
/Respiration
Inflow
DO
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NH4 → NO3
Nitrification
Degradation
of organics
Sediment Oxygen Demand
Sediments

Fig. 1

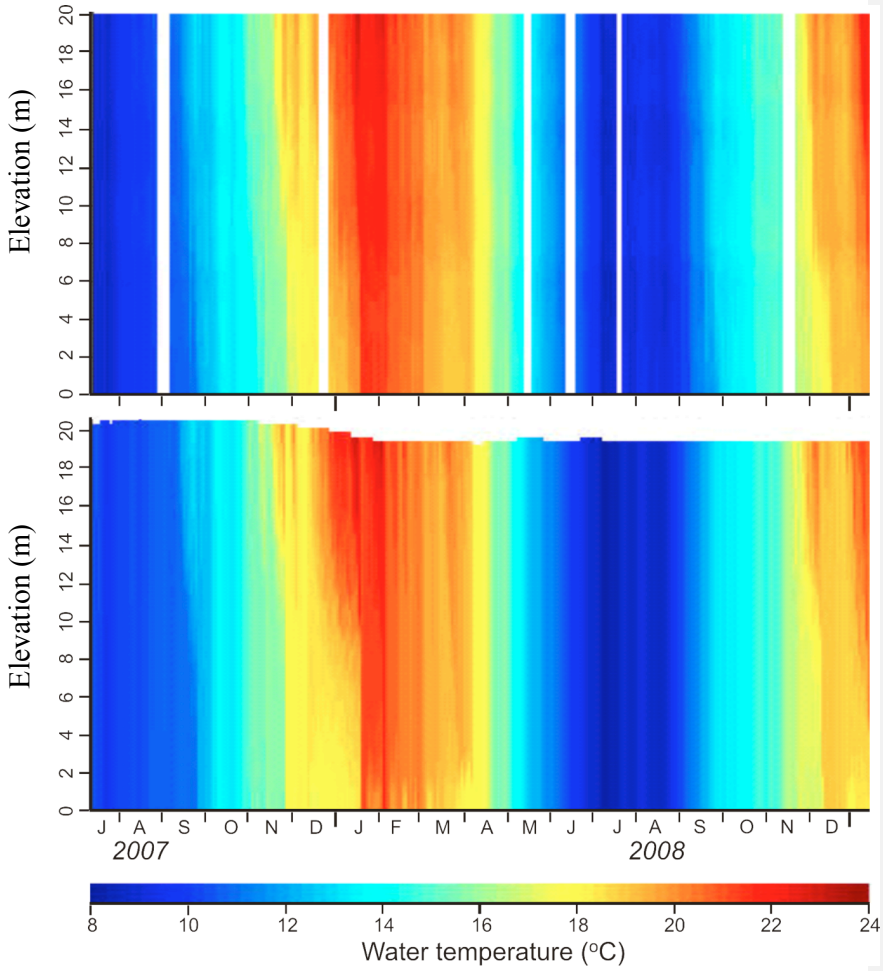

Fig. 2

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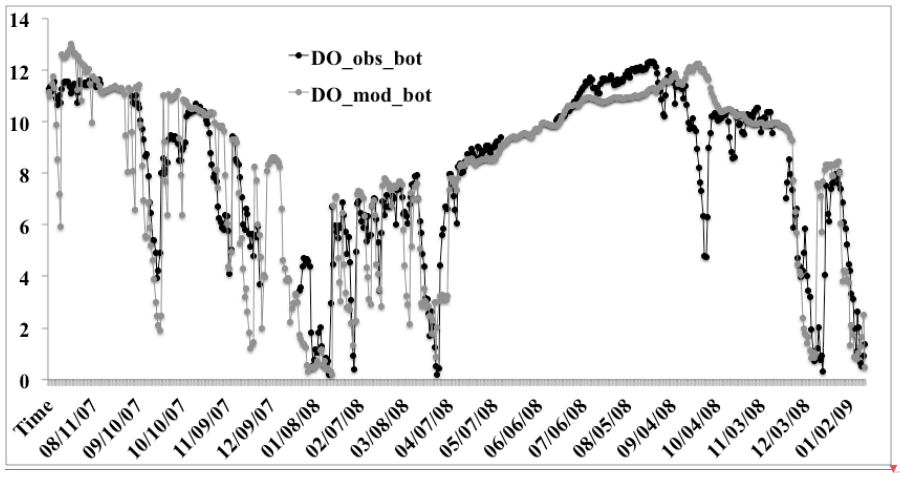

Fig. 3

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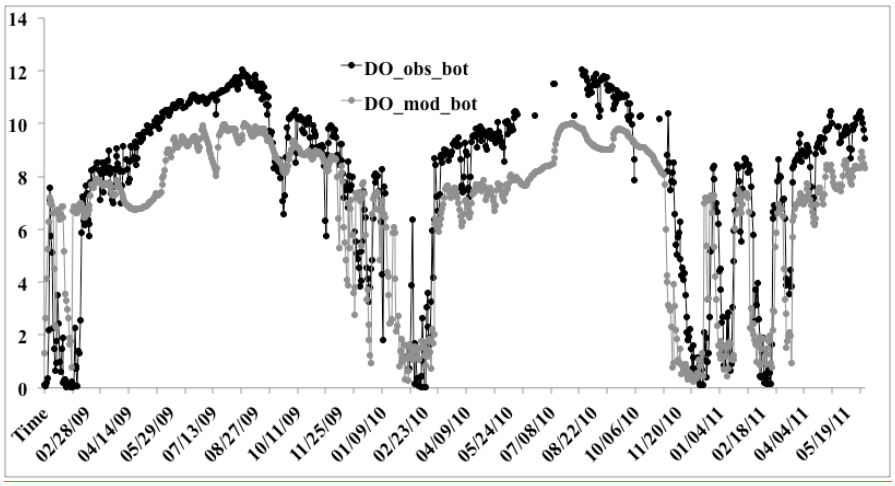

Fig. 4

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