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A Novel Objective Function DYNO for Automatic Multi-variable Calibration and Application to Assess Effects of Velocity versus Temperature Data for 3D Lake Models Calibration

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Abstract. This study introduced a novel Dynamically Normalized objective function (DYNO) for multi-variable (i.e., temperature and velocity) model calibration problems. DYNO combines the error metrics of multiple variables into a single objective function by dynamically normalizing each variable's error terms using information available during the search. DYNO is proposed to dynamically adjust the weight of the error of each variable hence balancing the calibration to each variable during optimization search. The DYNO is applied to calibrate a tropical hydrodynamic model where temperature and velocity observation data are used for model calibration simultaneously. We also investigated the efficiency of DYNO by comparing the result of using DYNO to results of calibrating to either temperature or velocity observation only. The result indicates that DYNO can balance the calibration in terms of water temperature and velocity and that calibrating to only one variable (e.g., temperature or velocity) cannot guarantee the goodness-of-fit of another variable (e.g., velocity or temperature). Our study suggested that both temperature and velocity measures should be used for hydrodynamic model calibration in real practice. Our example problems were computed with a parallel optimization method PODS but DYNO can also be easily used in serial applications.

1. Introduction

Hydrodynamic models simulate the hydrodynamic and thermodynamic processes in lakes and reservoirs that are important for simulating water quality in aquatic eco-systems (Chanudet et al., 2012). These simulation models (e.g., hydrodynamic modelling) play a critical role in managing water bodies (e.g., rivers, lakes, and coastal areas), as they are built to simulate the spatial and temporal distributions of specific water quality variables, and to study the response of a water body to different future management scenarios. The parameters of these models usually need to be calibrated to measured data to adequately represent local effects and hydrodynamic processes. Model calibration is a vital step in complex hydrodynamic modelling of lakes and other aquatic systems.

Model calibration of hydrodynamic models is mainly done manually (also called trial and error), where experts tune the parameters and simultaneously evaluate the goodness-of-fit between the simulation output and observations. This process is subjective, time-intensive and requires extensive expert knowledge (Afshar et al., 2011; Xia et al., 2021; Solomatine et al., 1999; Fabio et al., 2010; Baracchini et al., 2020). The challenges associated with manual calibration have encouraged the application of auto-calibration to hydrodynamic models, where the calibration is set up as an inverse problem to minimize the error between the simulation and observations. Some studies (e.g., Gaudard et al. (2017), Luo et al. (2018), Ayala et al. (2020) and Wilson et al. (2020)) have applied automatic calibration to one-dimensional hydrodynamic lake models where water temperature is the variable that is simulated and calibrated. These one-dimensional models are relatively cheap to run, allowing the use of automatic calibration methods that typically require many simulation evaluations to determine suitable parameter sets (e.g., differential evolution used in Luo et al. (2018) and Monte Carlo sampling used in Ayala et al. (2020)). However, one-dimensional models are unable to simulate the spatial distribution of some water variables, and thus may not be suitable for certain studies. Consequently, 2-dimensional or 3-dimensional models are preferred for studying the spatial-temporal distribution of water variables and are increasingly used to study lakes around the world (Chanudet et al., 2012; Galelli et al., 2015; Hui et al., 2018; Soulignac et al., 2017; Wahl and Peeters, 2014; Xu et al., 2017; Baracchini et al., 2020) . The calibration of 3-dimensional models, though, is considerably more challenging than calibration of one-dimensional models, since 3-dimensional models are significantly more computationally expensive and also involve more complicated physical processes (such as advection of flows).

The computationally expensive character of 3-dimensional models makes traditional optimization methods, such as differential evolution and Monte Carlo sampling, unsuitable for automatic calibration because these methods usually require many evaluations to get an acceptable solution. Surrogate-based optimization is highly suitable for such problems (Bartz-Beielstein and Zaefferer, 2017; Lu et al., 2018; Razavi et al., 2012) and recent studies have applied surrogate-based optimization methods to parameter estimation of hydrodynamics models. Surrogate-based optimization methods use a cheap-to-run surrogate approximation model (of the calibration objective) fitted with all known (i.e., already evaluated) values of the original expensive objective function, to guide the optimization search and reduce the number of evaluations required on the expensive simulations. For example, Xia et al. (2021) proposed a new optimization method called PODS (parallel optimization with dynamic coordinate search using surrogates) suitable for computationally expensive problems, and applied it to automatic calibration of a three-dimensional lake hydrodynamic models. More elaborate discussions on surrogate-based optimization algorithms can be found in Xia et al. (2021), Xia and Shoemaker (2021), Razavi et al. (2012), Bartz-Beielstein and Zaefferer (2017) and Haftka et al. (2016).

Computational intensity is not the only critical challenge associated with parameter estimation of 3-dimensional hydrodynamic models. Parameter estimation of these models is also a multi-site & multi-variable calibration problem, i.e., observation data is usually available at multiple locations and the underlying models simulate multiple variables (e.g., temperature and velocity). Moreover, simultaneous calibration of multiple variables is desired due to complex interactions between the different variables. For instance, temperature and velocity are inter-dependent variables of a lake hydrodynamic model, since water temperature affects the movement of water, and water velocity affects the distribution of water temperature. However, most prior research studies have calibrated hydrodynamic models to only temperature. This might because temperature measurements are relatively less expensive to get compared with velocity measurements and often temperature measurements are available to help predict water quality phenomenon. Wahl and Peeters (2014) use the measured water temperatures to calibrate a 3-dimensional hydrodynamic model of Lake Constance. Kaçıkoç and Beyhan (2014) calibrate the temperature of Lake Egirdir hydrodynamic model, the flow simulation of which is used for the lake

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water quality modeling. Marti et al. (2011) and Xue et al. (2015) also only used temperature data for lake hydrodynamic model calibration. Moreover, these studies use manual calibration for parameter estimation. Xia et al. (2021) use automatic calibration for parameter estimation, but only use water temperature observations in the calibration process. Reproducing water level is also a parameter estimation approach that pseudo-considers flow dynamics in calibration; however, a calibrated model that correctly simulates observed water level does not necessarily reproduce the observed 3D flow field accurately (Wagner and Mueller, 2002; Parsapour-Moghaddam and Rennie, 2018).

Hydrodynamics models predict the velocities throughout the water body. These results are important to understand the spatial distribution of water quality problems in sizeable lakes. For the purposes of model calibration it is useful to know whether efforts to measuring velocity directly are justifiable if temperature data is already available. We will examine the extent to which direct measurement of velocities justify the extra effort by giving more accurate results for hydrodynamics models and also look at the error associated with calibrating (for hydrodynamics) to temperature only, which is rarely studied in literature.

There are a few studies that attempt to calibrate hydrodynamic models to both temperature and velocity. Chanudet et al. (2012) attempt to calibrate both temperature and velocity sequentially (using manual calibration), i.e., they calibrate water temperature first and then the current velocities. Baracchini et al. (2020) performed two sequential steps in the automatic calibration of temperature and velocity, and the velocity calibration is based on the results obtained from temperature calibration. However, one problem with such two-step sequential approaches, either by manual or auto-calibration is that the calibration of the second variable might significantly alter the calibration quality of the first variable. This is especially true for multi-variable calibration problems, where the multiple variables being calibrated are sensitive to the parameters being calibrated. Other examples of such multi-variable calibration problems include watershed model calibration (Franco et al., 2020) and seawater intrusion model calibration (Coulon et al., 2021) etc. These multi-variable problems desire calibration frameworks that allow simultaneous calibration of all variables rather than calibrating one and then the second.

There are prior studies that simultaneously calibrate both temperature and velocity variables of hydrodynamic models. However, these use a trial and error (manual) mechanism for calibration (Råman Vinnå et al., 2017; Soulignac et al., 2017; Jin et al., 2000; Paturi et al., 2014). Manual calibration of multiple hydrodynamic variables simultaneously, is even harder than calibration of a single variable. A key challenge for automatic calibration of multi-variable calibration problems is in defining a suitable objective function to calibrate multiple variables simultaneously. Traditional approaches using automatic methods typically formulate the goodness-of-fit of multiple variables into a single objective function by adding weights between the goodness-of-fit of multiple variables (Afshar et al., 2011; Pelletier et al., 2006). However, a drawback of this approach is that the relative error magnitude of each variable of the new solutions found will probably varying during the search making it difficult to determine appropriate weights since they need to be determined / defined *a prior*, i.e., before optimization.

Another approach for calibration of multi-variables is using multi-objective optimization techniques (Afshar et al., 2013). However, multi-objective techniques are commonly used to optimize multiple sub-objectives that have a trade-off between each sub-objective (Akhtar and Shoemaker, 2016; Reed et al., 2013; Alfonso et al., 2010; Giuliani et al., 2016; Herman et al., 2014). While for the multi-variable hydrodynamic calibration problems, it is not apparent that there is usually a trade-off between the fit of multiple variables. Moreover, Multi-Objective

Optimization (MOO) is considerably more computationally difficult than Single Objective Optimization (SOO) and typically requires many more objective function evaluations. Thus, MOO may not be desired for computationally expensive calibration problems, especially when a significant trade-off between the objectives may not be present. Consequently, multi-variable calibration utilizing efficient SOO algorithms, while balancing the calibration to each variable equally during calibration, is a research area of significant value.

We introduce a new Dynamically Normalized Objective Function (DYNO) for automatic multi-variable calibration problem. The error of each variable (e.g., temperature and velocity of hydrodynamic models) is dynamically normalized by using the information about variable error of the evaluations found during the optimization search process. In this way, the balance between calibration of each variable is dynamically adjusted. We tested the efficiency of DYNO on a computationally expensive hydrodynamic lake model of a tropical reservoir, which takes 5 hours to run per simulation. DYNO is coupled into a recent parallel surrogate optimization algorithms PODS (Xia et al., 2021) and successfully applied for the calibration of multiple variables of the hydrodynamic model. Using DYNO, we investigate the impact of using temperature and/or velocity observations on model accuracy.

2. Methodology

2.1 Multi-variable Calibration Problems Description

The calibration problems investigated in this study are multi-site (i.e., observations are available from multiple locations), multi-variable (e.g., temperature and velocity for hydrodynamics) problems, and are defined, mathematically, as follows (the variable and function definition are given in Table 1):

$$\min_{\boldsymbol{X}\in\Theta} F(\boldsymbol{X}|\boldsymbol{K}) = F(\{f_k(\boldsymbol{X})|k \in \boldsymbol{K}\}) \tag{1}$$

$$f_k(\boldsymbol{X}) = f_k(\{g_j(sim_j^k(\boldsymbol{X}), obs_j^k)|j = 1, \cdots, M\}) \tag{2}$$

Note that the notation $\{z_i\}$ in Eq. (2) is simply meant to imply the function on the left depends on the finite series of quantities inside the braces $\{\bullet\}$.

Table 1. Notation and definitions of variables and functions in Eq. (1) and (2).

Variable	Description
$\boldsymbol{K}$	The set of variables the observation data of which is used in calibration. For example, $\boldsymbol{K} = [Tem]$ means that water temperature observation is used for calibration, i.e., water temperature is the variable that is being calibrated; $\boldsymbol{K} = [\overrightarrow{Vel}]$ means velocity observation is used for calibration; $\boldsymbol{K} = [Tem, \overrightarrow{Vel}]$ means that both temperature and velocity observations are used for model calibration
k	The symbol for elements in $\boldsymbol{K}$ variable (e.g., water temperature or velocity, $k = Tem$ or $k = \overrightarrow{Vel}$).$k \in \boldsymbol{K}$
$\boldsymbol{X}$	A d dimensional parameter vector restricted to parameter space Θ, where d is the number of parameters to be optimized
Θ	The parameter space is defined by the upper and lower limits on each parameter ($\boldsymbol{X}^{max}$and $\boldsymbol{X}^{min}$, respectively)
M	The total number of observation locations (or sites).
j	The index for observation location. $j = 1, \ldots, M$
$Sim_j^k(\boldsymbol{X})$	The simulation output of variable k at location $j$at times $t = 1, \ldots, N$ given the parameter vector $\boldsymbol{X}$
Obs_j^k	The observation (data) of variable k at location j at times $t = 1, \ldots, N$

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N	The total time steps of the observation data
t	The index for time steps. $t = 1, \ldots, N$
Function	**Description**
$F(\boldsymbol{X}\|\boldsymbol{K})$	The calibration objective function given the observation data of variables in K for calibration. $F(\boldsymbol{X}\|K)$ is a composite function of $f_k(\boldsymbol{X})$
$f_k(\boldsymbol{X})$	The error function of variable k over multiple site. $f_k(\boldsymbol{X})$ is a composite function of $g_j(Sim_j^k(X), Obs_j^k)$ for sites $j = 1, \ldots, M$
$g_j(Sim_j^k(\boldsymbol{X}), Obs_j^k)$	Goodness of fit between simulation output $Sim_j^k(\boldsymbol{X})$ and observation Obs_j^k of variable k at location j. When $k = Tem$, Normalized Root Mean Square Error (NRMSE) is utilized for $g_j(\bullet)$. When $k = \overrightarrow{Vel}$, normalized Fourier Norms of Root Mean Square Error (FNs) is used for $g_j(\bullet)$.

The set of parameters $\boldsymbol{X}$ being calibrated in this study includes nine parameters ($d = 9$). Details of these parameters are provided in Table 2 in section 2.4. The two variables are calibrated in this study are velocity and temperature for which data exists for different spatial location and time points.

We investigate different calibration formulations, where either one or both of these variables are calibrated. Consequently, $\boldsymbol{K} = [Tem]$ means that water temperature observation is used for calibration, i.e., water temperature is the variable that is being calibrated; $\boldsymbol{K} = [\overrightarrow{Vel}]$ means velocity observation is used for calibration; $\boldsymbol{K} = [Tem, \overrightarrow{Vel}]$ means that both temperature and velocity observations are used for model calibration, i.e., both variables are being calibrated simultaneously. The objective function in each scenario is discussed in section 2.5.

2.2 DYNO for Model Calibration with Multiple Variables

One major issue for model calibration with multiple variables is how to formulate the error of multiple variables into a single objective function. In practice, different variables (e.g., temperature and velocity) usually have different physical units and magnitudes of error. Their error functions cannot be summed up directly into a single objective function if we wish to give the error of each variable an equal weight in the overall objective function. The respective error functions have to be normalized. There are goodness-of-fit metrics that can normalize the error of different variables (for example Normalized Root Mean Square Error (NRMSE) and Kling-Gupta Efficiency (KGE, (Gupta et al., 2009))). However, it is still possible that the highest attainable NRMSE (or KGE) value (and the distribution of NRMSE (or KGE) value across the parameter space) for one variable maybe be much higher than the highest attainable NRMSE (or KGE) value (and the distribution of NRMSE (or KGE) value) of another variable. Hence how to balance such differences among multiple variables is still important even when the normalized goodness-of-fit metrics are used.

We propose a new general objective function, Dynamically Normalized Objective Function (DYNO), for the multi-variable calibration problem (e.g., calibrating temperature and velocity simultaneously). DYNO (as shown in Eq. (3)) normalizes the error of each variable $f_k(\boldsymbol{X})$ with its upper and lower bound, f_k^{max} and f_k^{min} of all evaluations found so far $\boldsymbol{\psi}$. Since true values of bounds are not known, f_k^{max} and f_k^{min} are dynamically updated during the optimization search after each iteration. Mathematical formulation of the multi-variable calibration problem, with the Dynamically Normalized Objective Function, is as follows:

$$min\, F(\boldsymbol{X}|\boldsymbol{K}) = \sum_{k \in K} \frac{f_k(\boldsymbol{X}) - f_k^{min}(\boldsymbol{X})}{f_k^{max}(\boldsymbol{X}) - f_k^{min}(\boldsymbol{X})} \tag{3}$$

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$$f_k^{max}(\boldsymbol{X}) = \max\{f_k(\boldsymbol{X})\ for\ all\ \boldsymbol{X} \in \boldsymbol{\psi}\} \quad (4)$$

$$f_k^{min}(\boldsymbol{X}) = \min\{f_k(\boldsymbol{X})\ for\ all\ \boldsymbol{X} \in \boldsymbol{\psi}\} \quad (5)$$

where $f_k^{max}(\boldsymbol{X})$ and $f_k^{min}(\boldsymbol{X})$ are the maximum and minimum values of $f_k(\boldsymbol{X})$ for all evaluation in $\boldsymbol{\psi}$, which is a set of all the evaluations evaluated so far and hence they have to be updated dynamically in each iteration during optimization. The detailed description of the implementation of Eq. (3) in the algorithm (i.e., PODS) tested in this study is given in Section 2.6 (the Algorithm Description section).

2.3 Study Site and Data

We use a 3-dimensional model of a tropical reservoir as an example to test the efficiency of DYNO for multi-variable calibration problems and to study the impact of using temperature and/or velocity data for model calibration. The horizontal boundary of the studied reservoir is given in Fig. 1 (a) and (b). One online water quality profiler station (STN. A1) was installed in the middle of the reservoir. The water temperature data at the station are available at various depths. The measured temperature data is used for model calibration in a previous study (Xia et al., 2021). We use this calibrated model to create synthetic observation data since the real velocity measurements are not available. We first assume a set of "true" model parameters $\boldsymbol{X}^R$. The value of $\boldsymbol{X}^R$ is based on an expert's guess and is listed in Table 2. The spatial and temporal observation data for the hypothetical lake is synthetically generated based on the "true" model parameters $\boldsymbol{X}^R$. The synthetic observation data for the hypothetical temperate lake is generated by running the simulation model for one year with a vector of model parameters $\boldsymbol{X}^R$. The simulation output is then saved hourly in N time steps for multiple variables, i.e., temperature and velocity ($\boldsymbol{K} = [Tem, \overrightarrow{Vel}]$) at M locations (specified in Fig. 1). In our study case, $N = 8761$ and $M = 12$ with different depths of five hypothetical sensor stations (STN. A1 and STN. B1-4 as shown in Fig. 1 (a) and (b)).

The saved hourly simulated output time series is denoted as $\Gamma = \{Sim^k(\boldsymbol{X}^R), k \in \boldsymbol{K} = [Tem, \overrightarrow{Vel}]\}$, which as defined (in Table 1) contains information for each time step, $t = 1, \dots, N$. So Γ is used as observation data for model calibration, i.e., $Obs^k, k \in \boldsymbol{K} = [Tem, \overrightarrow{Vel}]$ in Eq. (1). In the test of optimization for calibration, the true value of the parameter vector $\boldsymbol{X}^R$ is not provided to the optimization. The optimization will, instead, search for a best value of $\boldsymbol{X}$ that will minimize objective function $F(\boldsymbol{X}|\boldsymbol{K})$, where $\boldsymbol{K} = [Tem], [\overrightarrow{Vel}], or [Tem, \overrightarrow{Vel}]$. So the goal of automatic calibration via optimization is to obtain an optimum calibration $\boldsymbol{X}^*$ that results in simulation model output, $Sim^k(\boldsymbol{X}), k \in \boldsymbol{K}$, (see Eq. (1) and Eq. (2)) that is close to the synthetical observation time series data in $\boldsymbol{\Gamma}$.

The temperature and velocity simulation results based on the "true" model parameters (shown in Table 2) show temporal and spatial variation, as shown in Fig. 1 (a)-(d). Figure 1 (a) and (b) show the temperature and horizontal velocity distribution at the surface layer. Figure 1 (c) and (d) show the distribution of temperature and velocity magnitude at STN. A1. There is obvious temperature stratification in the vertical direction (as shown in Fig. 1(c)). We have the sampling locations across the reservoir where the observations can be used to calibrate the model parameters.

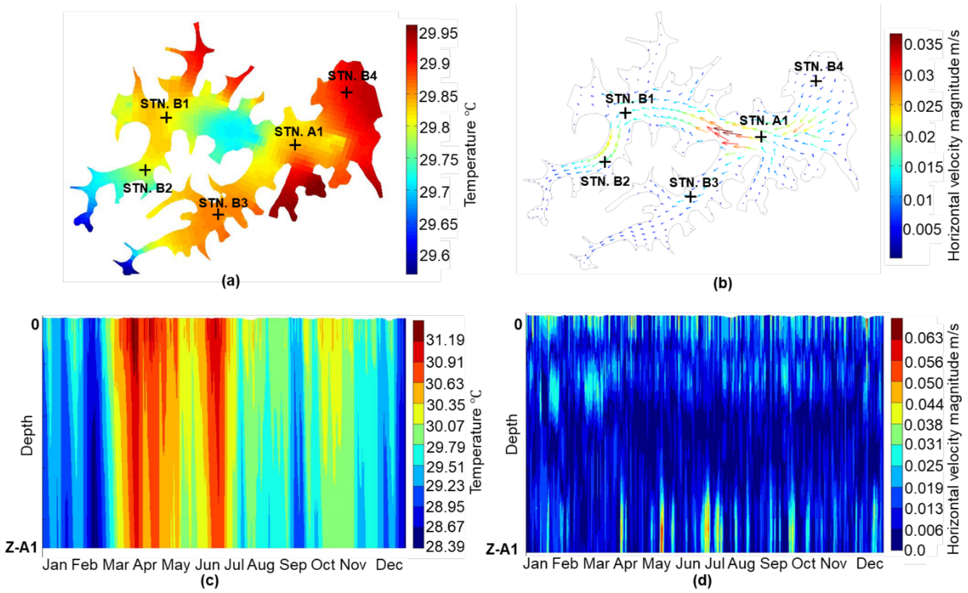

Figure 1. (a) Simulated (with "true" model parameters) temperature spatial distribution with sampling locations. (b) Simulated velocity spatial distribution with sampling locations. (c) Time-depth plot of simulated temperature at STN. A1. (d) Time-depth plot of velocity magnitude at STN. A1. Z-A1 is the maximum water depth at station A1.

2.4 Hydrodynamic Model and Calibration Parameters

The description of the hydrodynamic model is given in Xia et al., (2021). The hydrodynamic model is built with Delft3D-FLOW (Hydraulics, 2006). The Delft3D-Flow hydrodynamic model used was set up by the water utilities' employees and consultants, including the domain construction, input data preparation, and model configuration. The grid coordinate system is based on Cartesian coordinates (Z-grid), which has horizontal co-ordinate lines that are almost parallel with density interfaces to reduce artificial mixing of scalar properties such as temperature. The number of grid points in the x-direction is 65, the number of grid points in the y-direction is 67, and the number of layers in vertical is 19. A single 1-year simulation takes about 5 hours to run in serial on a windows desktop with CPU Intel Core i7-4790.

There are nine tunable model parameters (listed in Table 2) in the model. The first five parameters in Table 2 are related to the turbulence calculation. The k-ε closure model (Uittenbogaard et al., 1992) was chosen as the turbulence closure model to calculate the viscosity and diffusivity of the water. The calculation of the viscosity and diffusivity involves five parameters: 1) background viscosity in horizontal v_H^{back} , 2) vertical v_V^{back}, 3) the background eddy diffusivity in horizontal D_H^{back} , 4) vertical D_V^{back} and 5) the Ozmidov length L_{oz}. These parameters affect both the velocity and the temperature. The vertical exchange of horizontal momentum and mass is affected by vertical eddy viscosity and eddy diffusivity coefficient (Elhakeem et al., 2015). The horizontal velocities are affected by the horizontal eddy viscosity and diffusivity coefficients (Chanudet et al., 2012). Chanudet et al. (2012) highlighted that the most impactful parameter for temperature is the background vertical eddy viscosity and the Ozmidov length L_{oz} also has a significant effect on the thermal stratification by affecting the vertical temperature mixing. The bottom roughness, which has a direct impact on velocity, is computed

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according to Manning formulation with Manning's coefficient (n) given, which is a parameter that also should be calibrated.

The next three parameters in Table 2 are related to the simulation of surface heat flux. In the heat flux model, the evaporative heat flux and heat convection by forced convection is parameterized by the Dalton number c_e and Stanton number c_H , respectively, which are also in the list of calibration parameters. The Secchi depth H_{Secchi} (also included in Table 2) is another parameter required by the Ocean heat flux model. Secchi depth is related to the transmission of radiation in deeper water and thus affects the vertical distribution of heat in the water column (Chanudet et al., 2012). Heat fluxes through the reservoir bottom were not simulated in the current model. The last parameter is the manning coefficient, which affects the roughness of the bottom of the lake.

All these nine parameters affect (either directly or indirectly) the thermal and current activity in the water body, and thus, are included in the calibration process. The calibration range for these parameters (given in Table 2) is suggested by Singapore water utilities employees and consultants.

Table 2. Model parameter used in calibration. $\boldsymbol{X}^R$ denotes the true solution used to generate synthetical temperature and velocity observations at multi-sites.

Parameter vector $\boldsymbol{X}$	Parameter	Description (unit)	Physical process	Range	$\boldsymbol{X}^R$
x_1	ν_H^{back}	Background viscosity in horizontal (m^2/s)	3D turbulence	0.1-1.0[a,b,d,e]	0.5
x_2	D_H^{back}	Background eddy diffusivity in horizontal (m^2/s)		0.1-1.0[a,b,d,e]	0.5
x_3	ν_V^{back}	Background viscosity in vertical (m^2/s)		0-0.005[a,b,c,e]	5.00E-05
x_4	D_V^{back}	Background eddy diffusivity in vertical (m^2/s)		0-0.005 [a,b,c,e]	5.00E-05
x_5	L_{oz}	Ozmidov length scale (m)		0-0.05[a,b, e]	0.015
x_6	H_{Secchi}	Secchi depth (m)	Heat flux	0.1-2.0[a,e,f]	1
x_7	c_e	Dalton number (-)		0.001-0.002[a,b,c,e]	0.0013
x_8	c_H	Stanton number (-)		0.001-0.002 [a,b,c,e]	0.0013
x_9	n	Manning coefficient (m$^{-1/3}$s)	Roughness	0.02-0.03[a,b,e]	0.022

[a]Deltares (2014); [b]Chanudet et al. (2012); [c]Wahl and Peeters (2014); [d]Råman Vinnå et al. (2017); [e]Soulignac et al. (2017); [d]Pijcke (2014)

2.5 Calibration Problem Formulation

Three scenarios are considered to investigate the impact of model calibration against temperature and/or velocity observations: 1) calibrating to temperature data only (Cali-Tem), 2) calibrating to velocity data only (Cali-Vel), and 3) calibrating to both temperature and velocity together (Cali-Both). This corresponds to optimizing the problem $F(\boldsymbol{X}|\boldsymbol{K})$ in Eq. (1), where $\boldsymbol{K} = [Tem]$, $[\overrightarrow{Vel}]$, and $[Tem, \overrightarrow{Vel}]$ respectively for the three scenarios. The first two scenarios calibrate to only one variable, and the last scenario calibrates both variables simultaneously.

2.5.1 Model Calibration with One Variable

The objective functions for Cali-Tem and Cali-Vel scenarios are summarized in Eq. (6)-(8) and Eq. (9)-(11), respectively, where only observations of one variable are included in the calibration.

$$F(\boldsymbol{X}|\boldsymbol{K} = [Tem]) = f_{Tem}(\boldsymbol{X}) \tag{6}$$

$$f_{Tem}(\boldsymbol{X}) = \sum_{j=1}^{M} NRMSE_j^{Tem}(\boldsymbol{X}) \tag{7}$$

$$NRMSE_j^{Tem}(\boldsymbol{X}) = \frac{\sqrt{\frac{1}{N}\sum_{t=1}^{N}\left[Sim_{t,j}^{Tem}(\boldsymbol{X}) - Obs_{t,j}^{Tem}\right]^2}}{\frac{1}{N}\sum_{t=1}^{N} Obs_{t,j}^{Tem}} \tag{8}$$

$$F(\boldsymbol{X}|\boldsymbol{K} = [\overrightarrow{Vel}]) = f_{\overrightarrow{Vel}}(\boldsymbol{X}) \tag{9}$$

$$f_{\overrightarrow{Vel}}(\boldsymbol{X}) = \sum_{j=1}^{M} FNs_j^{\overrightarrow{Vel}}(\boldsymbol{X}) \tag{10}$$

$$FNs_j^{\overrightarrow{Vel}}(\boldsymbol{X}) = \frac{\sqrt{\frac{1}{N}\sum_{t=1}^{N}\left\| Sim_{t,j}^{\overrightarrow{Vel}}(\boldsymbol{X}) - Obs_{t,j}^{\overrightarrow{Vel}} \right\|_2}}{\sqrt{\frac{1}{N}\sum_{t=1}^{N}\left\| Obs_{t,j}^{\overrightarrow{Vel}} \right\|_2}} \tag{11}$$

where, $NRMSE_j^{Tem}(\boldsymbol{X})$ and $FNs_j^{\overrightarrow{Vel}}(\boldsymbol{X})$ denote the Normalized Root Mean Square Error (NRMSE) of temperature (described in Eq. (8)), and normalized Fourier Norms (FNs) of velocity vectors (described in Eq. (11)) at locations j. $Sim_{t,j}^{\overrightarrow{Vel}}(\boldsymbol{X})$ and $Obs_{t,j}^{\overrightarrow{Vel}}$ denote the simulated velocity given a parameter vector $\boldsymbol{X}$ and observed velocity, respectively, at time step t and location j. $Sim_{t,j}^{\overrightarrow{Vel}}(\boldsymbol{X})$ and $Obs_{t,j}^{\overrightarrow{Vel}}$ are 3-dimensional vector. $\|-\|_2$ in Eq. (11) is the Euclidean norm used to quantify the size of a vector.

The temperature and velocity data are taken at different depths of multiple stations, and their magnitude at different locations might be different due to spatial variation. Hence, the fitness at each location should be normalized before being summed into the objective function. For water temperature, Normalized Root Mean Square Error (NRMSE, as described in Eq. (8)) is used to quantify and normalize the error between the simulated and observed data. For velocity, normalized Fourier Norms of RMSE (FNs, as described in Eq. (11)) are used to measure the error between the model-simulated and observed data (corresponding simulated and observed velocity data points are three-dimensional vectors). The calculation of the Fourier Norm follows the description in Beletsky et al. (2006), Huang et al. (2010), Paturi et al. (2014) and Råman Vinnå et al. (2017).

2.5.2 DYNO for Model Calibration with Multiple Variables

In the Cali-Both scenario, both temperature and velocity are calibrated simultaneously, which can be treated as a bi-objective function problem. The objective function in the Cali-Both scenario (as shown in Eq. (12)) applies the DYNO proposed in Eq. (3). The error functions for water temperature, i.e., $f_{Tem}(\boldsymbol{X})$, and velocity, i.e., $f_{\overrightarrow{Vel}}(\boldsymbol{X})$, are the objective functions of the Cali-Tem scenario (Eq. (7) and the Cali-Vel scenario (Eq. (10), respectively. The temperature and velocity errors are dynamically normalized with their upper and lower bounds during the search of the optimization algorithm before being summed them into a single objective function. The mathematical formulation of the objective function in the Cali-Both Scenario (based on Eq. (3)) is as follows:

$$F(\boldsymbol{X}|\boldsymbol{K} = [Tem, \overrightarrow{Vel}]) = \frac{f_{Tem}(\boldsymbol{X}) - f_{Tem}^{min}(\boldsymbol{X})}{f_{Tem}^{max}(\boldsymbol{X}) - f_{Tem}^{min}(\boldsymbol{X})} + \frac{f_{\overrightarrow{Vel}}(\boldsymbol{X}) - f_{\overrightarrow{Vel}}^{min}(\boldsymbol{X})}{f_{\overrightarrow{Vel}}^{max}(\boldsymbol{X}) - f_{\overrightarrow{Vel}}^{min}(\boldsymbol{X})} \tag{12}$$

where the maximum and minimum of $f_{Tem}(\boldsymbol{X})$ and $f_{\overrightarrow{Vel}}(\boldsymbol{X})$ are updated after each optimization iteration (since new parameter sets are sampled in each optimization iteration). As the number of iterations increases, the denominators in Eq. (12) also increase since the optimization method finds better minimum objective function values. Hence the individual objective function components (for each variable) scale dynamically to maintain a roughly equal weight of the terms related to temperature and velocity.

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As defined in Eq. (6) to Eq. (12), three calibration formulations are investigated in this study. Table 3 gives a summary of these calibration formulations.

Table 3. Summary of Objective function formulation for different calibration scenarios.

Scenario Name	Variables used for calibration	Objective Function	Objective Function Formula
Cali-Tem	Temperature	$F(\boldsymbol{X}\vert\boldsymbol{K}=[Tem])$	Eq. (6)~(8)
Cali-Vel	Velocity	$F(\boldsymbol{X}\vert\boldsymbol{K}=[\overrightarrow{Vel}])$	Eq. (9)~(11)
Cali-Both	Temperature and Velocity	$F(\boldsymbol{X}\vert\boldsymbol{K}=[Tem,\overrightarrow{Vel}])$	Eq. (12)

2.6 Optimization Methods

2.6.1 PODS

We use a new efficient parallel surrogate algorithm PODS (Xia et al., 2021), a synchronous parallel version of serial DYCORS introduced by (Regis and Shoemaker, 2013). The serial optimization algorithm, DYCORS, is designed for global (with multiple local minima) black-box optimizations problems that are high-dimensional and have computationally expensive objectives (Regis and Shoemaker, 2013). Regis and Shoemaker (2013) show that serial DYCORS is considerably more efficient than other global optimization methods in obtaining good solutions with fewer objective function evaluations, which is very important for expensive objective functions like hydrodynamics models (Regis and Shoemaker, 2013). DYCORS uses RBF (Radial Basis Function) surrogates to guide the algorithm search towards promising solutions within the solution domain to reduce the number of evaluations (Regis and Shoemaker, 2007). Furthermore, DYCORS inherits the dynamic coordinate search idea from DDS (Tolson and Shoemaker, 2007) to improve its effectiveness and efficiency for high dimensional problems. PODS parallelized the serial DYCORS algorithm by following the general framework of the Synchronous Master-Worker Parallel Stochastic RBF Method introduced by Regis and Shoemaker (2009). This parallelization strategy of the algorithm allows simultaneous function evaluations on multiple processors (cores) in batch mode and can greatly speedup the calibration of computationally expensive models by reducing the calibration time and making the calibration of some extremely expensive models computationally tractable.

2.6.2 Implementation of Dynamically Normalized Objective Function in PODS.

The implementation procedure for incorporating the Dynamically Normalized Objective Function into the optimization algorithm PODS is described in Fig. 2. In the PODS algorithm, after each iteration, the sampling points for the next iteration are generated around the best solution found so far, in terms of the objective function value (in Eq. (1)). The use of DYNO affects the selection of the best solution found so far and also the fit of the surrogate model. When only one variable is considered in the objective function, the best solution is the evaluation with the lowest error between the simulation output and observations of the variable considered. In cases where multiple variables are considered in calibration, the best solution should be the evaluation after considering the error of multiple variables (as shown in Eq. (3)). Since the maximum and minimum value of the error of each variable $f_k^{max}(\boldsymbol{X})$ and $f_k^{min}(\boldsymbol{X})$ is dynamically changing after new evaluated simulations are available, the objective function value in Eq. (3) will be recalculated for all evaluated solutions after each iteration. Hence the surrogate model that is an approximation of the real objective function fitted by (F($\boldsymbol{X}\vert\boldsymbol{K}$), $\boldsymbol{X}$) is also rebuilt with

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these new objective function values of all evaluated solutions. Refitting of the surrogate model is computationally inexpensive compared with the runtime of the expensive objective function. Hence it does not affect overall algorithm runtime.

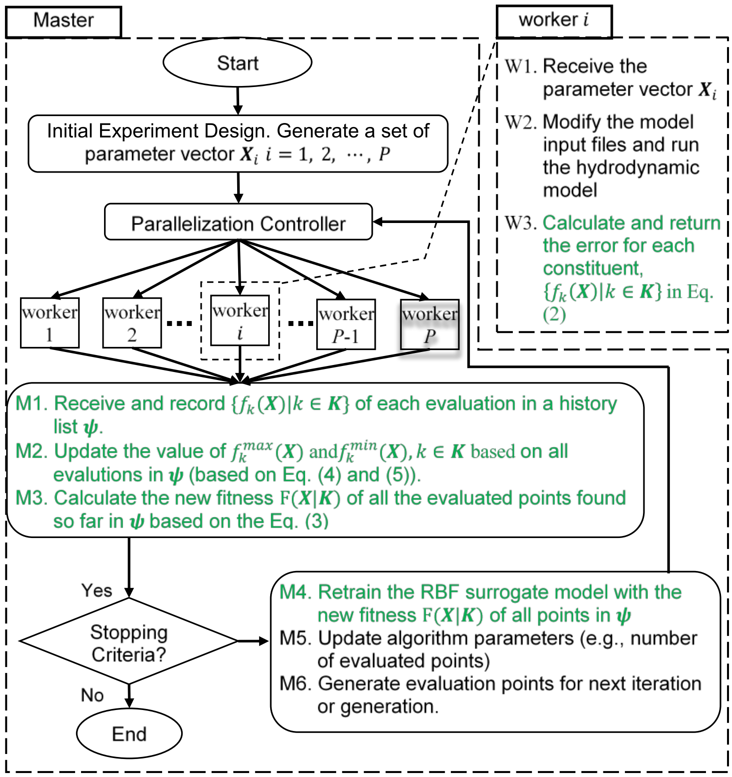

Figure 2. Diagram of the implementation of the Dynamic Normalized Objective Function with the parallel algorithm PODS. P is the number of processors available. The green texts (i.e., steps W3, M1-4) are changes made on PODS to incorporate DYNO. The rest part follows the original PODS method.

2.7 Experiments Setup

All computational experiments in this study are implemented on a single node on the National Supercomputer Center (NSCC) of Singapore, which is a Linux-based platform with dual Intel Xeon E5-2690 v3 Processors, with each node having 24 cores. Hence, we set the number of processors P to be 24. Due to the stochastic nature of the optimization algorithm (i.e., PODS) used in this study, multiple optimization runs are executed for each calibration experiment in Table 3. Considering that the calibrated hydrodynamic model in this study is extremely expensive, we perform three optimization trials for each calibration experiment (see Table 3 for a list of experiments). Furthermore, to remove any initial sampling bias, each concurrent optimization trial for the three calibration experiments is initialized with the same Latin Hypercube experimental design (so the calibration in each scenario is starting from the same initial solutions). We also investigated the performance of different forms of DYNO on the Cali-Both scenario (i.e., calibrating to both temperature and velocity data).

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3. Numerical Results and Discussion

3.1 Comparison of Calibrating to Temperature and/or Velocity

3.1.1 Final Solutions in Goodness-of-fit Metrics

We first compare the three calibration formulations in terms of goodness-of-fit metrics for both temperature and velocity. Table 4 summarizes this comparison for the three formulations, i.e., i) Cali-Tem (calibrate temperature only), ii) Cali-Vel (calibrate velocity only) and iii) Cali-Both (calibrate temperature and velocity simultaneously) (see definition in Table 3), with PODS used as the optimization algorithm and with a budget of 192 simulations.

The mean as well as the standard deviation of both temperature error $f_{Tem}(\boldsymbol{X}^*|\boldsymbol{K})$ (calculated as Eq. (7)) and velocity error $f_{\overrightarrow{Vel}}(\boldsymbol{X}^*|\boldsymbol{K})$ (Calculated as in Eq. (10)) over three trials are reported in Table 4, for all three calibration scenarios. $\boldsymbol{X}^*$ in Table 4 denotes the optimal calibration solution obtained by PODS in each trial for a given scenario (defined by the set of variables $\boldsymbol{K}$). The solution with the lowest variable error ($f_{Tem}(\boldsymbol{X}^*)$ or $f_{\overrightarrow{Vel}}(\boldsymbol{X}^*)$) is highlighted in bold in Table 4. Table 4 reports the variable errors of both temperature and velocity for all formulations to understand the impact of ignoring or including a variable in the calibration formulation. Please note that the temperature error, $f_{Tem}(\boldsymbol{X}|\boldsymbol{K}=[Tem])$, reported in Table 4, is exactly the calibration objective function in the Cali-Tem scenario ($F(\boldsymbol{X}|\boldsymbol{K}=[Tem])$ as shown in Eq. (7)). Similarly, the velocity error $f_{\overrightarrow{Vel}}(\boldsymbol{X}|\boldsymbol{K}=[Tem])$ is exactly the calibration objective function in the Cali-Vel scenario (i.e., $F(\boldsymbol{X}|\boldsymbol{K}=[\overrightarrow{Vel}])$ as shown in Eq. (10)). We use the word variable error instead of objective function value when referring to the values in Table 4 in subsequent discussions since we are in part looking at the impact of using data from one variable to predict another variable for which we don't have data.

Table 4 shows that the solution obtained when calibrating to temperature observation only (Cali-Tem) has smaller temperature errors but larger velocity errors than that if calibrating to velocity observation data only (Cali-Vel). However, it is surprising that when calibrating to both temperature and velocity (Cali-Both), the solution obtained by PODS has the lowest temperature and lowest velocity error compared with calibrating to either temperature observation or velocity observation only. This might be because calibrating to temperature will help to improve the fit of velocity and vice versa. This makes sense because water temperature and velocity are two related variables in hydrodynamic modeling, and they are affecting each other. Velocity is the fundamental variable of hydrodynamics with directional information not provided by temperature; temperature (via the heat flux model) may also affect the velocity field since it affects water density. This might explain calibrating both temperature and velocity simultaneously gives the best results.

Table 4. Summary table of the solution obtained by PODS for each scenario (Cali-Both, Cali-Vel, and Cali-Tem). $f_{Tem}(\boldsymbol{X}^*|\boldsymbol{K})$ and $f_{\overrightarrow{Vel}}(\boldsymbol{X}^*|\boldsymbol{K})$ are the temperature error $f_{Tem}(\boldsymbol{X}^*)$ and velocity error $f_{\overrightarrow{Vel}}(\boldsymbol{X}^*)$ (calculated in Eq. (7) and Eq. (10), respectively, with the optimal solution $\boldsymbol{X}^*$ obtained in each trial). The mean and standard deviation of $f_{Tem}(\boldsymbol{X}^*|\boldsymbol{K})$ and $f_{\overrightarrow{Vel}}(\boldsymbol{X}^*|\boldsymbol{K})$ among three trials are reported. The variable error is bolded in each scenario when the observation of the variable is included in the calibration in each scenario. (Some terms defined in Table 1)

Scenarios	The composite error of each variable (Temperature or Velocity)	
	$f_{Tem}(X^*\|K)$ Mean (Std.)	$f_{\overrightarrow{Vel}}(X^*\|K)$ Mean (Std.)
Cali-Both $K=[Tem,\overrightarrow{Vel}]$	**0.014 (0.003)**	**1.939 (0.165)**
Cali-Vel $K=[\overrightarrow{Vel}]$	0.087 (0.023)	2.809 (0.319)
Cali-Tem $K=[Tem]$	0.024 (0.005)	5.888 (1.435)

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3.1.2 Visual Comparison of Calibration Errors

The above analysis is based on the average variable error statistics only (i.e., $f_{Tem}(\boldsymbol{X}^*|\boldsymbol{K})$ and $f_{\overrightarrow{Vel}}(\boldsymbol{X}^*|\boldsymbol{K})$), of the best results obtained from PODS (over multiple trials) for all calibration scenarios. In order to further analyze the difference between calibration formulations (in terms of their effectiveness in calibrating both temperature and velocity), we visually compare the best calibration solutions ($\boldsymbol{X}^*$) obtained by PODS for each scenario, i.e., Cali-Tem, Cali-Vel and Cali-Both. We select one representative optimal solution ($\boldsymbol{X}^*$) from 3 trials in each scenario for this comparison.

The objective function value in terms of temperature and velocity composite error (over multiple locations) ($f_{Tem}(\boldsymbol{X})$ and $f_{\overrightarrow{Vel}}(\boldsymbol{X})$, as formulated in Eq. (7) and (10), respectively) and the corresponding parameter configuration ($\boldsymbol{X}^*$) of the selected solution (among three trials) are reported in Table 5. The horizontal velocity error $\Delta\overrightarrow{Vel}$ (2-dimensional) between simulated velocity $Sim_{t,j}^{\overrightarrow{Vel}}(\boldsymbol{X}^*)$ and observed velocity $Obs_{t,j}^{\overrightarrow{Vel}}$ (in the horizontal plane) is plotted as scatter plots of time-series in Fig. 3 (for all calibration scenarios). The temperature error ΔTem between simulation temperature $Sim_{t,j}^{Tem}(\boldsymbol{X}^*)$ and observed temperature $Obs_{t,j}^{Tem}$ is plotted as a time series (for each calibration scenario) in Fig. 4.

The error plots for the two sampling locations at multiple depths (i.e., surface layers of station STN. A1 and STN. B1 as shown in Fig. 1 (a)) are visualized in Fig. 3 and 4 (for one year). Since the velocity error $\Delta\overrightarrow{Vel}$ at a particular time and location is a vector (and not a scalar like temperature) and velocity error in 3 dimensions (for a time-series) is hard to represent visually, Fig. 3 only plots the velocity error (for one year) $\Delta\overrightarrow{Vel}$ in the horizontal plane (i.e., X and Y directions only). Moreover, each dot represents the error at one point in time within the study period.

Figure 3 plots the difference between the simulated velocity (for the optimized parameter values obtained from Cali-Tem (red scatter points), Cali-Vel (black scatter points), and Cali-Both (green scatter points) scenarios) and observed velocity. Ideally, the error for each scatter point should be zero, i.e., at the intersection of the two lines Figure 3 illustrates that calibrating to temperature data only (red scatter plot) results in the velocity error $\Delta\overrightarrow{Vel}$ scatter that diverges from the zero velocity error(i.e., the intersection point of the black lines), in comparison to the corresponding velocity error scatter plots of solutions obtained from calibrating to velocity data only (Cali-Vel scenario, i.e., black scatter plot) or to both velocity and temperature data (Cali-Both scenario, i.e., green scatter plot).

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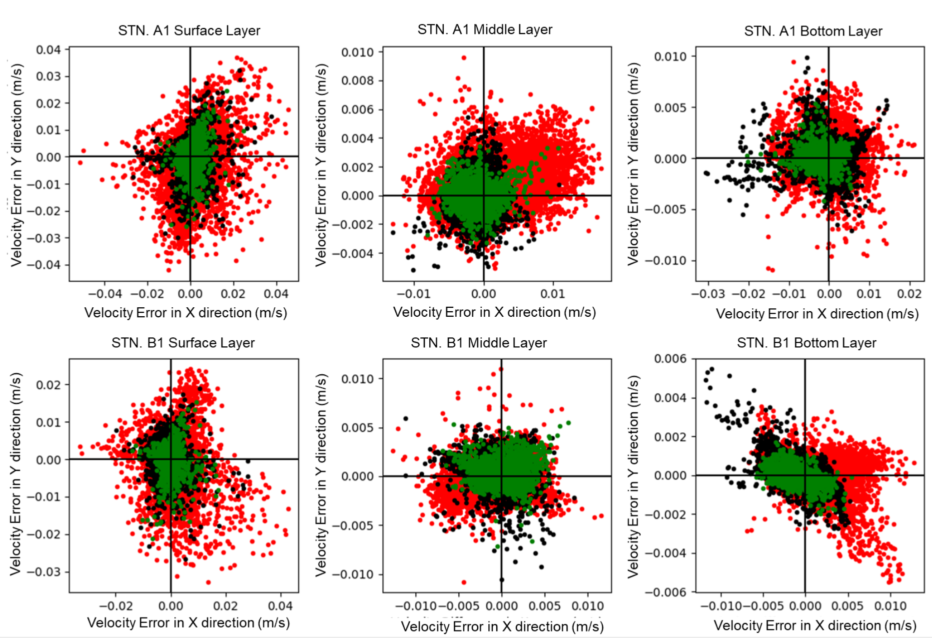

Figure 3. Scatter plot of velocity error $\Delta\overrightarrow{Vel}$ in horizontal (X and Y direction) between simulated velocity $Sim_{t,j}^{\overrightarrow{Vel}}(\boldsymbol{X}^*)$ and observed velocity $Obs_{t,j}^{\overrightarrow{Vel}}$ at location j. Each dot denotes the velocity error $\Delta\overrightarrow{Vel}$ of location j at one time step. j = surface layer of STN. A1 for upper panel and j = STN. B1 for lower panel. $\boldsymbol{X}^*$ is the optimal solution found by PODS in each scenario: Cali-Tem (red dots); Cali-Vel (black dots) and Cali-Both (green dots) as listed in Table 6. The “True” solution is on or near the intersection of the two perpendicular black lines.

Figure 4 shows the temperature error of solutions from three different calibration scenarios: Cali-Tem (red time-series), Cali-Vel (black time-series) and Cali-Both scenarios (green time-series). The errors between simulated and observed water temperature at the surface, middle and bottom layers of two stations (STN. A1 and STN B1) are plotted. In general, the temperature error of the solution in Cali-Both scenario is generally close to zero °C for all the layers and stations shown. The solution in Cali-Tem scenario also got temperature error close to zero °C at the middle and bottom layer at STN. A1, but it has larger temperature error than solution in Cali-Both at surface layer of STN. A1 and all layers of STN. B1. The solution in Cali-Vel scenario generally overestimated the water temperature in all locations (i.e., all the surface, middle and bottom layers at both stations). The temperature error of solution in Cali-Vel is much larger than solution in Cali-Tem and Cali-Both scenarios in the middle and bottom layer of both stations. The temperature error at most times, for the Cali-Vel scenario, is greater than 0.1 °C. This might be because both the Stanton and Dalton numbers are underestimated in the Cali-Vel scenario when compared with the True solution ($\boldsymbol{X}^R$) (As shown in Table 5). The Dalton number C_e affects the evaporative heat flux modeling and the Stanton number C_H influences the convective heat flux modeling in the Delft3D-FLOW model (Hydraulics, 2006). For the solution in Cali-Vel, a smaller Stanton number C_H= (shown in Table 5) might lead to underestimated convective heat flux, which will lead to the overestimated of the water temperature. In summary, calibrating to temperature and velocity (i.e., Cali-Both) give the best solution in terms of temperature error compare with calibrating to temperature or velocity only (i.e., Cali-Tem or Cali-Vel). Calibrating to velocity only (Cali-Vel) gives the worst result in terms of temperature fit.

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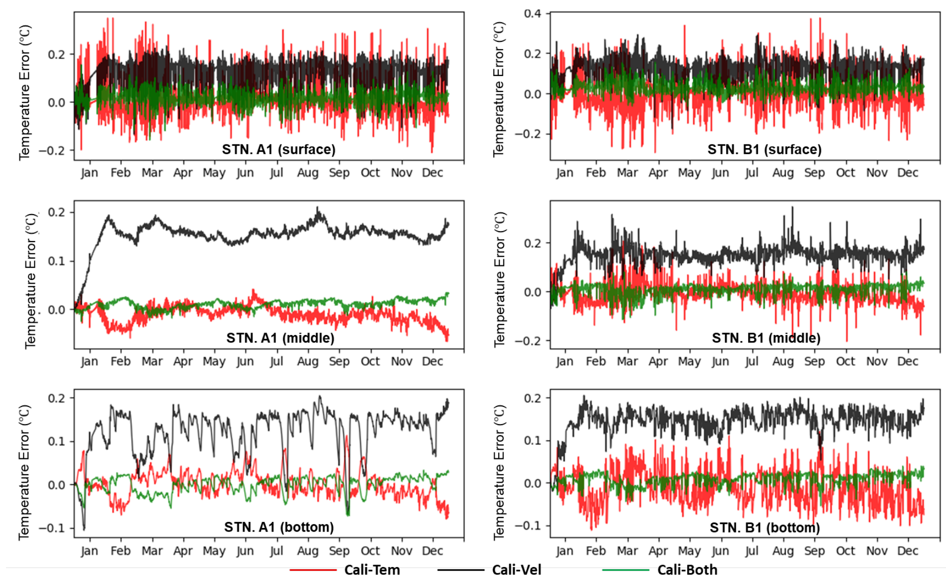

Figure 4. Time-series plots of temperature error *ΔT* between simulated water temperature and $Sim_{t,j}^{Tem}(X^{*})$ and observed water temperature ($Obs_{t,j}^{Tem}$) at location *j* where *j* = surface layer of STN4 for left panel and *j* = STN1 for the right panel. $X^{*}$is the optimal solution found by P-DYCORS in each scenario: Cali-Tem (Red lines); Cali-Vel (Black lines) and Cali-Both (green lines) as listed in Table 5.

Table 5. The composite error of each variable and the corresponding parameter configuration of the selected optional solution obtained via PODS in three calibration scenarios (Cali-Tem, Cali-Vel and Cali-Both). True solution ($\boldsymbol{X}^{R}$) defined in Table 2 is given for reference. The parameter symbols are defined in Table 2.

		True Solution ($\boldsymbol{X}^{R}$)	Cali-Tem	Cali-Vel	Cali-Both
Composite error of each variable[1]	$f_{Tem}(\boldsymbol{X})$	0	0.0202	0.0601	0.0108
	$f_{\overline{Vel}}(\boldsymbol{X})$	0	5.1945	2.7390	1.8006
Computed Parameter Vector ($\boldsymbol{X}$*)	$\boldsymbol{v_H^{back}}$ (m²/s)	0.5	0.7107	0.5084	0.4516
	$\boldsymbol{D_H^{back}}$ (m²/s)	0.5	0.1930	0.8427	0.4562
	$\boldsymbol{v_V^{back}}$ (m²/s)	5.00E-05	3.96E-04	3.40E-05	3.00E-05
	$\boldsymbol{D_V^{back}}$ (m²/s)	5.00E-05	1.12E-04	6.08E-06	2.98E-05
	$\boldsymbol{L_{oz}}$ (m)	0.015	0.0110	0.0490	0.0340
	$\boldsymbol{H_{Secchi}}$ (m)	1	0.5902	1.4147	1.1358
	$\boldsymbol{c_e}$ (-)	0.0013	0.0017	0.0013	0.0011
	$\boldsymbol{c_H}$ (-)	0.0013	0.0013	0.0012	0.0013
	$\boldsymbol{n}$ ($m^{-1/3}s$)	0.022	0.0229	0.0209	0.0243

[1]Smaller variable errors ($f_{Tem}(\boldsymbol{X})$ (see Eq. (7)) and $f_{\overline{Vel}}(\boldsymbol{X})$ (see Eq. (10))) are better, and the variable errors of the true solution $\boldsymbol{X}^{R}$ are zero (for both $f_{Tem}(\boldsymbol{X})$ and $f_{\overline{Vel}}(\boldsymbol{X})$).

3.2 Optimization Search Dynamics under Different Calibration Scenarios

We further analyze calibration progress of PODS for Cali-Tem, Cali-Vel and Cali-Both, to understand calibration convergence speeds of the three formulations. The purpose of the calibration progress analysis is to visualize the

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improvement in calibration quality of both temperature and velocity variables from the initial Latin Hypercube Designs (LHD), for all three formulations.

Figure 5 plots the calibration progress of the three formulations (i.e., Cali-Tem, Cali-Vel and Cali-Both) using PODS. Each subplot within Fig. 5, corresponds to the different concurrent optimization trials (i.e., trials of the stochastic optimization method using the same initial points from LHD) for each formulation. The best solutions are near the origin of each graph. Moreover, Fig. 5 plots the progress (quantified by visualizing both temperature and velocity errors) of the best solution found (measured in terms of the objective function value in each calibration scenario) during the search. Figure 5 indicates that when calibrating to temperature or velocity only, the optimization search cannot guarantee the improvement of the fit of another variable. For example, in Fig. 5 (a), when calibrating to velocity only, the temperature error of the best solution found at the end of the optimization search stage is worse than the temperature error of the best solution found after initial LHD, even though there is improvement in terms of velocity fit. Similarly, when calibrating to temperature only, the improvement on velocity fit is also not significant (for instance, in Fig. 5 (a)). When calibrating to the fit of both temperature and velocity using the DYNO formulation, the fit of both temperature and velocity improves in all trials, and the improvement remains balanced during the optimization search. Figure 5 also indicates that the final solution found in Cali-Both scenarios dominates the best solution found by PODS in Cali-Tem and Cali-Vel in terms of both temperature and velocity fit.

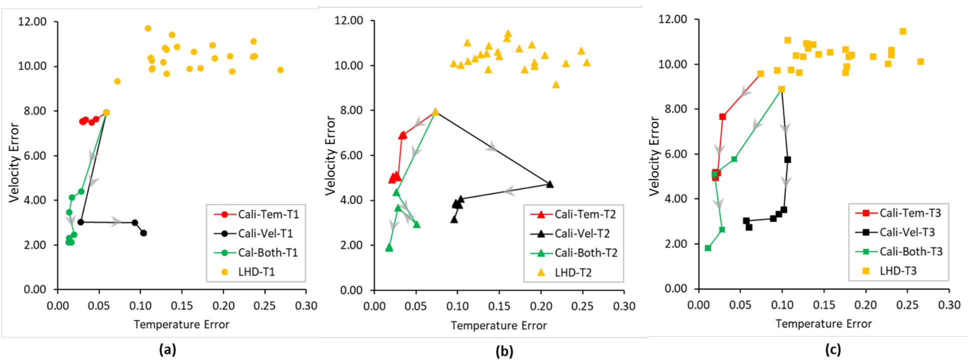

Figure 5. Calibration progress plot of the best solution found (in term of objective function value) during optimization search by PODS when calibrating to temperature only (Cali-Tem), calibrating to velocity only (Cali-Vel), and calibrating to both temperature and velocity (Cali-Both). Three random trials (i.e., T1, T2, and T3) are plotted in (a), (b), and (c). Lower velocity and temperature error are better. The yellow makers are evaluation point in initial experiment design using Latin Hypercube Design (LHD). Besides solutions in LHD, only the best solution in each of the optimization iterations are plotted (i.e., makers lined with lines). The line links the best previous solution in one iteration to the best solution in next iteration. The arrow indicates the direction from the previous solution to the next solution.

It is also important to understand the 'frequency' or likelihood with which PODS can find good temperature and velocity calibrations via the three different formulations proposed in this study. Hence, we also do a comparative frequency analysis of the errors (for velocity or temperature) of all evaluated points ($\boldsymbol{X}_i, i = 1, \dots, 3 * N_{max}$) from all trials (3 trials) of PODS when using difference calibration formulations (see Table 3). The purpose of this frequency analysis is to understand the likelihood with which the three different formulations can obtain good velocity and temperature calibrations. The frequency analysis results are presented in Fig. 6 via

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visualizations of empirical histograms of both velocity error and temperature error (from all solutions of 3 trials of PODS) for each calibration scenario.

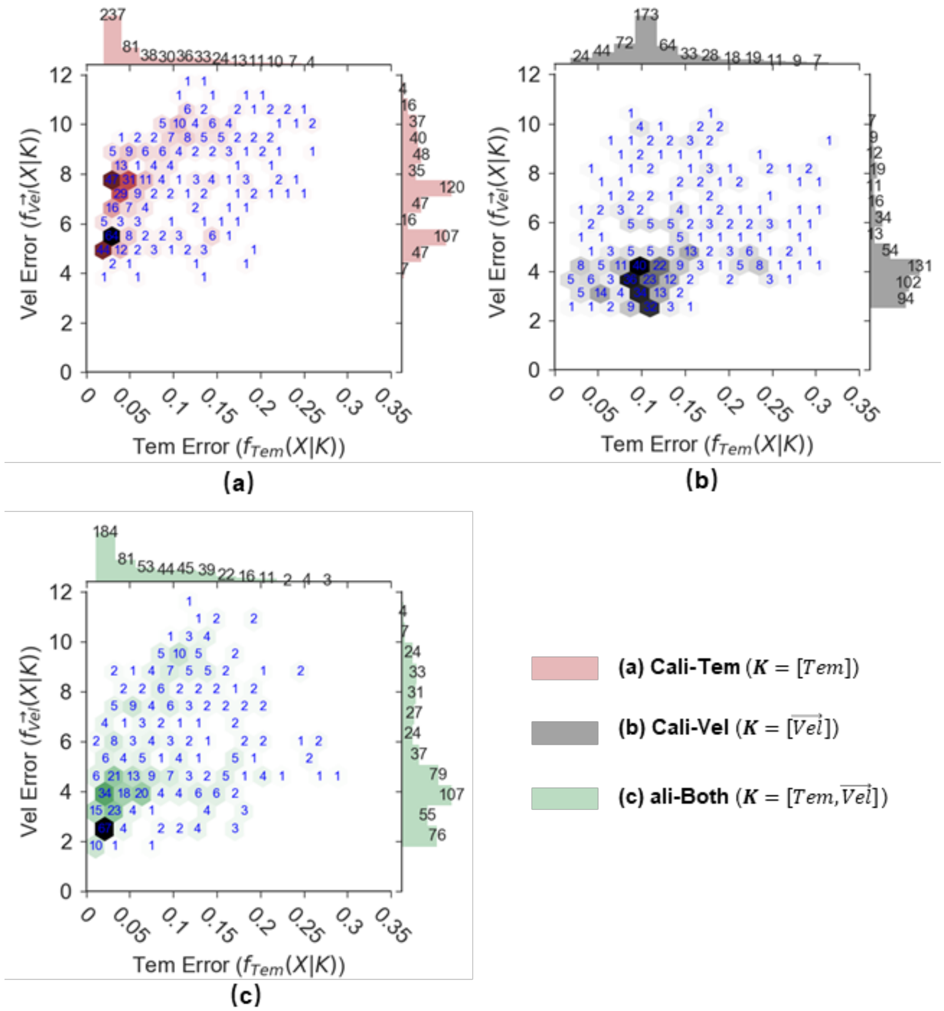

Figure 6. Distribution plot of all the evaluated points found by PODS (over 3 trials) in terms of temperature composite error $f_{Tem}(\boldsymbol{X}|\boldsymbol{K})$ and velocity composite error$f_{\overrightarrow{Vel}}(\boldsymbol{X}|\boldsymbol{K})$ in each scenario: Cali-Tem ($\boldsymbol{K} = [Tem]$), Cali-Vel ($\boldsymbol{K} = [\overrightarrow{Vel}]$), and Cali-Both ($\boldsymbol{K} = [Tem, \overrightarrow{Vel}]$). The number inside each hexagon represent the number of evaluated points located in that hexagon (e.g. with the combination temperature and velocity error associated with the corresponding values on the axes.) Darker color in hexagon means larger number of evaluated points located in that hexagon. The bar plot along the upper x axis ($f_{Tem}(\boldsymbol{X}|\boldsymbol{K})$) are the distribution of the evaluation points in terms of temperature error only. The bar plot along y axis ($f_{\overrightarrow{Vel}}(\boldsymbol{X}|\boldsymbol{K})$) are the distribution of the evaluation points in terms of velocity error only. The number above the bar shows how many evaluated points located in that bin. Smaller error ($f_{Tem}(\boldsymbol{X}|\boldsymbol{K})$ or$f_{\overrightarrow{Vel}}(\boldsymbol{X}|\boldsymbol{K})$) is better. The true solution ($f_{Tem}(\boldsymbol{X}^R|\boldsymbol{K}), f_{\overrightarrow{Vel}}(\boldsymbol{X}^R|\boldsymbol{K})$) is the origin of each subplot.

Figure 6 plots the error distribution of all the evaluated points over three trials (576 evaluations) for each scenario: Cali-Tem ($\boldsymbol{K} = [Tem]$), Cali-Vel ($\boldsymbol{K} = [\overrightarrow{Vel}]$), and Cali-Both ($\boldsymbol{K} = [Tem, \overrightarrow{Vel}]$). The different subplots in Fig. 6 provide a visualization of the velocity (vertical axis) and temperature (horizontal axis) error distribution

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via hexagonal bin (hexbin) plots (inside the square) and error histograms (outside the square) for each of the calibration scenarios. The number inside each hexbin denotes the number of evaluated points (for that combination of temperature error and velocity error) located in that hexbin. Furthermore, the hexbin with a larger number of evaluated points is highlighted with a darker color shade. The temperature histogram columns (above the square) represents the sum of all the hexbins inside the square directly beneath the number in the column. For velocity histogram (on right side of square), the column height depends on the sum of all the hexbins in the row to the left of the number.

The temperature and error velocity distribution visualizations of Fig. 6 clearly show that calibrating to both temperature and velocity data (see Fig. 6 (c), i.e., error distribution for the Cali-Both scenario), provides good temperature and velocity calibrations with a higher frequency. Figure 6 (c) shows that it is highly likely that both temperature and velocity errors are lower (indicated by darker hexbins with temperature error $f_{Tem}(\boldsymbol{X}|\boldsymbol{K})$ less than 0.05 and velocity error $f_{\overline{Vel}}(\boldsymbol{X}|\boldsymbol{K})$ less than 4). Consequently, Fig. 6(c) also illustrates that the newly proposed DYNO (see Eq. (3)) works effectively, in this case, to calibrate multiple variables simultaneously.

Figure 6 also illustrates that it is better to calibrate the hypothetical hydrodynamic model to velocity data rather than temperature data (see Fig. 6(a) and Fig. 6(b)) (if data for both variables is not available). Figure 6(a) indicates that calibrating to temperature only (i.e., the Cali-Tem scenario) results in a high chance that velocity error would be high (see the velocity error histogram in Fig. 6(a)). However, Fig. 6(b) illustrates that the errors in temperature when calibrating to velocity only (Cali-Vel) are likely to be relatively small in magnitude (see the temperature error histogram of Fig. 6(b)).

From the above discussion, we can conclude that calibrating to both temperature and velocity data with the newly proposed DYNO (implemented within the efficient surrogate algorithm PODS) is effective in obtaining a balanced calibration of both temperature and velocity variables. In real-world lake hydrodynamic applications, if available, both temperature and velocity data should be used for lake hydrodynamic model calibration. However, the very common practice of calibrating only to temperature data is shown to be unable to reproduce the flow dynamics well. This supports extra effort and expense to collect velocity data is expected to give a beneficial effect.

3.3 Impact of Different Forms of Normalization on the Performance of DYNO

This section investigates the impact of using different forms of normalization in the new objective function DYNO on optimization search performance. In Eq. (3), the error of each variable is normalized by the maximum and minimum values $f_k^{max}(\boldsymbol{X})$ and $f_k^{min}(\boldsymbol{X})$ of $f_k(\boldsymbol{X})$ among all the evaluations evaluated so far. One concern of using the maximum value $f_k^{max}(\boldsymbol{X})$ is that the objective function can be affected by extremely bad evaluations points. Another approach is to use the median value $f_k^{median}(\boldsymbol{X})$ of $f_k(\boldsymbol{X})$ among all the evaluations evaluated so far as a replacement of $f_k^{max}(\boldsymbol{X})$ to normalize the error of each variable. We refer to DYNO using the median value $f_k^{median}(\boldsymbol{X})$ as DYNO-N2 (as shown in Eq. (13)) to differentiate it from DYNO using the maximum value $f_k^{max}(\boldsymbol{X})$ (as shown in Eq. (3)), which we refer to as DYNO-N1 in the following text.

$$F(\boldsymbol{X}|\boldsymbol{K}) = \sum_{k\in\boldsymbol{K}} \frac{f_k(\boldsymbol{X}) - f_k^{min}(\boldsymbol{X})}{f_k^{median}(\boldsymbol{X}) - f_k^{min}(\boldsymbol{X})} \tag{13}$$

$$f_k^{median}(\boldsymbol{X}) = \text{med}\,\{f_k(\boldsymbol{X})\ for\ all\ \boldsymbol{X} \in \boldsymbol{\psi}\} \tag{14}$$

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where $f_k^{median}(\boldsymbol{X})$ and $f_k^{min}(\boldsymbol{X})$ are the median and minimum values of $f_k(\boldsymbol{X})$ among all the evaluations evaluated so far, and hence they are updated dynamically in each iteration during optimization.

The implementation of DYNO-N2 is similar to the implementation of DYNO-N1 (Eq. (3)). The only change is replacing the calculation related to $f_k^{max}(\boldsymbol{X})$ with $f_k^{median}(\boldsymbol{X})$. We tested relative efficacies of DYNO-N1 and DYNO-N2, by comparing three calibration trials, of each DYNO variant (using PODS), where each concurrent calibration trial was initialized using the same LHD. Figure 7 shows the progress of PODS with the two forms of DYNO as the objective functions. Figure 7 is similar in design to Fig. 5, and indicates that both forms of DYNO are able to balance the calibration on temperature and velocity. There are two trials where PODS with DYNO-N1 (using $f_k^{max}(\boldsymbol{X})$ for normalization) found a better solution than PODS with DYNO-N2 (using $f_k^{median}(\boldsymbol{X})$ for normalization).

The results here indicate that DYNO-N1 seems not adversely affected by the bad solution. A reason for this may be that PODS typically do not generate extremely bad solutions (i.e., outlier solutions with extremely large errors), since algorithm search is concentrated around the best solution found so far. However, if other optimization algorithms are used for calibration especially algorithms that explore the search space more, there maybe a higher likelihood of encountering outlier /extremely bad solutions during optimization search. Consequently, the performance of such algorithm with DYNO-N2 might be better than with DYNO-N2, which might need further investigation. The outlier solutions here mean solutions (obtained during the optimization search phase) that have much larger errors than other solutions found so far. Outlier or extremely bad solutions are also like for calibration problems where the model output is very sensitive to the calibration parameters (i.e., a small change in model parameters can cause huge changes in the model output that leads to much worse solutions).

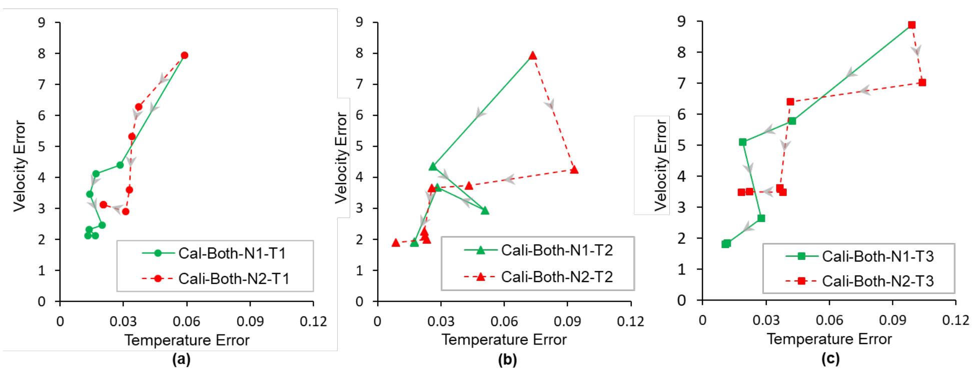

Figure 7. Calibration progress plot in terms of the best solution found during optimization search when using DYNO-N1 and DYNO-N2 as the objective function. Three random trials (T1, T2, and T3) are plotted in (a), (b), and (c). Lower velocity and temperature error are better. Figure 7 uses the same format as Figure 5.

3.4 Value of Velocity Measures in 3D Lake Model Calibration

High quality hydrodynamic simulations (e.g., thermal structure, current velocities, flow advection and vertical mixing) are vital for accurate spatial modelling of water quality in lakes. The hydrodynamic process influences the transport & production or transformation of biological and chemical components. Hence, if the simulation of

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flow dynamics is not adequately accurate, there is no way to achieve accuracy in the simulation of water quality. Previous studies use mostly temperature observations for the 3D lake hydrodynamic model calibration. Whereas, velocity data is less commonly used compared with temperature data for model calibration.

Our results in section 3.1 indicate that calibrating to temperature data only cannot guarantee accuracy in velocity simulation. Not using velocity data in model calibration (i.e., using temperature data in model calibration only) thus, may lead to large velocity errors (as indicated in the Figure 3). The inclusion of velocity measurements in calibration not only reduces velocity error but also helps improving the temperature fit. For example, in Fig. 4, when calibrating to both temperature and velocity data, the temperature error is smaller than the temperature error when calibrating to temperature data only. This is most obvious in the surface layers of both STN. A1 and STN. B1, where the temperature error when calibrating to both temperature and velocity (i.e., Cali-Both) is much smaller compared to calibrating to temperature only (i.e., Cali-Vel). The better result (better fit of temperature as well as velocity) in Cali-Both demonstrates the effectiveness of using velocity measures in 3D hydrodynamic lake model calibration. The comparison of calibrated parameter values in Cali-Both and Cali-Tem scenarios (in Table 5) also demonstrates the value of using velocity data besides temperature data in model calibration. In Table 5, we can see that the calibrated value of viscosity and diffusivity parameters in Cali-Both is much closer to the true value than that in Cali-Tem. This shows that the use of velocity measures helps to improve the calibrate of these viscosity and diffusivity parameters.

The risk of using only temperature data without velocity data, even for accurately simulating water temperature, is that temperature simulation is affected by both the flow dynamics and the heat transfer process. The fit of temperature data is a result of the combination of these two processes. However, the fit of the temperature data cannot guarantee accurate simulation of each of the processes, though accurate simulation of each process does guarantee the fit of temperature data. The velocity observation hence is valuable to help improve the flow dynamics simulation of the model, which is not only important for temperature simulation but also other water quality substances simulation (e.g., these biological and chemical components). Our research implication of the use of velocity observations is also in line with the study of Baracchini et al. (2020), where they also suggest have both temperature and current velocity for a complete system calibration.

3.5 Possibilities for Other Applications

In this study, we only demonstrate how DYNO can be incorporated into PODS parallel surrogate global optimization algorithm. (see section 2.6). However, the new objective function DYNO could also be easily utilized with other heuristic optimization methods (e.g., serial or parallel versions of Genetic Algorithm (Davis, 1991) and Differential Evolution (Tasoulis et al., 2004)) for effectively calibrating other multi-variables calibration problems. We have not provided a precise methodology for incorporating DYNO into other optimization methods though, since incorporation of DYNO depends on the structure of an optimization method, and structures of optimization methods vary a lot. We did illustrate in section 2.6 and Figure 3 on how components of parallel PODS are modified in order to use DYNO. Other optimization methods could be modified in a similar way to incorporate DYNO for use in multi-variable calibration.

Also, there are numerous other model calibration paradigms in general hydrology and water resources (besides the hydrodynamic model calibration) where simultaneous multi-variable and multi-site calibrations are required. Some examples of such multi-variable & multi-site calibration problems include watershed model

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calibration (Franco et al., 2020; Odusanya et al., 2019), seawater intrusion model calibration (Coulon et al., 2021), and water quality model calibration (Xia and Shoemaker, 2021) etc. In these problems, there are usually multiple constituents (e.g., substances) to be calibrated and the observations are usually available at multiple locations. Our new DYNO can potentially be used to calibrate them simultaneously. A popular calibration strategy for such problems in general hydrology is to use multi-objective calibration where it is assumed that a trade-off exists between multiple hydrologic responses (e.g., high flow, low flow, water balance, water quality etc.).

Using multi-objective algorithms, however, for calibrating hydrologic and watershed quality models may not be the most suited strategy for some case studies because i) multi-objective calibration can be computationally intensive if underlying simulations are computationally expensive and ii) meaningful trade-offs between different objectives may not exist. Kollat et al. (2012) demonstrate that prior multi-objective calibration exercises may have over-reported the number of meaningful trade-offs in hydrologic model calibration. DYNO is a reasonable alternative to classical multi-objective calibration in calibration problems where the trade-off between multiple component calibration objectives is not significant, because i) a balance between multiple constituent objectives is maintained with DYNO and ii) a single objective algorithm can be used with DYNO, which is computationally more efficient than a multi-objective algorithm. This is especially true for multi-constituent watershed model calibration problems where the achievable objective functions ranges for different constituents (e.g., flow, sediment, phosphorus etc.) are quite different. Multiple prior studies (Moriasi et al., 2012; Moriasi et al., 2015) highlight that achievable ranges of statistical calibration measures (e.g., Nash Sutcliffe Efficiency (NSE), bias etc.) are significantly different for different constituents (e.g., streamflow, sediment, total phosphorus etc.). Moriasi et al. (2015) note that in most watershed model case studies, the achievable range of NSE for streamflow is higher than the achievable range for total phosphorus. Hence, DYNO may be extremely effective in balancing simultaneous calibration of streamflow and phosphorus for such case studies. We believe that there is immense potential in the application of DYNO for multi-constituent watershed model calibration.

4 Conclusions

We conclude that the Dynamically Normalized Objective Function we propose is a new effective way to balance the calibration to different variables (i.e., temperature and velocity) in optimization-based -calibration. It is possible that the magnitudes of goodness-of-fit measures for different variables are very different (which may fluctuate during the optimization search), and thus the optimization search cannot maintain balance between different variables. Hence DYNO dynamically modifies the objective function, for multi-variable calibration, so that the error for each variable is being dynamically normalized in each iteration. This is to ensure that the search is giving approximately equal weight to each variable (e.g., velocity and temperature).

The proposed DYNO is tested in this study for simultaneous temperature and velocity calibration of a lake model. Moreover, DYNO is integrated with the PODS algorithm for testing on expensive lake hydrodynamic model calibration in parallel. Results indicate that using DYNO ensures a balanced calibration between temperature and velocity. We provide a detailed analysis to illustrate that DYNO balances the weight between different objectives dynamically, and thus allows for a balanced parameter search during optimization.

We conclude that calibrating to the error of one variable (either temperature or velocity) cannot guarantee the goodness-of-fit of another variable. Of course, the most accurate predications can be obtained by having both temperature and velocity data. These comparisons are possible because we have, via synthetic simulation, the true

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solution for the lake model. Our analysis suggests that in real practice, both temperature and velocity data are important for model calibration. The common practice of calibrating only to temperature data is not sufficient to reproduce the flow dynamics accurately and extra effort and expense to collect velocity data is expected to give a beneficial effect.

There are many possible future areas for application of this method. The Dynamically Normalized objective function (DYNO) would be effective for other multi-variable and multi-site calibration problems (especially for problems with many variables). Future research could apply the DYNO methods on other problems and using other optimization algorithms.

Code and Data availability

The tropical reservoir hydrodynamic numerical model and data were provided by PUB, Singapore's National Water Agency (https://www.pub.gov.sg/). The Delft3D open source code could be downloaded from https://oss.deltares.nl/web/delft3d/source-code. The PODS open source code could be download from https://github.com/louisXW/PODS. The code for objective function can be download from https://github.com/louisXW/DYNO-pods.

Author contributions

WX took responsibility for the methodology, software, formal analysis, investigation, original draft preparation, and visualization. WX, TA, CAS discussed the design and results and edited the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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