Hydrodynamical Modeling

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Introduction

We model lakes to visualize and quantify fluid flow, mass transport, and thermal structure. Understanding the evolving physical state (e.g., surface elevation, density, temperature, velocity, turbidity) is necessary for modeling fluxes of nutrients, pollutants, or biota in time-varying fields of one, two, or three space dimensions (1D, 2D, or 3D). Hydrodynamic modeling provides insight into spatial–temporal changes in physical processes seen in field data. For example, Figure 1 shows temperature profiles simultaneously recorded at different stations around Lake Kinneret (Israel). Extracts from model results (Figure 2) provides a context for interpreting these data as a coherent tilting of the thermocline. A time series of the thermocline can be animated, showing the principal motion is a counter-clockwise rotation of the thermocline. The complexities of the thermocline motion can be further dissected by using spectral signal processing techniques to separate wave components, illustrating a basin-scale Kelvin wave, a first-mode Poincaré wave, and a second-mode Poincaré wave.

It is said we build by 'measuring with micrometer, marking with chalk, then cutting with an axe'. However, hydrodynamic modeling inverts this process: we take an axe to the real world for our governing equations; we chalk a model grid on our lake, then numerically solve to micrometer precision. Thus, the governing equation approximations, grid selection, and numerical method all affect how a model reflects the physical world. Selecting an appropriate model requires understanding how model construction may affect the model solution.

As a broad definition, hydrodynamic modeling is the art and science of applying conservation equations for momentum, continuity, and transport (Figure 3) to represent evolving velocity, density, and scalar fields. The modeling science is founded upon incompressible fluid Newtonian continuum mechanics, which can be reduced to (1) any change in momentum must be the result of applied forces, and (2) the net flux into or out of a control volume must balance the change in the control volume. The modeling art is in selecting approximations, dimensionality, and methods that fit the natural system and provide adequate answers to the question asked.

Tables 1–4 list some of the 1D, 2D, and 3D lake modeling work from the mid-1990s to the present in the refereed literature. Unfortunately, much of the details of model development have been relegated to technical reports that are often either unavailable or difficult to obtain. Similarly, modeling applications conducted by or for government agencies often does not reach refereed publication. However, technical reports are generally detailed and valuable resources for applying and analyzing results; the reader is encouraged to seek out these publications before applying any model.

Dimensionality and Capabilities

Lake and reservoir models range from simple representation of thermocline evolution to multidimensional modeling of transport and water quality. Averaging (or integrating) the governing equations across one or more spatial dimensions provides representation of larger areas with less computational power. Such reduced-dimension models require less boundary condition data but more parameterization/calibration data. The simplest lake models average over horizontal planes (i.e., x and y directions) to obtain a 1D-model of the vertical (z-axis) lake stratification. Narrow reservoirs are modeled in 2D by laterally-averaging across the reservoir, thereby representing both vertical stratification and horizontal gradients from the headwaters to the dam. In shallow lakes, 2D-models in the x-y plane are used to examine depth-averaged circulation (without stratification). These reduced-dimension approaches cannot directly simulate variability in an averaged direction. However, such variability may be parameterized where processes are sufficiently well understood; in contrast, where processes are not understood or cannot be parameterized, the missing variability affects calibration and model results. Modelers must be careful not to simply parameterize or calibrate a poorly understood process by arbitrarily altering model coefficients.

Increasing model dimensionality and complexity reduces the time-scale over which a lake can be modeled. Typically, 1D-models can be applied for decades; 2D-models over multiple years to decades; 3D-models over days/weeks/months (but have been applied for longer in a few cases). This inverse relationship between dimensionality and time is not simply a function of computational power, but is inherent in the effects of stratification, mixing parameterizations, and model data requirements. For 1D-models,

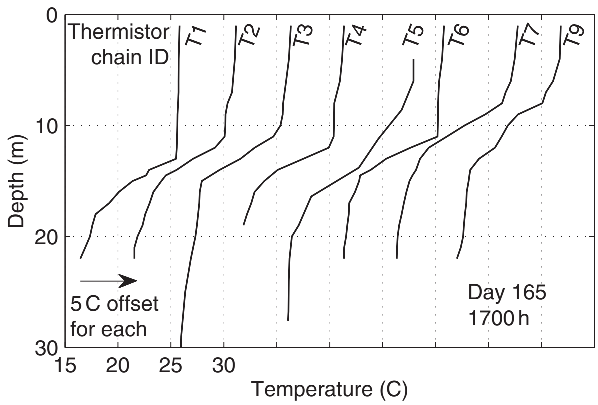

Figure 1 Temperature profiles collected in Lake Kinneret in 1997 (data of J. Imberger, Centre for Water Research, University of Western Australia).

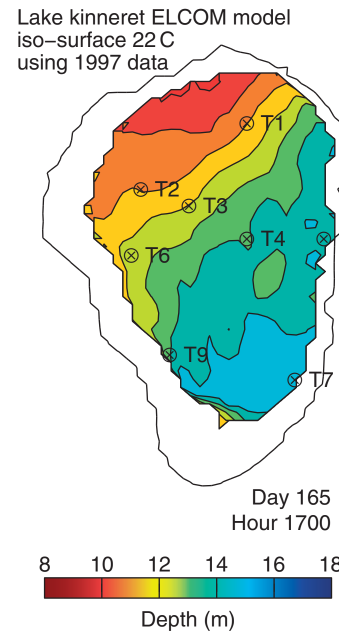

Figure 2 Modeled depth of temperature isosurface in the thermocline. Results from 3D-model at same time as field data collected in **Figure 1**.

vertical mixing is readily parameterized or calibrated to maintain sharp thermal stratification. However in 2D- and 3D-models, vertical mixing is caused by both the turbulence model and numerical diffusion of mass (a model transport error). Numerical diffusion always leads to weakening the thermocline, which affects modeled circulation and mixing that further weakens the thermal structure in a positive feedback cycle. Thus, longer-term 2D- and 3D-models require careful setup and analysis or results may be dominated by model error that accumulates as excessive mixing across the thermocline, resulting in poor prediction of residence time, mixing paths, and lake turnover.

For 1D-models (Table 1), we distinguish between turbulent mixing models derived from energy principals (e.g., DYRESM) or averaging transport equations (e.g., k-epsilon models) and pure calibration models that simply fit coefficients to nonphysical model equations (e.g., neural networks). Between these extremes are vertical advection/diffusion models (e.g., MINLAKE), which represent hydrodynamics by an advection/diffusion equation that requires site-based calibration. To the extent that more mechanistic models have all physical processes represented and correctly parameterized without site-specific calibration, they can be reasonably used for long-term predictions and readily transferred from lake to lake. Models relying solely on parameter fitting are questionable outside the calibration range, but are often easier to apply when sufficient calibration data is available. Although mechanistic models are arguably preferred, we rarely have sufficient data for a completely calibration-free mechanistic model; thus, in practical application such models are generally calibrated to some extent.

Laterally-averaged 2D-models (Table 2) are the workhorse of reservoir hydrodynamic/water quality modeling. For a narrow reservoir, the lateral-averaging paradigm is successful in capturing the bulk thermal/hydrodynamic processes, which are dominated by the large pelagic volume. However, where water quality processes are dependent on concentrations in shallow littoral regions, such models must be used carefully and with some skepticism. For example, a littoral algae bloom may depend on high nutrient concentrations that result from reduced circulation in the shallows. To correctly represent the bloom, a 2D water quality model must distort the biophysical relationships between growth rate and concentration. Furthermore, any scalar (e.g., toxic spill) represented simply by a concentration will automatically be diffused all the way across the reservoir, whether or not there is sufficient physical transport. Thus, a laterally averaged model will represent a toxic spill that mixes as a function of the reservoir width rather than physical processes.

Although 3D-models (Table 3) provide good representations of lake physics, they are notoriously complicated to set up and run. Although their operation is becoming easier with more established models, the progression to 'black box' modeling (i.e., where the user is not intimately familiar with the model itself) remains problematic. The interaction of the lake physics with the numerical method, governing equation approximations, time step, grid size, and initial/boundary condition data provides a wide scope for model inaccuracies. The effectiveness of a 3D-model

Momentum:

$$\underbrace{\frac{\partial u_i}{\partial t}}_{\text{Unsteady velocity}} + \underbrace{\sum_{j=1}^{3} u_j \frac{\partial u_i}{\partial x_j}}_{\text{Nonlinearity}} = \underbrace{-g_i}_{\text{Gravity force}} \underbrace{- \frac{1}{\rho_0}\frac{\partial P_{nh}}{\partial x_i}}_{\text{Non-hydrostatic pressure gradient}} \underbrace{-g\frac{\partial \eta}{\partial x_i}}_{\text{Free-surface or 'barotropic' pressure gradient}} \underbrace{-\frac{g}{\rho_0}\frac{\partial}{\partial x_i}\int_{z}^{\eta} \Delta\rho \, dx_3}_{\text{Stratification or 'baroclinic' pressure gradient}} + \underbrace{\sum_{j=1}^{3} \nu \frac{\partial^2 u_i}{\partial x_j^2}}_{\text{Viscous force}} \quad : \; i=1, 2, 3$$

Continuity:

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} = 0$$

Free surface evolution

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x_1}\int_{B}^{\eta} u_1 dx_3 + \frac{\partial}{\partial x_2}\int_{B}^{\eta} u_2 dx_3 = 0$$

x_i	Cartesian space (i = 1, 2 are horizontal; i = 3 is vertical)
u_i	Velocity
η	Free surface elevation
B	Bottom elevation
g	Gravitational acceleration
ν	Kinematic viscosity
P_{nh}	Non-hydrostatic pressure
ρ_0	Reference density
$\Delta\rho$	Difference between local density and reference density

Figure 3 General 3D incompressible flow equations (with the Boussinesq approximation) that are the basis for most hydrodynamic models. Hydrodynamics in lake modeling also requires transport equations for temperature, salinity (if important), and an equation of state for density.

presently depends on the user's understanding of the model capabilities and limitations. It is doubtful that we will see scientifically dependable black box models for at least another decade or so. Development of such models depends on development of expert systems that can replace a modeler's insight and experience in diagnosing different error forms.

Boundary and Initial Conditions

A hydrodynamic model is a numerical solution of an initial-and-boundary-value problem of partial differential or integral–differential equations. The model solution is never better than the initial and boundary conditions used for model forcing. Lake boundary conditions include spatially-varying wind field, thermal and mass exchange with the atmosphere, river inflows/outflow, groundwater exchanges, local catchment runoff, and precipitation. Boundary conditions may be poorly known, so understanding the model sensitivity to possible perturbations boundary conditions is necessary for setting the bounds of model believability.

Initial conditions are a snapshot of the system at time $t = 0$ (the model start time). Problems arise from our inability to obtain the full data set necessary to initialize a model (a problem that increases with model dimensionality). These problems can be somewhat reduced by providing sufficient model 'spin-up' time so that the boundary forcing dilutes the initial condition error. However, spin-up is only successful when (1) the initial conditions are a reasonable approximation of $t = 0$ and (2) the boundary forcing dominates the initial conditions by the end of spin-up. For example, in 3D-models the velocity initial condition is usually zero and the spin-up time is approximated by the 'spin-down' time from typical circulation velocities (i.e., the time over which inertia can be expected to keep water moving). However,

Table 1 Examples of 1D hydrodynamic lake models

Model	*Name/source*	*Notes*	*Details*	*Applications*
AQUASIM		tu	15, 31	15, 31, 32
DLM	Dynamic Lake Model	tu	23	7, 23, 24, 27, 33
DYRESM	Dynamic Reservoir Simulation Model	tu	14, 21	1, 5, 6, 14, 16, 17, 18, 22, 26, 35, 36
MINLAKE	Minnesota Lake Model	adv/dif	9, 20, 25	8, 9, 10, 11, 12, 13, 19, 34
Other		adv/diff	4, 30, 37	2, 3, 4, 30, 37
Other		tu	28	28, 29

tu: turbulent transport model; adv/diff: calibrated advection/diffusion transport model.

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a lake model with temperature initial condition that does not reflect the initial real-world stratification cannot recover through spin-up.

Calibration

Ideally, hydrodynamic models should not require calibration; i.e., with sufficient data for boundary conditions, initial conditions and turbulence coefficients, a model should adequately represent the physics of the real system. Unfortunately, our data and parameterizations are often inadequate. Calibration may be either through adjusting turbulence coefficients (e.g., the various '*c*' values in a k-epsilon model) or by adjusting boundary conditions. Modelers often jump straight into adjusting a turbulence model rather than examining the sensitivity of the model to inaccuracies in the boundary conditions. For example, wind-driven lakes may have unknown spatial gradients of the wind, or the wind sensor may be biased (e.g., in the wind shadow of a building). If the applied wind data under-predicts the actual wind forcing, then calibrating the turbulence model could lead to the 'right' answer for the wrong reason! There should be evidence that the calibrated process is the data mismatch problem (not just the solution). Furthermore, naïve calibration of turbulence coefficients can lead to unphysical values (e.g., an efficiency greater than unity should be a warning sign that something has been missed).

Hydrostatic Approximation

Horizontal length scales are larger than vertical scales in lakes and reservoirs, so the hydrostatic approximation is generally employed. This approximation neglects vertical acceleration ($\partial u_3/\partial t$) and nonhydrostatic pressure gradients ($\partial P_{\mathrm{nh}}/\partial x_i$). Note that vertical transport may be reasonably represented in a hydrostatic model, even while vertical acceleration is neglected. Vertical transport has multiple causes: continuity applied to divergence/convergence in the horizontal plane, turbulent mixing, and vertical inertial effects; only the latter is hydrostatically neglected.

Although large-scale free surface motions and the resulting circulations are well-represented by a hydrostatic model, internal seiches are more problematic. Tilting of a pycnocline (e.g., a thermocline) may be relatively steep and ensuing basin-scale waves may evolve in a nonhydrostatic manner. However in a hydrostatic model, the numerical dispersion errors may mimic nonhydrostatic behavior. Thus, physically correct wave dispersion may be serendipitously achieved when numerical dispersion is similar to physical dispersion. Such results must be used with caution as they are highly grid-dependent and the serendipitous confluence of errors may disappear when the model grid is refined. When model results show greater disagreement with the physical world as the model grid is made finer, this type of error may be a suspect.

Applying nonhydrostatic models for large-scale natural systems requires significantly more computational time, model complexity, and modeling expertise than for similar hydrostatic models. An extremely fine model grid and time step is necessary resolve vertical accelerations and nonhydrostatic pressure gradients. Nonhydrostatic lake and ocean models are actively under development, but their widespread application is not imminent.

Model Grid

Overview

Hydrodynamic modeling requires discretizing physical space on a model grid. The size and characteristics of the grid determine the scales of what a model can and cannot represent. In the horizontal plane, there

Table 2 Examples of 2D hydrodynamic lake models

Model	*Name/Source*	*Notes*	*Details*	*Applications*
CE-QUAL-W2	U.S. Army Corps of Engineers	fd, la, Ca		1, 2, 3, 7, 8, 9, 10, 17, 19, 20, 21, 24
RMA2	Research Management Associates	fe, da, cu		14, 23
HYDROSIM	Hydrodynamic Simulation Model	fe, da, cu	11	18
others		la	5, 26	5, 12, 13, 26
others		da	4, 16, 22	4, 6, 16, 22

Numerical Method: fd = finite difference; fe = finite element

Horizontal Grid: Ca = Cartesian grid; cu = curvilinear grid

2D form: da = depth-averaged; la = laterally-averaged

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Table 3 Examples of 3D hydrodynamic lake models

Model	*Name*	*Notes*	*Details*	*Applications*
CH3D	Curvlinear Hydrodynamics in 3-Dimensions	cfd, cu, zl/ sg, ms	10, 34	16
EFDC	Environmental Fluid Dynamics Code	cfd, cu, zl, ms		9, 12, 13, 14, 15
ELCOM	Estuary and Lake Computer Model	cfd, Ca, zl, si	11	2, 7, 8, 11, 17, 18, 19, 20, 21, 23, 25, 26, 27, 28
GLLVHT	Generalized Longitudinal Lateral Vertical Hydrodynamic and Transport Model	fd, cu, we, si		24, 36
POM; ECOM	Princeton Ocean Model; Estuary and Coastal Ocean Model	cfd, cu, sg/ zl, ms/si	1	1, 3, 4, 5, 33, 35, 37
RMA10	Research Management Associates 10	fe, un, zl		6, 29
SI3D	Semi-Implicit 3D	cfd, cu, zl, si	31	30, 31, 32

Numerical Method: cfd – conservative finite difference; fd – finite difference; fe – finite element.

Horizontal Grid: Ca – Cartesian grid; cu – curvilinear grid; un – unstructured grid.

Time-stepping: ms – mode-splitting; si – semi-implicit.

Vertical Grid: zl – z-level vertical grid; sg – sigma grid.

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are three grid systems: Cartesian, curvilinear, and unstructured. For models including a vertical dimension, the vertical grid may be terrain-following (sigma coordinate), Cartesian (z-level) or isopycnal (Lagrangian). Unstructured grids can also be used in the vertical plane, but have not been widely adopted.

Grid Size and Convergence

The local grid size controls the 'resolution' of local processes; e.g., a single grid cell has only a single velocity on a simple Cartesian finite-difference grid. Thus, the grid mesh is a top-level control on the resolvable physics and transport. For example, if only two grid cells are used across a narrow channel the transport may be theoretically either unidirectional or bidirectional; however, two grid cells cannot represent a deep center channel flow with return flows along both shallow banks. A useful exercise is to consider how many grid cells are necessary to represent 1.5 periods of a sine wave: although three cells is clearly the minimum, the resulting discrete pattern will not be particularly sinusoidal. Arguably, 10–15 grid cells should be the minimum resolution for most important flow features. An effective model grid resolves the key physical features at practical computational cost. Grid design should be an iterative process wherein model results at different grid scales are compared to gain insight into model performance. A model grid is 'converged' when further grid refinement does not significantly change model results. Unfortunately, obtaining a converged grid is not always practical; indeed, most large-scale models suffer from insufficient grid resolution. Such models may still have validity, but grid-scale effects may dominate physical processes.

Horizontal Grid Systems

Cartesian grids are obtained with a square or rectangular mesh (Figure 4(a)). The mesh structure allows simple model coding since a grid cell's neighbors are easily determined. For multidimensional models, simple Cartesian grids cannot be applied with fine resolution in some regions and coarse resolution in others. These deficiencies can be addressed with 'plaid' structured meshes (i.e., nonuniform Cartesian grid spacing), domain decomposition or nested grid (e.g., quadtree) techniques. To use an efficient rectangular mesh on a sinuous reservoir, the topography may be straightened along the channel centerline before applying the Cartesian mesh.

Curvilinear grids in the horizontal plane are structured meshes (similar to a Cartesian grid) that smoothly distort the quadrilateral elements throughout horizontal space (Figure 4(b)). The distortion between physical (x,y) space and curvilinear (ξ,η) space requires transformation of the governing equations. Curvilinear meshes allow fine grid resolution in one area and coarse resolution in another, as long as the mesh changes smoothly between regions. The smoothness and orthogonality of the mesh (as seen in physical space) will affect the model solution. Reasonable rule-of-thumb criteria are (1) adjacent grid

Table 4 Model applications

Lake	*1D*	*2D*	*3D*
Akkajaure Reservoir (Sweden)	28		
Lake Alpnach (Switzerland)	15		
Lake Baldegg (Switzerland)	15		
Lake Balaton (Hungary)		4	
Lake Baikal (Russia)		5, 12	
Bassenthwaite Lake (UK)	2		
Lake Belau (Germany)		22	
Lake Beznar (Spain)	27		
Brenda Pit Lake (Canada)	16		
Brownlee Reservoir (USA)		24	
Lake Burragorang (Australia)	26		26, 27, 28
Cheatham Lake (USA)		1	
Clear Lake (USA)		23	30, 32
Lake Constance (Germany/Switzerland)			2
Cummings Lake (Canada)	24		
Dexter Pit Lake (USA)	1		
East Dollar Lake (Canada)	24		
Entrepenas Reservoir (Spain)	37		
Lake Erie (Canada/USA)		3	22
Flint Creek Lake (USA)			36
Great Slave Lake (Canada)			21
Hartwell Lake (USA)			9
Hume Reservoir (Australia)	33		
Isikli Reservoir (Turkey)		10	
Kamploops Lake (Canada)		13	
Lake Kinneret (Israel)	5, 14		11, 18, 20, 23
Lake Ladoga (Russia)			3
Lake Maracaibo (Venezuela)			17, 19
Lake Michigan (Canada/USA)			33
Lake Monoun (Cameroon)	22		
Mundaring Weir (Australia)			25
Lake Neusiedl		16	
Lake Nyos (Cameroon)	22, 23, 31, 32		
Lake Ogawara (Japan)			7
Lake Okeechobee (USA)			12, 13, 14, 15
Onondaga Lake (USA)			1
Orlik Reservoir (Czech Republic)	35		
Otter Lake (USA)	19		
Lake Paldang (South Korea)			24
Pareloup Reservoir (France)	30		
Pavin Crater Lake (Canada)	16		
Prospect Reservoir (Australia)	26		
Lake Rinihue (Chile)	6		
Rochebut Reservoir (France)	30		
Lake Saint Pierre (Canada)		6, 18	
Salton Sea (USA)			6
Sau Reservoir (Spain)	18		
Schoharie Reservoir (USA)		7, 8	
Lake Shasta (USA)		2, 9, 21	
Lower Shaker Lake (USA)		14	
Shihmen Reservoir (Taiwan)		25	
Slapy Reservoir (Czech Republic)	35		
Lake Soyang (Korea)		15	
J. Strom Thurmond Lake (USA)		20	
Lake Superior (Canada/USA)			5, 37
Lake Tahoe (USA)	7		31
Te Chi Reservoir (Taiwan)		17, 26	
Tseng-Wen Reservoir (Taiwan)		17	
Lake Victoria (Kenya/Tanzania/Uganda)			35
Villerest Reservoir (France)	3, 4		
Lake Washington (USA)			16
Wellington Reservoir (Australia)			8
Lake Yangebup (Australia)	36		

Numbers correspond to notes from **Tables 1, 2,** and **3** for 1D, 2D and 3D models, respectively.

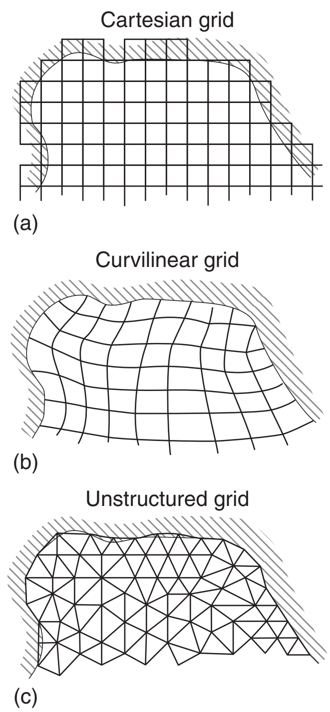

Figure 4 Plan view illustrating different horizontal grid systems.

cells should have increased/decreased volume by no more than 10% and (2) off-orthogonal transformation metrics should be an order of magnitude smaller than orthogonal metrics. Smooth curvilinear meshes can be manually designed with simple drafting tools, but stand-alone mesh creation software is generally used. Some models require orthogonality or near-orthogonality for the mesh, which severely constrains mesh creation.

Unstructured grids in the horizontal plane are composed of n-sided polygons (Figure 4(c)); triangular and quadrilateral elements are typically preferred or required. An unstructured mesh is the easiest for fitting complicated topography and arguably has the greatest flexibility for providing fine resolution in some areas with coarse resolution in others. However, model solutions are still affected by local gradients of grid cell volume and grid orthogonality. Creating a good unstructured grid is an art, requiring separate grid creation software and a lengthy trial-and-error process. It is often necessary to carefully examine model performance on several different unstructured grids to gain an understanding of how different grid choices affect the solution. Finite difference and finite volume models for unstructured meshes are relatively recent developments, but have not yet seen extensive use in lakes or reservoirs.

Vertical Grid Systems

Z-level grids are the simplest vertical system, using layers with whose thickness is uniform across the horizontal plane (Figures 5(a)). Layer thicknesses may vary in the vertical, but should do so smoothly (i.e., no more than about 10% expansion of thickness in adjacent layers). Z-level grids are generally preferred for 2D and 3D lake models due to their simplicity. A disadvantage is that steep bottom slopes are represented as discrete stair steps, which distorts along-slope flow. Coupling a 2D- or 3D-model with a benthic boundary layer model can overcome the stair-step problem, albeit by increasing model complexity and introduction of empiricism and ad hoc coupling mechanisms.

Sigma-coordinate (terrain following) vertical grid systems are commonly used in oceanic-scale modeling (e.g., the Great Lakes), but have significant drawbacks for inland waters. Sigma-coordinate systems divide each water column into a fixed number of layers, resulting in thick layers in deep water and thin layers in shallow water (Figures 5(b)). For sloping boundaries, the sigma-coordinate system must be truncated or a singularity occurs where the depth goes to zero. Sigma-coordinates are preferred for modeling along-slope processes, but may distort internal wave dynamics along the slope.

Isopycnal coordinate systems require a moving grid that tracks the Lagrangian movement of predefined isopycnals (Figures 5(c)). This approach is common for 1D lake models as a means of easily tracking stratification creation and destruction. Multidimensional isopycnal models have been developed for ocean simulations to limit numerical diffusion that otherwise weakens stratification; these models have not seen wide application in lakes or reservoirs.

Time Step

Unsteady models take an initial density/velocity field and advance these forward in time (subject to the boundary conditions of the system). A model that is stable at a large time step is often prized as being more computationally efficient. The model time step is generally limited by a Courant–Lewy–Friedrichs (CFL) condition, defined as $u \Delta t \Delta x^{-1} < C_a$, where u is a velocity (fluid or wave), Δt is the time step, Δx is the grid spacing (in the same direction as u), and C_a is a constant that depends on the numerical method (typically $C_a \leq 1$). Some models also have a viscous limitation controlled by the turbulent vertical eddy viscosity (ν_z) such that $\nu_z \, \Delta t \, \Delta z^{-2} < C_\nu$. It is possible to design stable numerical methods for $C_a > 1$ or $C_\nu > 1$; however stability at large time step does not imply accuracy. For example, a reservoir that is 10 m deep × 10 km length will have a surface seiche period of ∼30 min; the physics of this seiche cannot be modeled with a 20 min time step, even if the model is stable. Thus, the model time step should be chosen *both* for model stability and to accurately resolve the time-scale of processes. In particular, a large model time step will mask the cumulative effect of nonlinearities from short-time-scale processes.

Numerical Methods

There are three basic methods for discretizing the governing equations on a model grid; in order of increasing complexity these are: (1) finite difference, (2) finite volume, and (3) finite element. *Finite difference methods* represent spatial derivatives by discrete gradients computed from neighboring grid cells. *Finite volume methods* pose an integral form of the governing equations for conservative cell-face fluxes. Both finite difference and volume methods provide a set of discrete algebraic equations representing the continuous governing equations. For a model with a sufficiently refined grid and time step, the solution of the discrete equations is an approximate solution of the continuous equations. In contrast, *finite element methods* directly approximate the *solution* of the governing equations rather than the governing equations themselves. Finite element methods are often characterized as being appropriate for unstructured grids, whereas finite difference methods are often characterized as appropriate for structured grids; this outdated canard needs to be put to rest. Finite difference and finite volume methods have both been successfully applied on unstructured grids, and finite element methods can also be successfully applied to structured grids. The choice of grid and numerical method are entirely independent in model development. However, most models are designed for only one type of grid.

The finite element method is mathematically appealing but requires considerable computational effort, especially for density-stratified flows. Because temperature gradients are directly coupled to momentum through density and hydrostatic pressure gradients, a pure finite element discretization requires simultaneous solution of momentum, temperature transport, and an equation of state. As a further complication, global and local conservation is not always achieved in finite element methods; i.e., local scalar transport fluxes into and out of an element may only approximately balance the scalar accumulation in the element, and the integrated global scalar content may not be conserved. These effects can create problems for water quality models that are directly coupled to finite element hydrodynamic models as source/sink water quality terms may be dominated by numerical nonconservation. Note that consistent finite element methods may be implemented for global scalar conservation, but many existing codes have not been tested or proven consistent.

Finite difference and finite volume methods are conceptually quite different, but may be very similar in the model code. Finite differences are often described as point-based discretizations, whereas finite-volume methods are described as cell-based. However, most multidimensional hydrodynamic models apply a hybrid approach: momentum is discretized with finite differences, but continuity is discretized on a staggered grid, which is discretely equivalent to a volume integral (i.e., a finite volume approach). Thus, these hybrid or ‘conservative finite difference’ methods ensure exact volume conservation for fluxes into and out of a grid cell. This exact local and global scalar transport conservation, along with their simplicity, has made these methods the most popular 3D-modeling approaches.

Order of Accuracy

Multidimensional models are often judged by the ‘order of accuracy’ of their time and space discretizations for the governing equations. This order reflects how the error changes with a smaller time step or smaller grid spacing. For example with 2nd-order spatial discretization, model error reduces by two orders of magnitude for each magnitude reduction in grid size. Higher-order methods are generally preferred, although they are more computationally expensive than low-order methods for the same number of grid cells. There is a trade-off when computational power is limited: a higher-order method may only be possible with a larger time step and/or grid cell size than a lower-order model. It is generally thought that for converged grids the absolute error of a higher-order method on a coarse grid will be less than the absolute error of a lower-order method on a fine grid. However, this idea presupposes that both the model grids provide converged solutions. When the grid cannot be fully converged due to computational constraints (often the case for practical problems), the comparative efficiency of high-order or low-order methods must be determined by experimentation.

As a general rule, 1st-order spatial discretizations (e.g., simple upwind) are too numerically diffusive for good modeling. Spatial discretizations that are 2nd-order (e.g., central difference) often have stability issues, so 3rd-order (e.g., QUICK) is generally preferred. The best 3rd-order spatial methods include some form of flux limiting (e.g., TVD or ULTIMATE) to reduce unphysical oscillations at sharp fronts. Fourth-order and higher spatial discretization methods can be found in the numerical modeling literature, but have not been applied in any common lake models.

For time discretizations, 2nd-order methods (e.g., Crank–Nicolson) are preferred, but many models are only 1st-order due to the complexity of higher-order methods. In general, if one process is modeled with a 1st-order time-advance, then the entire scheme is 1st-order. As a note of caution, some semi-implicit 2nd-order methods may be only 1st-order accurate (albeit stable) for CFL > 1.

Model Errors

We separate the idea of 'model error' from 'data error'; the latter is associated with incorrect or unknown boundary/initial conditions, while the former is inherent in the model itself. Model errors are not randomly distributed. Instead, models provide an exact solution of an approximation of the governing equations, so the errors are determined by the discrete approximations. Three different types of fundamental errors will occur in any sufficiently complicated transport field: numerical diffusion of mass, numerical dissipation of energy and numerical dispersion of waves.

Numerical diffusion of mass occurs when advection of a sharp density gradient causes the gradient to weaken (as if mass diffusivity were greater). In a stable model, this error is has a net bias towards weakening sharp gradients and can be a significant problem for representing the evolution of stratification when an active internal wave field is modeled.

Numerical dissipation of energy occurs when momentum is numerically diffused (as if viscosity were greater). This effect is generally referred to as 'numerical viscosity'. It typically occurs near sharp velocity gradients and tends to weaken the gradients. A stable model requires nonnegative numerical dissipation, as negative (or anti-) dissipation leads to positive feedback and the exponential growth of kinetic energy (i.e., the model 'blows up').

Numerical dispersion of waves occurs when a model propagates a wave component (free surface or internal) at the wrong speed. This effect can have interesting consequences for hydrostatic models (as discussed in Hydrostatic Approximation above).

In general, higher-order models have smaller errors, but may lead to antidiffusion (i.e., artificial resharpening of a gradient) or antidissipation (i.e., artificial increase in energy) that can destabilize a model. For any model to be reliable, the numerical diffusion of mass should be an order of magnitude smaller than turbulent mixing, and numerical dissipation of energy should be an order of magnitude less than turbulent dissipation.

Modeling Turbulence and Mixing

The governing equations for lake and reservoir hydrodynamic modeling are generally the Reynolds-Averaged Navier Stokes (RANS) equations, although some Large-Eddy Simulation (LES) methods may be suitable for future applications. With either method, processes smaller than the grid and time scales are empirically-modeled rather than directly simulated. Local values for eddy viscosity and eddy diffusivity are generally used to represent the nonlinear turbulent advection of momentum (viscosity) and scalars (diffusivity). As turbulence varies in both time and space, constant and uniform values of eddy viscosity are rarely appropriate. In particular, the ability of stratification to suppress vertical turbulence and mixing leads to nonuniform profiles with near-zero values at strong stratifications. A wide variety of RANS turbulence models are in use, the most popular being $k-\varepsilon$, $k-l$, and mixed-layer approaches, which must be modified to account for stratification. Performance of turbulence models may be highly dependent on the model grid resolution, so grid selection must be combined with selection of the appropriate turbulence model and settings. A key difficulty is that discretization on a coarse model grid (often required due to computational constraints) leads to high levels of numerical dissipation and diffusion. Indeed, it is not unusual to find that the model error dominates the turbulence model, particularly in the horizontal flow field. The relative scales of numerical dissipation and diffusion may also have an impact. If numerical dissipation is dominant, then internal waves may be damped before they cause significant numerical diffusion of mass. Thus, a 2D- or 3D-model that artificially damps internal waves may provide a 'better' long-term representation of the thermocline, but at the cost of poorly representing the 2D or 3D transport processes!

Similarities and Differences between Lake and River Modeling

Although the focus of this article is on lake models, many of the underlying discussions of model types and errors are equally applicable to river modeling. Such models can also be 1D, 2D, or 3D, may be hydrostatic or nonhydrostatic, and have difficulties with turbulence modeling and grid resolution (especially at finer scales). River models are perhaps easier to validate because there is a single major flux direction (downstream) that quantitatively dominates the hydrodynamics; this directionality is in dramatic contrast to the unsteady oscillatory forcings in a lake that make collecting sufficient validation data a complex and time-consuming task. On the other hand, the higher flow rates typical of rivers lead to bed motion and sediment transport that may strongly affect the flow patterns. At high flows, rivers may be geomorphically active and the use of simple fixed-bed models (appropriate for lakes over shorter time scales) may be entirely unsuitable. Thus, knowledge gained in lake modeling cannot always be transferred directly to rivers or vice versa – each discipline has its own key challenges. For lakes, modeling evolving temperature stratification is the critical requirement; for a river model, the correct representation of the riverbed geometry and its geomorphologic evolution is critical.

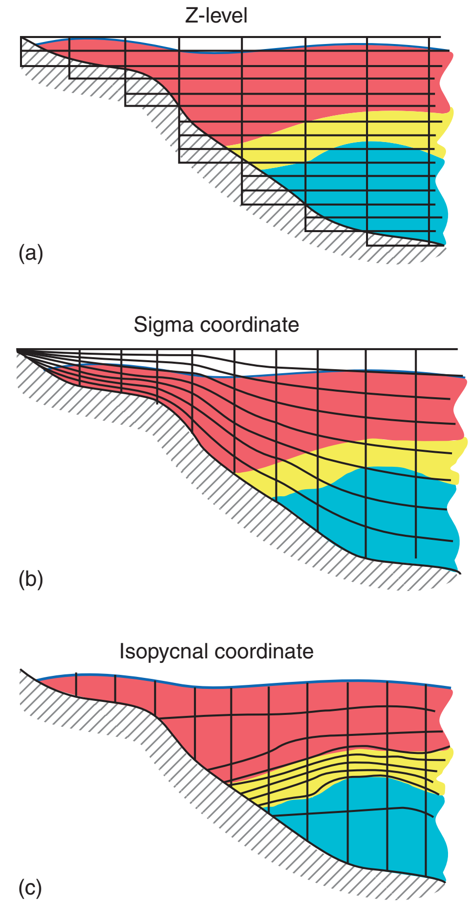

Figure 5 Elevation view illustrating different vertical grid systems relative to a stratified lake with warm (red) surface water, thermocline (yellow) and cooler (blue) hypolimnetic water.

Summary and Future Directions

Selecting whether to use a 1D-, 2D-, or 3D-model depends on the water body, available computational power, available field data and the type of answers desired. Applying 1D-models is always fastest and simplest, whereas 3D-models are computationally intense and require the greatest user skill and effort. 2D- and 3D-models need extensive field data to drive spatially-varying model boundary conditions and provide validation. In contrast, 1D-models need less extensive boundary condition data, but may require field studies to parameterize variability in the averaged directions. Whether a 3D-model is 'better' than a 1D-model will depend on the physics of interest. For example, if the physics of internal waves in a lake are unknown, a 3D-model may be needed to understand their effects. However, if the basic internal wave physics are already understood, then a 1D lake model (appropriately parameterized) may be adequate. The ideal conjunction of 1D and 3D lake models has yet to be attempted: the strength of 3D-models lies in quantifying the short-time, space-varying lake response to an event. Theoretically, such a model could be used to develop better parameterizations of 1D-models, increasing our understanding of how short-term events modify longer-term system behavior.

In considering hydrodynamic models coupled to water quality models, the ability to adequately capture bulk transport of hydrodynamic fields (e.g., velocity, temperature) should not be taken as proof of the ability to capture greater complexities in scalar biogeochemical distributions. Modeling the temperature is relatively easy because the problem is bounded and provides negative feedback. That is, lake temperatures are typically between 4 and 35 °C with the warm side facing up, and any attempt to turn the warm side downwards leads to horizontal density gradients and pressure forces that oppose overturning. Similarly, warming of the lake surface leads to increased heat loss to the atmosphere, which tends to moderate and limit errors. Velocity is also subject to large-scale forcing (wind) and is a bounded problem as unphysically large velocities will cause a model to blow up. Furthermore, dissipation is a limiting mechanism that works everywhere and at all times to bring the velocity towards zero. Thus, both velocity and temperature have preferred 'rest' states and model error cannot accumulate indefinitely without the results becoming obviously wrong. In contrast, scalar dispersion is driven by local turbulence and advection, without any global bounds to limit model error accumulation. Thus, even while the large-scale velocity and temperature fields look reasonable, a model may produce localized features that lead to unrealistic transport of scalars. Even simple passive tracer transport leads to complicated model-predicted gradient features as illustrated in Figures 6 and 7 and associated animations. Although such tracer fields illustrate model-predicted transport, there are relatively few field studies or methods for effective validation. These problems become even more pronounced for water quality models as biogeochemical scalar concentrations (such as phytoplankton biomass) are locally forced by nutrient concentrations, do not have a preferred 'rest' state, and have source/sink behaviors that may be affected by model transport errors. As such, 2D and 3D hydrodynamic/water modeling without validating field data should be considered cartoons that may be informative, but are also speculative and may be simply wrong!

As computers grow more powerful, there is a tendency to throw more grid cells at a system to improve model results. However, as the model grid is made finer, there is some point where neglect of the nonhydrostatic pressure is inconsistent with the grid scale – i.e., the model provides a better solution to the wrong equations. As a reasonable rule of thumb, if the horizontal grid scale is substantially smaller than the local depth of water, then the hydrostatic approximation may be inappropriate. Where internal wave evolution is important, nonhydrostatic pressure gradients should be included in future models. Although nonhydrostatic models presently exist, they have not yet been practically demonstrated for large-scale lake modeling.

Model calibration should be used carefully and in conjunction with sensitivity analyses. Indeed, the difference between an uncalibrated hydrodynamic model and field data may provide greater insight into the physical processes than a calibrated model. A careful modeler will estimate the uncertainty in various boundary conditions and conduct model sensitivity tests to understand how the uncertainty may affect results. Unnecessary calibration can be avoided by gaining a better understanding of the model error characteristics. Before applying any 3D-model to a lake or reservoir, the model should be tested on 2D rectangular domains at similar scales; e.g., simple models of internal waves, river inflows, and wind-driven mixing can provide relatively rapid insight into the relationship between model error, grid scale, time step and physics.

The horizontal grid for lake models may be Cartesian, curvilinear, or unstructured; these methods have

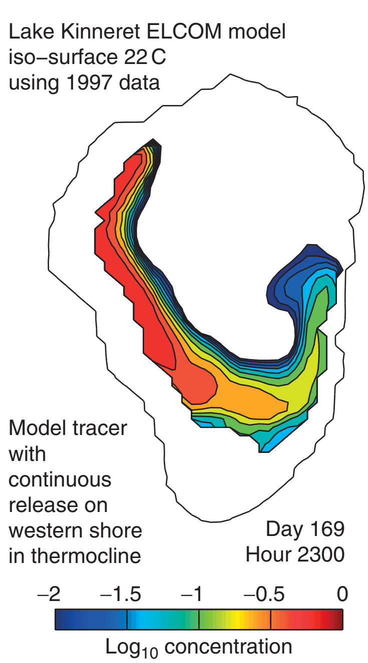

Figure 6 Modeled passive tracer concentrations in the thermocline of Lake Kinneret for a tracer concentration of 1.0 continuously released from the western boundary. This tracer motion is principally due to a basin-scale Kelvin wave.

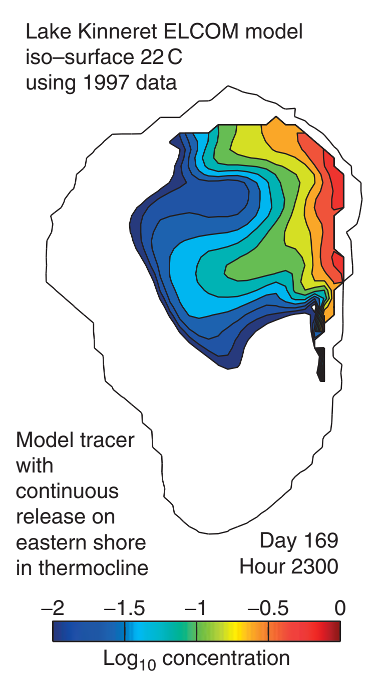

Figure 7 Modeled passive tracer concentrations in the thermocline of Lake Kinneret for a tracer concentration of 1.0 continuously released from the eastern boundary. This tracer motion is due to the combination of a Kelvin wave and a 2nd-mode Poincaré wave.

different strengths, weaknesses and complexities, such that the practical choice depends on the system, model availability and the modeler's bias. Where fine grid resolution is needed over a part of a domain (e.g., littoral zones), future developments in automated quadtree meshing of Cartesian grids may be easier to use than either curvilinear or unstructured grids.

Both *z*-level and sigma-coordinate vertical grids have significant drawbacks that remain unaddressed in the literature. Boundary layer sub-models have attempted to patch these problems, but are relatively complicated to develop and apply. Isopycnal methods may provide some future improvement, but it is not clear that they will be a panacea. Although a few isopycnal simulations have been made in lakes, we presently lack a thorough analysis of how isopycnal models represent internal wave dynamics at lake scales and along sloping boundaries.

There have been significant advances in ocean and estuarine modeling that have not yet appeared in lake models, but one must be careful about generalizing their applicability. Lake modeling faces two key problems: (1) long residence times allows model error to accumulate, unlike error that washes out with the tide in an estuary, and (2) the forcing is inherently unsteady in direction/amplitude, and may have sharp spatial gradients. Thus, methods suitable for a strong tidal exchange or a unidirectional ocean current with a smoothly varying wind field may not be effective for weak, unsteady forcing of a lake in the wind-shadow of a mountain. Indeed, despite our advances there remains significant work ahead before the art of hydrodynamic modeling is replaced by simple engineering.

Further Reading

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