

Literature Review on Nutrient-Related Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling

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Ben Cope
EPA Region 10
Seattle, Washington

Dr. Taimur Shaikh
EPA Region 6
Dallas, Texas

Rajbir Parmar, Project Officer
Office of Research and Development
Center for Environmental Measurement and Modeling
Athens, Georgia

The Cadmus Group

in collaboration with

HDR, Inc.

AQUA TERRA Consultants
(A Division of RESPEC Consulting and Services)

Dr. Steven Chapra, Tufts University

Dr. James Martin, Mississippi State University

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Kyle Flynn, Montana Dept. of Environmental Quality

Greg Pelletier, Washington Dept. of Ecology

Nuri Mathieu, Washington Dept. of Ecology

Jon Butcher, Tetra Tech

Steve Whitlock, EPA

EPA internal peer review:

Chris Knightes, EPA

Tim Wool, EPA

External peer review:

Kyle Flynn, CDM Smith

Scott Wells, Portland State University

Jon Butcher, Tetra Tech

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Disclaimer

This document provides guidance to those who develop, evaluate, and apply environmental models. It does not impose legally binding requirements; depending on the circumstances, it may not apply to a situation. The U.S. Environmental Protection Agency (EPA) retains the discretion to adopt, on a case-by-case basis, approaches that differ from this guidance.

This document has been reviewed by the U.S. Environmental Protection Agency, Office of Research and Development, and approved for publication.

1. Introduction

The 1985 Second Edition of *Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling* (Bowie et al. 1985; the Rates Manual) is a widely used source of information on kinetic formulations and associated rate constants and coefficients used in surface water quality modeling. One of the most common applications of this type of modeling is for Total Maximum Daily Load (TMDL) assessments conducted in support of the Clean Water Act. Advancements in water quality modeling over the last three decades have resulted in new and updated formulations not documented in the 1985 Rates Manual. Recent modeling and water quality process studies also have provided additional information on suitable values for rate constants and coefficients for model applications. Accordingly, this report presents the findings of a literature review reflecting the latest information on surface water quality modeling and rates, constants and kinetics for modeling related to several of the most commonly used for water quality management planning and development of TMDLs. It is the first step in a more comprehensive compilation of content for updating the entire 1985 Rates Manual.

Toward this end, EPA contracted with The Cadmus Group, Inc., in collaboration with HDR, Inc. (HDR), AQUA TERRA Consultants, Dr. Steven Chapra of Tufts University, and Dr. James Martin of Mississippi State University (hereafter referred to as “project team”) to compile and review literature and model rates, constants, and kinetics relevant to four water-quality models identified in the project scope of work: the Water Quality Analysis Simulation Program (WASP; Wool et al., 2003; Ambrose and Wool, 2017); CE-QUAL-W2 (Cole and Wells, 2018); Hydrologic Simulation Program-FORTRAN (HSPF, Bicknell et al., 2014); and the modernized stream and river quality model QUAL2K (Chapra et al., 2012) and the closely related QUAL2Kw (Pelletier and Chapra, 2008). The literature review consists primarily of evaluating model documentation and model application studies and will be supplemented by a more widespread review of laboratory and field studies in the future.

This report summarizes the project team’s literature compilation and review efforts. Included is a description of recent developments in dissolved oxygen, nutrient, and algae modeling in WASP, CE-QUAL-W2, HSPF, and QUAL2K/QUAL2Kw. These groups of parameters will be hereafter referred to as Group 1 parameters given that they are the first part of a planned multi-phase effort to gather rates, constants, and kinetic formulations for all the topics in the 1985 rates manual (Bowie et al., 1985). These Group 1 parameters were defined in the project scope of work. Also included in this report is a discussion of the literature selection and review steps that were taken to assess the applicability and thoroughness of model reports identified and considered. Future data review and compilation efforts may focus on other parameter groups for state-variables such as pH and alkalinity, temperature, zooplankton, macrophytes, and bacteria.

It is important to note that the tables of model parameter values developed for this effort do not include empirical data from experimental or laboratory studies. In this regard, the report and the tables that included herein are not an exhaustive presentation of all possible values, but rather describe coefficients that were used and calibrated in more recent well-documented model applications. The project team determined that it was not feasible within the scope of this work to pursue collection of updated field or laboratory data on rates and constants for water quality processes that are simulated in each model. Discussion of challenges associated with tabulating empirical data, as well as future work that could be conducted in tabulating those values, is included in Section 6 of this report.

The information presented in this report describes an assessment of the body of literature related to the application of the four models listed above. The report includes information on the geographic and environmental ranges of published modeling efforts as well as any gaps, in terms of location, modeled constituents, and environmental conditions, in the application of each model. Each model is also described with a focus on updates since 1985 and the results of the literature review related to each model. The second objective of this project was to review and compile rate, constant, and kinetic (RCK) parameters from relevant literature sources and tabulate this information for use by model practitioners.

This document and the accompanying parameter value tables do not constitute a complete replacement for sections of the 1985 Rates Manual related to the Group 1 parameters noted above, which includes more detail on species-specific algal rates as well as related nutrient parameters. It is important to note that there are fundamental similarities among the four models selected for this effort. Specifically, many of the post-1985 model enhancements to QUAL2K, CE-QUAL-W2, and WASP correspond to formulations that were already incorporated into HSPF in 1985.

The rate tables provided in this document contain study-specific metadata for each model application including: study location, geographic applicability, environmental conditions, purpose/model use, calibration period, and input data sampling plan. Details on model updates since the 1985 Rates Manual, as well as a discussion of available literature, potential data gaps, and limitations related to model application are included within the report.

2. Overview of Recent Developments in Rates, Constants, and Kinetic Formulations

Water quality models covered in this document along with the most recent version consulted and web page address as of 10/8/2019 are summarized in Table 1.

Table 1. Models Summarized in this Document

| Model | Version | Web Page |
|--|-------------------|---|
| WASP (Water Quality Analysis Simulation Program) | 8.32 (4/2/2019) | https://www.epa.gov/ceam/water-quality-analysis-simulation-program-wasp |
| CE-QUAL-W2 | 4.2 (9/20/2019) | http://www.cee.pdx.edu/w2/ |
| HSPF (Hydrologic Simulation Program – FORTRAN) | 12.5 (4/8/2019) | https://www.epa.gov/ceam/hydrological-simulation-program-fortran-hspf and https://www.epa.gov/ceam/basins-download-and-installation |
| QUAL2K | 2.12b1 (5/5/2016) | http://www.qual2k.com/ |
| QUAL2Kw | 6 (9/22/2016) | https://ecology.wa.gov/Research-Data/Data-resources/Models-spreadsheets/Modeling-the-environment/Models-tools-for-TMDLs |

2.1 WASP

Model Background

The Water Quality Analysis Simulation Program, WASP (Wool et al., 2003; Ambrose and Wool, 2017), has been used regularly both nationally and internationally since its development in the early 1980's. WASP is a generalized modeling framework based on the finite-volume concept for quantifying fate and transport of water quality variables in surface waters. While WASP has been applied to address a myriad of environmental problems, including pathogens, dissolved oxygen, eutrophication, and toxic contaminants, the focus of this project is on eutrophication and dissolved oxygen. WASP is capable of being applied in one, two or three dimensions to virtually any type of waterbody. Initially, WASP depended on the user to specify the model geometry and advective and dispersive transport, usually by trial-and-error calibration to observed spatial and temporal profiles of temperature and/or salinity, but with the latest releases of the code, WASP can use information from hydrodynamic models such as DYNHYD5 (Ambrose et al., 1993), RIVMOD (Hossenipour and Martin, 1990), DYRESM (Imberger and Patterson, 1981), EFDC (Hamrick, 1996), and SWMM (Rossman, 2015). This has significantly expanded WASP's capabilities and applications to more complex riverine and estuarine systems.

WASP is EPA-supported and has a long history of development and application, beginning with its release (DiToro et al., 1983) and continuing with its latest version, WASP8.32 (U.S. EPA, 2019; <https://www.epa.gov/ceam/water-quality-analysis-simulation-program-wasp>). As constructed at the time that the Rates Manual was published in 1985 (Bowie et al., 1985), the eutrophication kinetics present in WASP were based on the Potomac Estuary Model (PEM) developed by HydroQual (Thomann and Fitzpatrick, 1982). The following state variables were included in WASP at that time:

- Salinity;
- Phytoplankton biomass (two groups) as chlorophyll a or carbon;

- Dissolved and particulate inorganic phosphorus;
- Detrital dissolved and particulate organic phosphorus;
- Ammonia nitrogen;
- Nitrate nitrogen;
- Detrital total organic nitrogen;
- Carbonaceous biochemical oxygen demand (CBOD);
- Dissolved oxygen; and
- Suspended solids.

Fluxes of sediment oxygen demand and nutrients (inorganic phosphorus, ammonia nitrogen, and nitrate nitrogen) were specified as “boundary conditions” across the sediment–water interface.

Recent Model Additions

The most recent version of WASP has been expanded and includes the following state variables in addition to those listed above:

- Up to five phytoplankton groups (e.g., diatoms, greens, cyanobacteria);
- Up to three macrophyte/benthic algae groups;
- Detrital and dissolved organic nitrogen;
- Detrital and dissolved organic phosphorus;
- Detrital organic carbon and five types of CBOD;
- Biogenic and dissolved silica;
- Alkalinity/pH;
- Up to 10 inorganic solids;
- Water Temperature; and
- Predictive Light Module.

Algal System Modeling

Basic algal system modeling in WASP follows formulations that were already well established at the time of the 1985 Rates manual in which the specific algal growth rate is a function of the maximum 20 °C growth rate at optimal light and nutrient concentrations. The maximum growth rate is modified by multiplicative factors describing limits on growth imposed by temperature, light availability, and concentrations of dissolved inorganic phosphorus and dissolved inorganic nitrogen. These equations are not repeated here.

With the expansion of WASP to allow the user to model up to three phytoplankton groups, the user now also has the option to specify an alternative approach to model the effects of temperature on algal growth. Rather than just be limited to the traditional Arrhenius or “theta” (θ) model (Equation 2-1), the

user may also specify a set of temperature optimum curves (Equations 2-2a and 2-2b) in which the growth rate increases with temperature up to an optimum temperature and then decreases with higher temperatures.

$$\mu(T) = \mu_{20 \text{ deg C}} \cdot \theta^{T-20} \quad 2-1$$

Where:

$\mu(T)$ = algal growth rate at the ambient temperature
 T = temperature
 $\mu_{20 \text{ }^\circ\text{C}}$ = algal growth rate at 20 °C
 θ = temperature coefficient

$$\mu(T) = \mu_{T_{opt}} \cdot e^{-\beta_1(T-T_{opt})^2} \quad T \leq T_{opt} \quad 2-2a$$

$$\mu(T) = \mu_{T_{opt}} \cdot e^{-\beta_2(T_{opt}-T)^2} \quad T > T_{opt} \quad 2-2b$$

Where:

$\mu(T)$ = the algal growth rate at the ambient temperature
 T_{opt} = optimal temperature
 β_1, β_2 = parameters that determine the shape of the relationship of growth to temperature below and above the optimal temperature, respectively

With the modification of WASP to include additional phytoplankton species, rates and constants relevant to each phytoplankton group or species modeled are required for the following:

- Algal growth and respiration rate as a function of temperature and saturating light intensities;
- Rates of phytoplankton grazing by zooplankton;
- Algal settling rates for each algal group simulated;
- Michaelis-Menten constants for algal growth limitation by inorganic nitrogen, phosphorus, and silica; and
- Cell composition (stoichiometry) with respect to carbon, nitrogen, phosphorus, chlorophyll and, for diatoms, silica.

The most recent version of WASP also includes include the following new processes and kinetic formulations that impact Group 1 parameters:

- Sediment diagenesis nutrient flux model. Based on a model developed by DiToro and Fitzpatrick (1993) and DiToro (2001), and implemented into WASP by Martin et al. (2012), the sediment diagenesis nutrient flux model (SFM) computes the mass balance of organic and inorganic nutrients and oxygen between the water column and the sediment bed. The SFM accounts for the deposition of organic matter (phytoplankton and particulate organic matter [carbon, nitrogen, phosphorus, and biogenic silica]) from the water column to the sediment bed, the diagenesis or decomposition of this organic matter to its end-products (inorganic nitrogen,

phosphorus, and silica, and oxygen demanding materials), and the effects of sediment conditions on oxygen demand and nutrient fluxes to the overlying water column.

- A benthic algal model (Martin et al., 2006) that can simulate the inter-relationships between temperature, light, nutrients, and benthic algae or periphyton. In many shallow streams and rivers, it is the benthic algae or periphyton that are often of greater ecological and environmental importance than water column or floating phytoplankton.

The new state variables for particulate and dissolved organic nitrogen (replacing detrital total organic nitrogen) require rates and constants for:

- The hydrolysis of particulate organic nitrogen to dissolved organic nitrogen;
- The mineralization of dissolved organic nitrogen to ammonia nitrogen;
- The settling of particulate organic nitrogen; and
- The partitioning of phytoplankton respiration and death to particulate organic nitrogen, dissolved organic nitrogen and ammonia nitrogen.

As a consequence of adding detrital organic carbon to the model, the user must provide hydrolysis base rates (K_{hyd}) at 20 °C and temperature correction coefficients (θ 's) for the conversion of detrital (particulate) organic matter to dissolved organic carbon to CBOD, and the fraction of detrital organic carbon that goes to each of the three classes of CBOD because of hydrolysis of the detrital organic carbon.

The addition of silica state variables to the model, including the uptake and utilization of silica by diatom phytoplankton, requires rates and constants for the dissolution of biogenic silica to dissolved silica, the settling of biogenic silica, and the specification of the carbon to silica ratio for diatoms.

Sediment Flux Model

This section describes the governing equations for a sediment flux model (SFM) that was recently incorporated into WASP. The SFM is similar to the sediment diagenesis or sediment flux models used in other water quality models including QUAL2K and CE-QUAL-W2.

The SFM includes state variables for labile (G_1), refractory (G_2), and relatively inert (G_3) particulate organic carbon (C), nitrogen (N), and phosphorus (P), particulate or biogenic silica (BSi), inorganic nutrients (ammonia [NH_3], nitrate [NO_3], phosphorus [PO_4], silica [Si], hydrogen sulfide [H_2S], and methane [CH_4]). The rates and constants that need to be specified are related to two sets of processes that occur in the sediment bed: diagenesis (or decomposition) of the particulate organic matter that is delivered to the sediment bed, and the reactions that occur in the aerobic and anaerobic layers in the sediment, and the transfer that occurs between these layers due to particulate and dissolved mixing. The general form of the diagenesis mass balance equation follows (in implicit form) Equation 2-3,

$$\frac{C_{Gi}^{t+\Delta t} - C_{Gi}^t}{\Delta t} = \frac{J_{POMi}}{H_{sed}} - \frac{W_{bur}}{H_{sed}} C_{Gi}^{t+\Delta t} - K_{diagi} C_{Gi}^{t+\Delta t} \quad 2-3$$

Where:

- C_{Gi}^t = concentration of G_i (labile, refractory [relatively inert] carbon, nitrogen, or phosphorus) in the sediment bed at time t
 $C_{Gi}^{t+\Delta t}$ = concentration of G_i (labile and refractory carbon, nitrogen, or phosphorus) in the sediment bed at time $t+\Delta t$
 Δt = time step of the water quality model
 J_{POMi} = flux of G_i from the overlying water column to the sediment bed
 H_{sed} = depth of the active layer in the sediment bed
 W_{bur} = net burial or sedimentation
 K_{diagi} = diagenesis rate constant for G_i

The equations that govern the reactions that occur in the aerobic (layer 1) and anaerobic (layer 2) layers of the sediment, and the particulate and dissolved mixing between the two layers are provided below from the WASP user manual. Since the aerobic layer is quite thin, $H_1 \approx 1$ mm (10^{-3} m), and the surface mass transfer coefficient is on the order of $s \approx 0.1$ m/day, the residence in the layer is $H_1/s = 10^{-2}$ days. Because of the depth of the upper layer, it can be assumed to be at steady state without any loss in accuracy, and is expressed as follows (Equation 2-4):

Aerobic Layer (layer 1):

$$\begin{aligned}
 0 = & -s(f_{d1}C_{T1}^{t+\Delta t} - C_{d0}^{t+\Delta t}) + \omega_{12}(f_{p2}C_{T2}^{t+\Delta t} - f_{p1}C_{T1}^{t+\Delta t}) \\
 & + K_{L12}(f_{d2}C_{T2}^{t+\Delta t} - f_{d1}C_{T1}^{t+\Delta t}) - \omega_2 C_{T1}^{t+\Delta t} - \frac{\kappa_1^2}{s} C_{T1}^{t+\Delta t} \\
 & + J_{T1}^{t+\Delta t} + C_{T2}^{t+\Delta t} \dot{H}_1^+ - C_{T1}^{t+\Delta t} (\dot{H}_1 + \dot{H}_1^-)
 \end{aligned} \tag{2-4}$$

The anaerobic layer mass balance time-dependent implicit formula using the Euler method is in Equation 2-5:

Anaerobic Layer (layer 2):

$$\begin{aligned}
 H_2 \frac{C_{T2}^{t+\Delta t} - C_{T2}^t}{\Delta t} = & -\omega_{12} (f_{p2}C_{T2}^{t+\Delta t} - f_{p1}C_{T1}^{t+\Delta t}) \\
 & -K_{L12}(f_{d2}C_{T2}^{t+\Delta t} - f_{d1}C_{T1}^{t+\Delta t}) - \kappa_2 C_{T2}^{t+\Delta t} + \omega_2 C_{T1}^{t+\Delta t} \\
 & -\omega_2 C_{T2}^{t+\Delta t} + J_{T2}^{t+\Delta t} + C_{T1}^{t+\Delta t} \dot{H}_1^- - C_{T2}^{t+\Delta t} (\dot{H}_2 + \dot{H}_1^+)
 \end{aligned} \tag{2-5}$$

Where:

- s = surface transfer rate; $SOD/[O_2(0)]$, where SOD = sediment oxygen demand (SOD) rate and $O_2(0)$ is the overlying water concentration
 f_{d1} = fraction dissolved in layer 1
 f_{d2} = fraction dissolved in layer 2
 f_{p1} = fraction particulate in layer 1
 f_{p2} = fraction particulate in layer 2
 $C_{T1}^{t+\Delta t}$ = total concentration in layer 1 at time $t+\Delta t$
 $C_{T2}^{t+\Delta t}$ = total concentration in layer 2 at time $t+\Delta t$

| | |
|-----------------------|---|
| C_{T2}^t | = total concentration in layer 2 at time t |
| $C_{d0}^{t+\Delta t}$ | = concentration in overlying water column |
| K_{L12} | = mass transfer coefficient via diffusion |
| ω_{12} | = particle mixing coefficient between layers 1 and 2 |
| ω_2 | = sedimentation velocity for layer 2 |
| $J_{T1}^{t+\Delta t}$ | = source term for total chemical in layer 1 at time t+ Δt |
| $J_{T2}^{t+\Delta t}$ | = source term for total chemical in layer 2 at time t+ Δt |
| κ_1^2 | = square of reaction velocity in layer 1 |
| κ_2 | = reaction velocity in layer 2 |
| \dot{H}_1^- | = time derivative for H in layer 1 (not used; constant depth assumed) |
| \dot{H}_1^+ | = time derivative for H in layer 1 (not used; constant depth assumed) |
| \dot{H}_1 | = time derivative for H in layer 1 (not used; constant depth assumed) |
| \dot{H}_2 | = time derivative for H in layer 2 (not used; constant depth assumed) |
| H_2 | = thickness of layer 2 |
| Δt | = time step |

The fraction dissolved and particulate in the two layers are computed from Equations 2-6a through 2-6d:

Layer 1:

$$f_{d,1} = \frac{1}{1+\pi_{C1}S_1} \quad 2-6a$$

$$f_{p,1} = \frac{\pi_{C1}S_1}{1+\pi_{C1}S_1} \quad 2-6b$$

Layer 2:

$$f_{d,2} = \frac{1}{1+\pi_{C2}S_2} \quad 2-6c$$

$$f_{p,2} = \frac{\pi_{C2}S_2}{1+\pi_{C2}S_2} \quad 2-6d$$

Where:

| | |
|------------|---|
| π_{C1} | = partition coefficient for total chemical in layer 1 |
| π_{C2} | = partition coefficient for total chemical in layer 2 |
| S_1 | = solids concentration in layer 1 |
| S_2 | = solids concentration in layer 2 |

(Note: a more complete description of the SFM may be found in DiToro [2001] or Martin et al. [2006].)

The rates required by the SFM include: diagenesis or decay rates and temperature coefficients for particulate labile and refractory C, N, P, and BSi; freshwater and saltwater nitrification and denitrification reaction velocities; oxidation velocities for H₂S and CH₄; partition coefficients for NH₃, PO₄, Si and H₂S; and particulate and dissolved mixing coefficients. Note: the term “reaction velocities” is used for nitrification, denitrification, and oxidation because these values are formulated in the model as a product of a reaction rate times a depth, therefore having units of m/day.

Benthic Algal Model

The benthic algal or periphyton model includes state variables for bottom algal biomass (dry weight; DW) and internal cell nitrogen and phosphorus. The kinetic representations for benthic algae in WASP (beginning in version 7) were adopted from the QUAL2K model (Chapra, 2005). They differ from the representation of phytoplankton in two primary ways: (1) the benthic algal model uses an algal growth rate that is dependent on the intracellular nutrient content, following the Droop formulation (Droop, 1973), rather than external nutrients, and (2) space limitation effects are incorporated into bottom algae photosynthesis. As a result, there are a few more model constants or coefficients that are used to model the intracellular nutrient dynamics.

Benthic algal simulation was not covered in detail in the 1985 Rates Manual, so additional details are provided herein for WASP and the other three models discussed in this review. Bottom algae biomass, a_b , is represented as dry weight biomass (D) per unit area of available substrate. Bottom algal biomass increases due to photosynthesis and decreases with respiration and death, as calculated in Equation 2-7:

$$S_{ab} = (F_{Gb} - F_{Rb} - F_{Db}) A_b \quad 2-7$$

where S_{ab} is the total source/sink of algal biomass (g D/d [day]), F_{Gb} is the photosynthesis rate (g D/m²-d [per day]), F_{Rb} is the respiration loss rate (gD/m²-d), F_{Db} is the death rate (g D/m²-d), and A_b is the bottom substrate surface area (m²).

Two options are available to represent the bottom algal photosynthesis rate, F_{Gb} [gD/m²-d]. The first option, using Equation 2-8, is a temperature-corrected, zero-order maximum rate attenuated by nutrient and light limitation (simplified from Rutherford et al., 2000):

$$F_{Gb} = F_{Gb20} \varphi_{Tb} \varphi_{Nb} \varphi_{Lb} \quad 2-8$$

where F_{Gb20} is t

he maximum photosynthesis rate at 20 °C [gD/m²-d], φ_{Tb} is the photosynthesis temperature correction factor [dimensionless], φ_{Nb} is the bottom algae nutrient attenuation factor [dimensionless number between 0 and 1], and φ_{Lb} is the bottom algae light attenuation coefficient [dimensionless number between 0 and 1].

The second option, using Equation 2-9, uses a first-order, temperature-corrected rate constant, attenuated by nutrient, light, and space limitation:

$$F_{Gb} = k_{Gb20} \varphi_{Tb} \varphi_{Nb} \varphi_{Lb} \varphi_{Sb} a_b \quad 2-9$$

where k_{Gb20} is the maximum photosynthesis rate constant at 20 °C [d⁻¹], φ_{Sb} is the bottom algae space attenuation coefficient [dimensionless number between 0 and 1], and other terms are as defined above. Space limitation of the first-order growth rate is modeled as a logistic function, using Equation 2-10:

$$\varphi_{Sb} = 1 - \frac{a_b}{a_{bmax}} \quad 2-10$$

where a_{bmax} is the bottom algae carrying capacity, or maximum density [gD/m²].

Nutrient limitation of the photosynthesis rate is dependent on intracellular nutrient concentrations using a formulation shown in Equation 2-11, which was originally developed by Droop (1973):

$$\varphi_{Nb} = \min \left[\left(1 - \frac{q_{0N}}{q_N} \right), \left(1 - \frac{q_{0P}}{q_P} \right) \right] \quad 2-11$$

where q_N and q_P are cell quotas of nitrogen [mg N/gD] and phosphorus [mg P/gD], respectively, and q_{0N} and q_{0P} are the minimum cell quotas of nitrogen [mg N/gD] and phosphorus [mg P/gD], respectively. The minimum cell quotas are the levels of intracellular nutrient at which growth ceases.

Intracellular nutrient (nitrogen or phosphorus) concentrations, or cell quotas, represent the ratios of the intracellular nutrient to the bottom algal dry weight, and are calculated using Equations 2-12a and 2-12b, respectively:

$$q_N = 10^3 \frac{IN_b}{a_b} \quad 2-12a$$

$$q_P = 10^3 \frac{IP_b}{a_b} \quad 2-12b$$

where q_N and q_P are cell quotas [mg N/gD or mg P/gD], IN_b is intracellular nitrogen concentration [g N/m²], IP_b is intracellular phosphorus concentration [g P/m²], and 10^3 is a units conversion factor [mg/g].

The total source/sink terms for intracellular nitrogen (Equation 2-13a) and phosphorus (Equation 2-13b) in bottom algal cells [g/d] are controlled by uptake, excretion, and death:

$$S_{bN} = (F_{UNb} - F_{ENb} - F_{DNb}) * A_b \quad 2-13a$$

$$S_{bP} = (F_{UPb} - F_{EPb} - F_{DPb}) * A_b \quad 2-13b$$

where F_{UNb} and F_{UPb} are uptake rates for nitrogen and phosphorus by bottom algae [gN/m²-d and gP/m²-d], F_{ENb} and F_{EPb} are the bottom algae cell excretion rates [g N/m²-d and g P/m²-d], and F_{DNb} and F_{DPb} are loss rates from bottom algae death [g N/m²-d and g P/m²-d].

The N (Equation 2-14a) and P (Equation 2-14b) uptake rates depend on both external and intracellular nutrient concentrations as in Rhee (1973):

$$F_{UNb} = 10^{-3} \rho_{mN} \left(\frac{NH_4 + NO_3}{K_{sNb} + NH_4 + NO_3} \right) \left(\frac{K_{qN}}{K_{qN} + (q_N - q_{0N})} \right) a_b \quad 2-14a$$

$$F_{UPb} = 10^{-3} \rho_{mP} \left(\frac{PO_4}{K_{sPb} + PO_4} \right) \left(\frac{K_{qP}}{K_{qP} + (q_P - q_{0P})} \right) a_b \quad 2-14b$$

where NH_4 , NO_3 , and PO_4 are external water concentrations of ammonium N, nitrate N, and phosphate P [mg N/L and mg P/L], ρ_{mN} and ρ_{mP} are the maximum uptake rates for nitrogen and phosphorus [mg N/g D-d and mg P/gD-d], K_{sNb} and K_{sPb} are half-saturation constants for external nitrogen and phosphorus [mg N/L and mg P/L], K_{qN} and K_{qP} are half-saturation constants for intracellular nitrogen and phosphorus [mg N/gD and mg P/gD], and 10^{-3} is a units conversion factor [g/mg]. Note that nutrient uptake rates fall to half of their maximum values when external nutrient concentrations decline to the half-saturation constants, or when excess internal nutrient concentrations rise to the internal half-saturation constants.

The internal N (Equation 2-15a) and P (Equation 2-15b) excretion rates are represented using first-order, temperature-corrected kinetics:

$$F_{ENb} = K_{Eb20} \theta_{Eb}^{T-20} q_N a_b 10^{-3} \quad 2-15a$$

$$F_{EPb} = K_{Eb20} \theta_{Eb}^{T-20} q_P a_b 10^{-3} \quad 2-15b$$

where k_{Eb20} is the bottom algae cell excretion rate constant at 20 °C [d^{-1}] and Θ_{Eb} is the bottom algae excretion temperature coefficient [dimensionless].

The internal N (Equation 2-16a) and P (Equation 2-16b) loss rates from benthic algal death are the product of the algal death rate, F_{Db} [gD/m^2-d], and the cell nutrient quotas:

$$F_{DNb} = F_{Db} q_N 10^{-3} \quad 2-16a$$

$$F_{DPb} = F_{Db} q_P 10^{-3} \quad 2-16b$$

where 10^{-3} is a units conversion factor [g/mg].

WASP8 added capability to simulate floating surface and subsurface and submersed macroalgae, along with forms of macrophytes that obtain nutrients from the water column rather than from roots in the sediment. The kinetic formulations are similar to those for periphyton.

The additional rates and constants that need to be specified include:

- Benthic algal initial stoichiometry (i.e., DW:C, C:N, C:P and C:Chl-a ratios);
- Benthic algal growth, death, and respiration rates, and corresponding temperature coefficients;
- Saturating light intensity;
- Minimum cell quotas for internal N and P for cell growth;
- Maximum uptake rates for N and P;
- Half saturation uptake constants for intracellular and extracellular N and P; and
- Carrying capacity or maximum density for bottom biomass.

2.2 CE-QUAL-W2

CE-QUAL-W2 is a two-dimensional, laterally averaged hydrodynamic and water quality model that describes vertical and longitudinal distributions of hydrodynamics, heat, and selected biological and chemical materials in a water body through time. It was one of the first water quality models in which water quality was coupled with multi-dimensional hydrodynamics.

CE-QUAL-W2 has undergone continuous development since the early 1970s, first largely by the U.S. Army Corps of Engineers (USACE), and over the last several years by Dr. Scott Wells and others at Portland State University. CE-QUAL-W2 Version 1.0 was released in 1986 (Environmental and Hydraulics Laboratory, 1986) and its first application to De Gray Reservoir (Martin, 1988). Version 2 of the model was released in 1995 (Cole and Buchak, 1995) and the latest official release is Version 4.1 released October 2017 (Cole and Wells, 2018). The model has been widely applied throughout the world.

Portland State University (<http://www.ce.pdx.edu/w2/>) reports over 2,300 documented applications worldwide, including 935 applications in the United States and Canada.

Version 1.0 of CE-QUAL-W2 (Martin, 1988) allowed for simulation of the interactive dynamics of physical factors (such as flow and temperature regimes), chemical factors (such as nutrients), and an algal assemblage. The model structure allowed for the simulation of up to 20 water quality constituents in addition to temperature, density, and circulation patterns. Hydrodynamics and water temperatures could be simulated independently of, or in conjunction with, other water quality constituents.

Since its initial release there have been substantial improvements and modifications to the original code. Many of the modifications were related to the solution scheme, physical computations (e.g., the model can now be applied to riverine systems), addition of particle tracking, and the graphical user interface. However, there have been several updates and improvements to the water quality kinetics as well. The state variables in the latest release of CE-QUAL-W2 (Version 4.1; Cole and Wells, 2018) are tabulated in Table 2 in comparison to those from Version 1.0. In addition, model output includes over 60 derived variables (e.g., pH, TOC, DOC, TON, TOP, DOP; Cole and Wells, 2011) for comparison with observed data. The most notable improvements in the kinetics over Version 1.0 were the addition of multiple inorganic solids groups, dissolved inorganic and particulate biogenic silica, photodegradation of generic constituents, N₂ as a state variable to compute Total Dissolved Gas (TDG), multiple groups of algae, zooplankton, epiphytes, macrophytes, non-conservative alkalinity, a sediment diagenesis model (Prakash et al., 2011) including bubble formation and rise in the water column, sediment consolidation, and a variable sediment temperature, pH, and alkalinity and new state variables of metals, H₂S, and CH₄ in the water column and sediment (Cole and Wells, 2018).

With regards to rates and kinetics, primary producers in Version 1.0 of CE-QUAL-W2 were simulated using a single state variable taken to represent planktonic forms (e.g., phytoplankton). In the present version, multiple phytoplankton groups may be simulated. The latest version allows the user to select the number and kinds of algae and additional state variables have been added for periphyton and macrophytes. In Version 1.0, rates of change in phytoplankton biomass were computed from an optimal growth rate that was modified by light and nutrients and from losses due to natural mortality, dark respiration, excretion, grazing, and settling. The approach in the present version is similar, but this version allows for variable stoichiometry (versions prior to 3.5 used fixed stoichiometric constants for the ratios of nitrogen and phosphorus to organic matter), losses due to grazing by zooplankton (multiple zooplankton groups are simulated), mortality and excretion to particulate organic matter (POM) rather than detritus (labile and refractory particulate organic carbon, nitrogen, and phosphorus), and an ammonia preference.

The kinetic formulations for periphyton or epiphyton in the current version of CE-QUAL-W2 are based on the balance between growth, respiration, excretion, mortality, and burial. Epiphyton growth rate (Equation 2-17) is computed by modifying a maximum growth rate affected by epiphyton biomass, temperature, and nutrient availability:

$$K_{eg} = \gamma_{er} \gamma_{ef} \lambda_{min} K_{eg\ max} \quad 2-17$$

Where:

γ_{er} = temperature rate multiplier for rising limb of curve

γ_{ef} = temperature rate multiplier for falling limb of curve

λ_{\min} = multiplier for limiting growth factor (minimum of phosphorus, silica, nitrogen, and epiphyton biomass)

K_{eg} = epiphyton growth rate, sec^{-1}

$K_{eg\max}$ = maximum epiphyton growth rate, sec^{-1}

Rate multipliers for epiphyton growth are computed based upon available light, phosphorus, nitrogen, silica, and epiphyton biomass. Epiphyton biomass is included as a surrogate for light limited epiphyton self-shading.

The rate multiplier for light is based upon the Steele function (Equation 2-18):

$$\lambda_l = \frac{I}{I_s} e^{\left(\frac{I}{I_s} - 1\right)} \quad 2-18$$

Where:

I = available light, watts per square meter ($\text{W}\cdot\text{m}^{-2}$)

I_s = saturating light intensity at maximum photosynthetic rate, $\text{W}\cdot\text{m}^{-2}$

λ_l = light limiting factor

Rate multipliers limiting epiphyton growth due to nutrient limitations are computed using the Monod relationship (Equation 2-19):

$$\lambda_i = \frac{\Phi_i}{P_i + \Phi_i} \quad 2-19$$

Where:

λ_i = phosphorus or nitrate + ammonium concentration, g m^{-3}

P_i = half-saturation coefficient for phosphorus or nitrate + ammonium, g m^{-3}

The epiphyton preference for ammonium is modeled using Equation 2-20:

$$P_{NH_4} = \Phi_{NH_4} \frac{\Phi_{NOx}}{(K_{NH_4} + \Phi_{NH_4})(K_{NH_4} + \Phi_{NOx})} + \frac{K_{NH_4}}{(\Phi_{NH_4} + \Phi_{NOx})(K_{NH_4} + \Phi_{NOx})} \quad 2-20$$

Where:

P_{NH_4} = ammonium preference factor

K_{NH_4} = ammonia preference half-saturation coefficient, g m^{-3}

Φ_{NH_4} = ammonium concentration, g m^{-3}

Φ_{NOx} = nitrate–nitrite concentration, g m^{-3}

Epiphyton dark respiration is computed per Equation 2-21 using the rising limb of the temperature function:

$$K_{er} = \gamma_{er} \gamma_{ef} K_{er\max} \quad 2-21$$

Where:

K_{er} = epiphyton respiration rate

γ_{er} = temperature rate multiplier for rising limb of the curve

γ_{ef} = temperature rate multiplier for falling limb of the curve

$K_{er\max}$ = maximum dark respiration rate, sec^{-1}

Epiphyton excretion is evaluated in Equation 2-22 using an inverse relation to the light rate multiplier:

$$K_{ee} = (1 - \lambda_l) \gamma_{er} \gamma_{ef} K_{eemax} \quad 2-22$$

Where:

K_{ee} = epiphyton excretion rate

K_{eemax} = maximum excretion rate constant, sec^{-1}

Epiphyton mortality is defined in Equation 2-23:

$$K_{em} = \gamma_{er} \gamma_{ef} K_{emmax} \quad 2-23$$

Where:

K_{em} = epiphyton mortality rate

K_{emmax} = maximum mortality rate, sec^{-1}

This mortality rate represents both natural and predator mortality. Epiphyton growth does not occur in the absence of light. Epiphyton growth is not allowed to exceed the limit imposed by nutrient supply over a given timestep. Epiphyton excretion is not allowed to exceed epiphyton growth rates.

The epiphyton burial rate represents the burial of dead epiphyton to the organic sediment compartment. Currently, there is no sloughing of epiphyton into the water column as a function of velocity shear. This is a function of the biomass limitation term.

The epiphyton biomass is controlled by a biomass limitation equation based on Monod kinetics. The biomass limitation function, f , varies from 0 to 1 and is multiplied with the growth rate. This function is defined as in Equation 2-24:

$$f = \left[1 - \frac{B}{B + K_b} \right] \quad 2-24$$

Where:

B = epiphyton areal biomass, g/m^2

K_b = epiphyton areal biomass half-saturation coefficient, g/m^2

The macrophyte model in CE-QUAL-W2 can represent multiple submerged species and allows nutrients to be obtained from the water column or the sediments. If they are obtained from the sediments, the sediments are assumed to be an infinite pool that cannot limit growth. Plants grow upwards from the sediment through model layers. Growth upward is accomplished by moving the growth of a layer to the layer above if the concentration in the layer is greater than a threshold concentration and the concentration in the upper layer is less than the same threshold concentration. Macrophyte shading is modeled by making light attenuation as a function of macrophyte concentration. The remaining kinetics of the macrophyte model in CE-QUAL-W2 are similar to those used to represent epiphyton, except that macrophytes are not subject to burial.

Nutrients simulated in Version 1.0 of CE-QUAL-W2 included ammonia, nitrate-nitrogen, and inorganic phosphorus, with source terms including phytoplankton respiration, dissolved organic matter (DOM) decay (detritus and dissolved forms, labile and refractory), and anaerobic release from sediments (a zeroth order rate). Nutrient losses included algal uptake during growth and phosphorus settling of fractions sorbed to iron and solids. Nitrification and denitrification were additional losses for ammonia

and nitrate respectively. In the present version, dissolved and particulate biogenic silica are added as state variables. Additional loss terms for nutrients include uptake by macrophytes and epiphytes (like phytoplankton, there may be multiple groups of each). Additional source terms include zooplankton respiration, a 1st order sediment release (in addition to a zeroth order rate), and decay of labile and refractory DOM, POM, and CBOD.

For dissolved oxygen in Version 1.0, sources and sinks included phytoplankton growth and respiration, reaeration, detritus decay, DOM decay (labile and refractory), ammonia decay, mortality, and sediment oxygen demand (zeroth order rate). In the current version, additional sources and sinks include growth and respiration of macrophytes and epiphytes, respiration of zooplankton, and decay of sediments, DOM (labile and refractory), POM (labile and refractory state variables), CBOD (multiple groups), and oxidation of CH₄, H₂S, and reduced metals. Several new reaeration formulations have been added that are specific to rivers, lakes and reservoirs, estuaries, and aeration over large dam spillways/gates, small dams, and weirs. In the current version 4.1, the sediment diagenesis model is structured based on the equations presented in Section 2.1 and is a modification of the sediment diagenesis sub-model included as part of the CE-QUAL-ICM model (Cercio and Cole, 1994), which incorporates a mass-balance model in bottom sediments to predict sediment oxygen demand and nutrient flux. In addition, the model includes prediction of bubble formation and rise in the water column, which can be used in the evaluation of oxygen injection systems (see Martin and Cole [2000] for an example application for J. Percy Priest Reservoir, Tennessee).

Table 2. CE-QUAL-W2 Version 1 State Variables (Martin, 1988) compared to Version 4.1 (Cole and Wells, 2018)

| Version 1.0 Variables | Version 4.1 Variables |
|-------------------------------------|---|
| Water Temperature (including ice) | Water Temperature (including ice) |
| Conservative tracer | Any number of generic constituents defined by a 0 and/or a 1 st order decay rate and/or a settling velocity and/or an Arrhenius temperature rate multiplier and/or photo-degradation and/or gas transfer/volatilization that can be used to define any number of the following: conservative tracer, water age or hydraulics residence time, coliform bacteria, contaminants, N ₂ gas (for computation of TDG). |
| Coliform bacteria | |
| Total dissolved solids or salinity | Total dissolved solids or salinity |
| Inorganic suspended solids | Inorganic suspended solids groups ¹ |
| Dissolved inorganic carbon | Total Inorganic Carbon |
| Alkalinity (conservative) | Alkalinity (non-conservative) |
| Labile dissolved organic matter | Labile dissolved organic matter (three forms: N,P,C) |
| Refractory dissolved organic matter | Refractory dissolved organic matter (three forms: N,P,C) |
| Phytoplankton | Phytoplankton groups ¹ |

| Version 1.0 Variables | Version 4.1 Variables |
|--|---|
| Detritus | Labile particulate organic matter (three forms: N,P,C) |
| | Refractory particulate organic matter (N,P,CO) |
| Phosphate-phosphorus | Bioavailable phosphorus (commonly represented by orthophosphate or soluble reactive phosphorus) |
| Ammonia-nitrogen | Ammonia-nitrogen |
| Nitrate + nitrite-nitrogen | Nitrate + nitrite-nitrogen |
| Dissolved oxygen | Dissolved oxygen |
| Organic sediments | Organic sediments |
| Total Iron | Total iron |
| No further state variables in version 1.0; Version 4.1 included additional variables in the next column. | CBOD groups with separate settling, N, and P defined for each group ¹ |
| | Dissolved silica |
| | Particulate biogenic silica |
| | Zooplankton groups ¹ |
| | Epiphyton groups ¹ |
| | Macrophyte groups ¹ |
| | CH ₄ , SO ₄ , H ₂ S, reduced and oxidized Mn and Fe |

¹ Arbitrary number of state variables, set by user

2.3 HSPF

The Hydrological Simulation Program-FORTRAN (HSPF; Bicknell et al., 2014) is a watershed model developed under U.S. EPA sponsorship to simulate hydrologic and water quality processes in natural and man-made water systems. HSPF uses information such as the records of rainfall and temperature, computed evaporation, landscape characteristics to simulate watershed processes. The initial result of an HSPF simulation is a time series of the quantity and quality of water transported over the land surface and through soil zones. Runoff flow rate, sediment runoff, nutrients, pesticides, toxic chemicals, and other water quality constituent concentrations can be predicted. The model uses these runoff and infiltration results, coupled with stream channel information, to simulate instream flow and water quality processes. From this information, HSPF produces a time series of water quantity and quality at any point in the watershed.

HSPF was first released publicly in 1980 as Release No. 5 (Johanson et al., 1980) by the EPA Water Quality Modeling Center (now the Center for Exposure Assessment Modeling). Originally, HSPF was

designed based on the Stanford Watershed Model (SWM) developed in the early 1960s. SWM was expanded and refined in the early 1970s into the Hydrocomp Simulation Program (HSP), which built in nonpoint source loading and water quality simulation capabilities (Donigian and Imhoff, 2006). HSPF was developed to integrate functions of HSP, EPA’s Agricultural Runoff Management model, and EPA’s Nonpoint Source model. Throughout the 1980s, 1990s, and the 2000s, HSPF underwent a series of code and algorithm enhancements producing a continuous succession of updated code, culminating in the major upgrade of Version No. 12.2 in 2005 (Bicknell et al., 2005). The most recent version is 12.5, released in 2019 as part of the BASINS 4.5 package (<https://www.epa.gov/ceam/better-assessment-science-integrating-point-and-non-point-sources-basins>).

The structure of HSPF features four major “application modules”: PERLND for pervious land segments, IMPLND for impervious land segments, RCHRES for river reaches and well-mixed reservoirs, and BMP for simulating constituent removal efficiencies associated with implementing management practices. Of these four application modules, only one (RCHRES) falls within the topical domain (i.e., surface water quality modeling) of EPA’s Rates Manual. Some processes relevant to this project are included in HSPF application modules other than RCHRES, but are simulated using the waterbody science contained within RCHRES, and were included in this effort where applicable. The RCHRES module is a one-dimensional model with completely mixed segments. It incorporates state variables for inorganic and organic forms of N and P along with phytoplankton and periphyton biomass. The basic state variables relevant to nutrient simulation in HSPF are summarized in Table 3.

Table 3. State Variables Relevant to Instream Nutrient Simulation in HSPF

| Variable Name | Definition | Units |
|---------------|--|-------------------|
| BOD | Benthic oxygen demand at 20 °C | mg/L |
| DOX | Dissolved oxygen concentration | mg/L |
| SATDO | Dissolved oxygen saturation concentration | mg/L |
| NH3 | Dissolved concentration of NH ₃ | mg/L |
| NH4 | Dissolved concentration of NH ₄ | mg/L |
| NO2 | Dissolved concentration of NO ₂ | mg/L |
| NO3 | Dissolved concentration of NO ₃ | mg/L |
| PO4 | Dissolved concentration of PO ₄ | mg/L |
| SN4(3) | Storage of NH ₄ on sand, silt, clay | mg/mg |
| SPO4(3) | Storage of PO ₄ on sand, silt, clay | mg/mg |
| BALCLA | Benthic algal density (as chlorophyll a) | µg/m ² |
| BENAL | Benthic algal density (as biomass) | mg/m ² |
| ORC | Dead refractory organic carbon | mg/L |
| ORN | Dead refractory organic nitrogen | mg/L |
| ORP | Dead refractory organic phosphorus | mg/L |
| PHYCLA | Phytoplankton concentration (as chlorophyll a) | µg/L |
| PHYTO | Phytoplankton concentration (as biomass) | mg/L |
| POTBOD | Potential biochemical oxygen demand | mg/L |
| TORC | Total organic carbon | mg/L |
| TORN | Total organic nitrogen | mg/L |
| TORP | Total organic phosphorus | mg/L |
| ZOO | Zooplankton concentration | mg/L |

HSPF simulates a single phytoplankton type. HSPF first calculates a temperature-corrected maximum algal growth rate using linear interpolation between a minimum and maximum temperature for growth. Limitations on algal growth are then applied using a Michaelis-Menten half saturation approach to evaluate growth reduction due to availability of inorganic nitrogen, orthophosphorus and light. Algal growth may also be limited by insufficient water depth. Algal death rates can vary between a low and high unit death rate. The high death rates are applied when concentrations of inorganic nitrogen or orthophosphorus fall below a user specified limit, or when the concentration of phytoplankton (as chlorophyll a) exceeds a specified value. In the original formulation of HSPF, benthic algae are simulated as analogous to phytoplankton except that light availability is calculated at the bottom, rather than middle of the water column, a maximum benthic algae density is imposed, and growth and death rates may vary relative to phytoplankton by a fixed ratio. Unlike phytoplankton, benthic algae are not subject to advection. Instead, when the density of benthic algae exceeds a user-specified limit the excess benthic algal is added to the death rate to represent sloughing loss. HSPF does not explicitly simulate macrophytes, and their effects on water quality must be approximated using the benthic algal routines.

A major enhancement to the HSPF nutrient algorithms was introduced in Version 10 in 1993. The focus was on implementing a more robust representation of inorganic sediment–nutrient interactions for both suspended and bed sediment. While the enhancements were a significant improvement, the approach does not constitute a full diagenesis model. The focus of the enhancement was on a free-flowing riverine environment, one in which the adsorptive medium was expected to be predominantly non-organic. While the sediment–nutrient interaction enhancements were being implemented to support the EPA Chesapeake Bay Program, an upgrade in the computation and representation of additional nutrient processes was also introduced. In addition to model processes present in the original 1980 model, current features of the HSPF RCHRES module include:

- Adsorption/desorption of phosphate and ammonium to inorganic sediment fractions (sand, silt, clay) is represented using a linear relationship with a kinetic transfer rate. New state variables for concentration and mass of phosphate and ammonium in suspended sediment fractions and concentration of phosphate and ammonium in bed sediment are introduced.
- Nutrients adsorb/desorb from suspended sediment according to user-specified water column partition coefficients.
- Bed sediment fractions are assumed to have reach-specific, temporally constant nutrient concentrations. When nutrients adsorbed on suspended sediment are added to the bed via deposition, these nutrients join an infinite pool. When sediment and its adsorbed nutrients are scoured from the bed, the amount of nutrient entering the water column is proportional to the amount of re-suspended sediment at a constant nutrient concentration.
- Reduction of nitrate to nitrogen gas (i.e., denitrification) is represented in the water column using a first-order, temperature-dependent formulation dependent on water column nitrate concentration. A parameter is integrated that specifies the dissolved oxygen concentration above which denitrification (an anaerobic process) ceases; this threshold value is user-defined.
- Ionization of ammonia to ammonium is represented in the water column. New (or re-defined) state variables for ammonia, ammonium, and total ammonia are required.
- Ammonia volatilization is represented using a two-layer model that relates volatilization rate to oxygen reaeration rate.

With the modification of HSPF to include sediment–nutrient interactions, the following rates and constants are required: constant bed concentrations of ammonia-N and orthophosphorus-P adsorbed to each sediment fraction (sand, silt, and clay) and adsorption coefficients (K_d) for ammonia-N and orthophosphorus-P. Addition of the denitrification process required introducing two new rates and constants: temperature correction factor for denitrification rate, and a threshold value for DO concentration above which denitrification ceases. Addition of the ammonia volatilization process required constants to represent both the exponent in the gas layer and the liquid layer of the mass transfer equation.

In addition, a more sophisticated benthic algae simulation was introduced into the HSPF surface water quality algorithms in Version 12.2 in 2005. The new methods are based on periphyton kinetics contained in the DSSAMt water quality model (Caupp et al., 1998), and allow effective simulation of benthic algae in shallow streams and rivers. Up to four different algal types can be simulated simultaneously, and the processes these algae undergo are independent of phytoplankton processes. The process equations and assumptions are as follows:

- Benthic algae are assumed to grow only in portions of the stream that are classified by the user as riffles.
- Algal growth is a function of available nutrients, light, temperature, and the total density of benthic algae.
- Nitrogen-fixing (blue-green) algae can be represented, and algae are generally not permitted to reduce nutrients below a user-defined minimum.
- Respiration is dependent on temperature.
- Algae are lost or die (i.e., are removed) through grazing/disturbance by benthic invertebrates and through scouring or sloughing processes.
- The inorganic and organic nutrient pools in the water column reflect the growth, respiration, and removal processes.

The new routines can represent multiple types of benthic algae, each of which is simulated in a similar manner. For benthic algal type i , the overall mass balance equations are given by Equation 2-25:

$$\frac{d \text{BENAL}_i}{dt} = [\text{GROBA}_i - \text{RESBA}_i - \text{SLOF}_i] * \text{BENAL}_i - \text{REMBA}_i \quad 2-25$$

Where:

BENAL_i = biomass (mg biomass/m²)

GROBA_i = growth or production rate (/interval)

RESBA_i = respiration rate (/interval)

SLOF_i = biomass removal rate from scouring (/interval)

REMBA_i = removal rate (grazing and disturbance) (mg biomass/m²/interval)

The growth or production rate for type i is given by Equation 2-26:

$$\text{GROBA}_i = \text{MBALGR}_i * \text{TCMBAG}_i * \min\{\text{GROFN}_i, \text{GROFL}_i, \text{GROFD}_i\} \quad 2-26$$

Where:

MBALGR_i = production under optimal conditions
 TCMBAG_i = temperature limitation function
 GROFN_i = nutrient limitation function
 GROFL_i = light limitation function
 GROFD_i = density limitation function

The temperature limitation function is computed by an Arrhenius equation characterized by a coefficient for the temperature effect on the growth of each algal type at 20 °C.

If the inorganic nitrogen and phosphorus concentrations are greater than user-defined minimum values for growth (NMINGR and PMINGR), then growth can occur, and the nutrient limitation function is computed by Equation 2-27, a Michaelis-Menten equation for non-blue-green algae:

$$GROFN_i = \min \left\{ \frac{GROFV \cdot PO_4}{CMMP_i + GROFV \cdot PO_4}, \frac{GROFV \cdot MMN}{CMMN_i + GROFV \cdot MMN} \right\} \quad 2-27$$

Where:

GROFV = velocity limitation function for benthic algal nutrient availability (-)
 PO₄ = dissolved available phosphorus concentration (mg P/L)
 CMMP_i = half-saturation constant for phosphorus uptake (mg P/L)
 MMN = dissolved available inorganic nitrogen concentration (mg N/L)
 CMMN_i = half-saturation constant for nitrogen growth f (mg N/L)

For nitrogen-fixing (blue-green) algae, if the available nitrogen concentration is greater than a user-defined parameter (NMAXFX), fixation is suppressed and the above equation is used. Otherwise, fixation is assumed to occur and only the orthophosphate limitation is applied.

The velocity adjustment on nutrient limitation is computed as in Equation 2-28:

$$GROFV = \frac{BALVEL}{CMMV + BALVEL} \quad 2-28$$

Where:

BALVEL = water velocity in riffle sections of reach (ft/s or m/s)
 CMMV = half-saturation constant for velocity for algal nutrient availability (ft/s or m/s)

If the light intensity is greater than the user-specified minimum value for growth (LMINGR), then growth can occur, and the light limitation function on growth is computed as in Equation 2-29:

$$GROFL_i = \frac{BALLIT}{CSLIT_i} * \exp \left(1 - \frac{BALLIT}{CSLIT_i} \right) \quad 2-29$$

Where:

BALLIT = available light at the stream bottom (langley [ly]/interval)
 CSLIT_i = saturating light intensity for growth of benthic algal type i (ly/interval)

The density limitation function on growth is based on the total density of benthic algae of all types (SUMBA) as in Equation 2-30:

$$GROFD_i = \frac{CMMD1_i * SUMBA + CMMD2_i}{SUMBA + CMMD2_i} \quad 2-30$$

Where:

SUMBA = total benthic algal biomass for all algal types (mg biomass/m²)

CMMD1_i = coefficient in equation for density-limited growth

CMMD2_i = half-saturation constant for density-limited growth (mg biomass/m²)

If necessary, the growth of each benthic algal type is adjusted so that its density (mg/m²) does not go below the minimum value given by the input parameter MINBAL.

Respiration is calculated as in Equation 2-31:

$$RESBA_i = BALR20_i * TCBALR_i^{T_w - 20} + GRORES_i * GROBA_i \quad 2-31$$

Where:

BALR20_i = respiration rate at 20 °C (/interval)

TCBALR_i = temperature correction coefficient for respiration

T_w = water temperature (°C)

GRORES_i = fraction of respiration required to support growth

Benthic algae removal is assumed to occur as a result of grazing and disturbance by benthic invertebrates and scouring. These processes are computed in subroutine BALREM. The total removal rate of all benthic algae due to grazing and disturbance is computed as in Equation 2-32:

$$REMINV = CREMVL * TCGRAZ^{T_w - 20} * \frac{SUMBA}{SUMBA * CMMBI} * BINV \quad 2-32$$

Where:

REMINV = total removal of benthic algae (all types) due to grazing and disturbance (mg biomass/m²/interval)

CREMVL = removal rate due to grazing and disturbance of benthic algae by invertebrates (mg biomass/mg invertebrates/interval)

TCGRAZ = temperature correction coefficient for grazing of benthic algae by benthic invertebrates

CMMBI = half-saturation constant for benthic invertebrate grazing (mg biomass/m²)

BINV = biomass of grazing benthic invertebrates in the reach (mg invertebrates/m²)

The scouring loss rate (/interval) for each benthic algal type is computed as in Equation 2-33:

$$SLOF_i = CSLOF1_i * \exp(CSLOF2_i * BALVEL) \quad 2-33$$

Where:

CSLOF1_i = rate coefficient in scour regression equation for benthic algal type (/interval)

CSLOF2_i = exponent coefficient in scour regression equation for benthic algal type x (/interval)

Finally, the total removal is computed by allocating the total grazing removal to each of the types and adding the scouring removal rate as in Equation 2-34:

$$REMBA_i = [REMINV/SUMBA + SLOF_i] * BENAL_i$$

2-34

If necessary, the removal of each benthic algal type is adjusted so that its density (mg/m²) does not go below the minimum value given by the input parameter MINBAL.

The following rates and constants are required when simulating benthic algae using the newer method:

- Minimum benthic algae density (as biomass);
- Coefficient for the alternative nitrogen preference equation for benthic algae;
- Fraction of non-refractory nutrients resulting from benthic algae death/removal that are assumed to be immediately available as inorganic nutrients, plus refractory organic carbon;
- Concentration of available inorganic nitrogen in the water column above which nitrogen-fixation by benthic algae is suppressed;
- Maximum benthic algae growth rate for each benthic algae species;
- Temperature correction coefficient for growth for each species;
- Half-saturation constants for nitrogen- and phosphorus-limited growth for each species (if the value for the nitrogen limitation is set to zero, then growth is not limited);
- Coefficient for total benthic algae density in the density-limited growth equation for each species;
- Half-saturation constant for density-limited growth for each species;
- Saturation light level for each species;
- Benthic algae respiration rate at 20 °C for each species;
- Temperature correction coefficient for respiration for each species;
- Rate coefficient in the benthic algae scour equation for each species;
- Multiplier of velocity in the exponent in the benthic algae scour equation for each species;
- Fraction of photorespiration needed to support growth/photosynthesis for each species;
- Annual benthic algae grazing (removal) rate by invertebrates;
- Half-saturation constant for grazing by invertebrates;
- Temperature correction coefficient for macroinvertebrate grazing;
- Biomass of grazing invertebrates in the reach;
- Coefficient and exponent in the turbidity estimation equation;
- Coefficient and exponent in the light extinction equation;
- Fraction of the reach that is composed of riffles where benthic algae can grow;
- Half-saturation constant for riffle velocity in the nutrient availability equation for benthic algae;
- Critical flow levels (3) for riffle velocity and average depth; and
- Riffle velocity multipliers corresponding to the critical flow value and depth multipliers corresponding to the critical flow value

2.4 QUAL2K and QUAL2Kw

Model Background

QUAL2K (or Q2K) and QUAL2Kw (or Q2Kw) are closely related river and stream water quality models, developed primarily by Tufts University, the Washington State Department of Ecology, and the Montana Department of Environmental Quality, that are intended to represent modernized versions of the EPA-supported model QUAL2E (or Q2E) model (Brown and Barnwell 1987). The first version of the QUAL2K model (Chapra, 1999) was originally developed to address several major shortcomings of Q2E. Since then, it has been updated on a periodic basis with the current version documented by Chapra et al. (2015).

Q2Kw (w for Washington) is an alternative expression of the model developed by Pelletier et al. (2006) and Pelletier and Chapra (2008)¹. Most of the following discussion focuses on Q2K with a separate section devoted exclusively to the major distinguishing features of Q2Kw. For the purposes of this document, discussions of Q2K are also relevant to Q2Kw. Post-1985 enhancements to Q2K are equally applicable to Q2Kw, and are therefore not discussed separately. Features or components that are found in Q2Kw but not in Q2K are discussed as being Q2Kw-specific. Enhancements specific to Q2Kw are not specifically related to rates, constants, or kinetic formulations, as discussed in more detail later in this section.

The original impetus for Q2K stemmed from two major overriding factors: 1) Q2E had not been updated since it was issued in 1987 and hence had not kept up with advances in water-quality modeling and computing; and 2) Q2E was developed primarily for larger rivers in the Eastern United States and hence had some severe deficiencies for application in the Western United States. Key issues that needed to be addressed were:

- Q2E could not be applied to clear and shallow streams dominated by bottom algae;
- It did not mechanistically model sediment–water fluxes of oxygen and nutrients;
- It could not be used for anoxic systems (e.g., the model did not include denitrification and it allowed oxygen concentrations to go negative);
- It did not simulate pH and hence could not address pH-dependent processes such as ammonia toxicity; and
- It was not designed for modern personal computers, and new software advances offered an opportunity to move the program to a spreadsheet environment for ease of use and transparency.

The current release of Q2K (Chapra et al., 2012) is version 2.12 (www.qual2k.com). Q2K is similar to Q2E in the following respects:

- One dimensional – the channel is well-mixed vertically and laterally;
- Branching – the system can consist of a mainstem river with branched tributaries;

¹ The current version and documentation of Q2Kw is available from the Washington State Department of Ecology at <http://www.ecy.wa.gov/programs/eap/models.html>

- Steady-state hydraulics² – non-uniform, steady flow is simulated;
- Diel heat budget – the heat budget and temperature are simulated as a function of meteorology on a diel time scale. Solar radiation is computed at each time step as a function of date, time, latitude/longitude, and atmospheric conditions using solar equations;
- Diel water-quality kinetics – all water quality variables are simulated on a diel time scale; and
- Heat and mass inputs – point and non-point loads and withdrawals are simulated.

The Q2K framework includes the following elements not found in Q2E:

- Carbonaceous BOD speciation – Q2K uses two forms of carbonaceous BOD to represent organic carbon;
- Anoxia – Q2K accommodates anoxia by reducing oxidation reactions to zero at low oxygen levels. In addition, denitrification is modeled as a first-order reaction that becomes pronounced at low oxygen concentrations;
- Sediment–water interactions – Sediment–water fluxes of dissolved oxygen and nutrients can be simulated internally rather than being prescribed. That is, oxygen (SOD) and nutrient fluxes are simulated as a function of settling particulate organic matter, reactions within the sediments, and the concentrations of soluble forms in the overlying waters using a version of the sediment diagenesis framework (Di Toro and Fitzpatrick, 1993; Di Toro, 2001) developed by Martin and Wool (2012);
- Bottom algae – The model explicitly simulates attached bottom algae. These algae have variable stoichiometry;
- Light extinction – Light extinction is calculated as a function of suspended algae, detritus, and inorganic solids;
- pH – Both alkalinity and total inorganic carbon are simulated. The river’s pH is then computed based on these two quantities;
- Pathogens – A generic pathogen is simulated. Pathogen removal is determined as a function of temperature, light, and settling;
- Reach-specific kinetic parameters – Q2K allows you to specify many of the kinetic parameters on a reach-specific basis; and
- Weirs and waterfalls – The hydraulics of weirs are explicitly modeled as well as the effects of weirs and waterfalls on gas transfers (oxygen, carbon dioxide, and unionized ammonia).

The kinetic formulation for bottom algae in QUAL2K and QUAL2Kw is the same as the formulation used in current version of WASP and described in Section 2.1 because the WASP module was based on the representation in QUAL2K.

The model state variables are listed in Table 4.

² Although Q2K is limited to steady-state hydraulics, Q2Kw does not have this limitation. Q2Kw simulates non-steady, non-uniform flow using kinematic wave flow routing. Q2Kw is capable of continuous simulation with time-varying boundary conditions for periods of up to one year. Q2Kw also has the option to use repeating diel conditions similar to Q2K but with either steady or non-steady flows. See subsection QUAL2Kw-Specific Features.

Table 4. QUAL2K/QUAL2Kw Model State Variables

| Variable | Symbol | Units |
|----------------------------|-----------------|-----------------------------------|
| Conductivity | s | µmhos |
| Inorganic suspended solids | m _i | mg D ¹ /L |
| Dissolved oxygen | o | mg O ₂ /L |
| Slowly reacting CBOD | c _s | mg O ₂ /L |
| Fast reacting CBOD | c _f | mg O ₂ /L |
| Organic nitrogen | n _o | µg N/L |
| Ammonia nitrogen | n _a | µg N/L |
| Nitrate nitrogen | n _n | µg N/L |
| Organic phosphorus | p _o | µg P/L |
| Inorganic phosphorus | p _i | µg P/L |
| Phytoplankton | a _p | µg A ¹ /L |
| Phytoplankton nitrogen | IN _p | µg N/L |
| Phytoplankton phosphorus | IP _p | µg P/L |
| Detritus | m _o | mg D ¹ /L |
| Pathogen | X | cfu/100 mL |
| Alkalinity | Alk | mg CaCO ₃ /L |
| Total inorganic carbon | c _T | mole/L |
| Bottom algae biomass | a _b | mg A ¹ /m ² |
| Bottom algae nitrogen | IN _b | mg N/m ² |
| Bottom algae phosphorus | IP _b | mg P/m ² |

¹ In the current versions of the model, *A* represents mass as chlorophyll a and *D* represents mass as ash-free dry weight.

QUAL2Kw-Specific Features

QUAL2Kw (Q2Kw) began in 2004 as a modification of Q2K version 1.4. The current release is version 6 (Pelletier and Chapra, 2008; <https://ecology.wa.gov/Research-Data/Data-resources/Models-spreadsheets/Modeling-the-environment/Models-tools-for-TMDLs>). The development of Q2Kw is supported by the Washington State Department of Ecology and has occurred in parallel to development of Q2K, and the development team for Q2Kw includes the developers of Q2K. Q2Kw is used as the main modeling framework for TMDL studies in the state of Washington related to temperature and eutrophication in rivers (e.g., Carroll et al., 2006). Q2Kw has also been adopted by other states (e.g., Turner et al., 2009) to support their TMDL programs, and it is widely used worldwide (e.g., Kannel et al., 2011).

The parallel development of Q2Kw from 2004 to the present has led to the addition of several capabilities that are not available in Q2K. As discussed earlier in this section, post-1985 enhancements to Q2K related to rates, constants, and kinetic formulations are equally applicable to Q2Kw. In addition to the features of Q2K described above, the current version of Q2Kw (version 6) also has the following capabilities:

- Non-steady, non-uniform flow using kinematic wave flow routing – Q2Kw is capable of continuous simulation with time-varying boundary conditions for periods of up to one year. Q2Kw also maintains the option to use steady flow with repeating diel conditions, like Q2K;
- Transient storage zones – Q2Kw has the capability to simulate water quality in hyporheic transient storage (HTS) and/or surface transient storage (STS) zones attached to any reaches;
- Automatic calibration – Q2Kw includes a genetic algorithm to calibrate the kinetic rate parameters automatically within user-defined ranges for each parameter. Details on the autocalibration algorithm is included in the model manual;
- Monte Carlo simulation – Q2Kw is capable of Monte Carlo simulation to evaluate uncertainty or sensitivity with either of the following two add-ins for Microsoft Excel: 1) an open-source add-in called YASAIw supported by the Washington State Department of Ecology³, or 2) Oracle Crystal Ball⁴; and
- Sediment Flux Model (SFM) – Q2Kw employs the same SFM framework as WASP, following the governing equations described in Section 2.1.

The benthic and planktonic algal simulation routines are similar to those contained in the advanced eutrophication module of WASP (since version 7). The algorithms for predicting detrital and periphyton concentrations in WASP were adapted from the QUAL2K model. Unlike WASP, the QUAL2K and QUAL2Kw models do not contain separate macroalgae routines.

3. Methodology for Identifying Relevant Literature

To identify literature appropriate for developing tables of rates from modeling studies since the 1985 Rates Manual, the team conducted literature searches and contacted members of the modeling community. Internet searches were conducted using Google Scholar and Google to obtain both peer-reviewed published literature as well as grey literature (e.g., TMDL reports). Keywords were chosen based on our team's expertise and knowledge of the models and the water quality constituents of interest (i.e., dissolved oxygen, nutrients, and algae). A list of primary keywords used for the literature search is provided in Table 5. These keywords were combined and manipulated for multiple search efforts; this is not an exhaustive list of all keyword combinations. These keywords, and other permutations of them, were applied to Google Scholar, Web of Science, the USACE Engineering Research and Development Center (ERDC) library, EPA's TMDL Database, and other publication repositories. In addition, the available lists of model-centric publications were mined for additional literature to evaluate.

³ YASAIw, an open-source Monte Carlo simulation add-in for Microsoft Excel supported by the Washington Department of Ecology, is available for download from <http://www.ecy.wa.gov/programs/eap/models.html>

⁴ Oracle Crystal Ball is an add-in for Microsoft Excel available from Oracle at <http://www.oracle.com/us/products/applications/crystalball/overview/index.html>

Table 5. Primary keywords for literature identification

| Keyword | |
|---|--------------------------------------|
| [Model name] | Phytoplankton model rates |
| Application of [model name] | Dissolved oxygen model rates |
| Modeling studies using [model name] | Nutrient rate constant surface water |
| Parameter values TMDL models | Freshwater nutrient recycling |
| TMDL [model name] | Sediment nutrient diagenesis model |
| Surface water model calibration results | Water quality model parameters |

During the literature search and review phase, specific documents targeted included:

- **TMDL modeling studies**, in which one or more of the four models of interest were calibrated and validated as part of TMDL development;
- **General water quality modeling studies**, in which one of the four models was used to assess water quality separate from the development of a TMDL; and
- **Laboratory or field studies**, in which rates, constants, and kinetic parameters used in the models were measured under controlled conditions.

In addition to Internet searches, the project team reached out to the modeling community to obtain relevant literature. To do so, announcements (example shown in Exhibit 1) requesting relevant studies were posted on professional listservs identified for three of four models (

Exhibit 2). Several listserv members contacted the project team to provide documents that appeared relevant to this effort.

Exhibit 1. Example announcement posted to model listserv

To: HSPF-USERS@LISTSERV.UOGUELPH.CA
 Subject: Request for information for Rates, Constants, Kinect Formulations manual

Our team is supporting EPA on a research project to support updates to Rates, Constants, and Kinetic Formulations in Surface Water Quality Monitoring (Second Edition) (EPA/600/3-85/040). If you have applied any of the following models—QUAL2Kw, WASP, CE-QUAL-W2 or HSPF—in the development of nutrient TMDLs, we would be interested in obtaining any reports that discuss the application of those models in the TMDL development. In particular, we are looking for reports or peer-reviewed publications that provide information concerning the calibration of the model, its calibration data sets, and model coefficients used. Electronic or hard-copy versions of those reports would be appreciated.

Contact: [contact information]
 Thank you.

Exhibit 2. Listservs by model

| Model Name | Listserv |
|------------|---|
| WASP | http://www.Isoft.com/scripts/wl.exe?SL1=WASP-USERS&H=LISTSERV.UOGUELPH.CA |
| HSPF | http://www.Isoft.com/scripts/wl.exe?SL1=HSPF-USERS&H=LISTSERV.UOGUELPH.CA |
| CE-QUAL-W2 | http://w2forum.cee.pdx.edu/ |

The documents obtained from the Internet searches were screened and narrowed down further by applying the following criteria:

- **Publication date:** Studies published in 1985 or later were selected, to ensure the most recent information is used and that it reflects updates and changes to the models since the 2nd Edition of the Rates Manual was published. Issues may arise in comparing the values identified in the 1985 manual to values gathered for this project. In some instances, the values are not directly comparable, as some of the model formulations have changed (see, for example, Equation 2-1 vs. Equations 2-2a and 2-2b);
- **Specificity to models and constituents of interest:** Only studies specific to the four models and to Group 1 water quality constituents (dissolved oxygen, nutrients, and algae) were selected;
- **Availability of data on rates, constants, and kinetic parameters:** Studies that explicitly provided values of model rates, constants, and kinetic parameters, typically identified in tables and figures, were included; and
- **Representativeness of different waterbody types:** Studies that represented different waterbody types, such as lakes, rivers, estuaries, and streams, were selected.

It was outside the scope of this effort to research formally or make judgments on the quality control practices of the studies and reports identified through the literature review and included here as literature and data sources. For all models, the project team assumed that state and federal agencies and peer-reviewed journals publish studies and study data with acceptable quality control practices and data quality. To determine whether a paper or report was suitable for inclusion in the data tables, several criteria were considered to gauge completeness of documentation for the purposes of this project: tabulated final calibrated parameters; information on the data used for calibration; description of model setup and calibration procedures; and an evaluation by the authors of model output. Reports that did not include thorough documentation were removed from consideration. A study or paper that was deemed inappropriate for this project's data tables was not necessarily a poor-quality paper or poorly executed study; omission may merely indicate that the authors did not provide complete documentation of procedures and calibrated parameters, possibly due to journal space constraints or because the goals of the paper did not require in-depth documentation. The project team found that state and federal government reports often provide more complete descriptions of data acquisition and model development than peer-reviewed journal articles.

Selected documents were then reviewed for information on:

- Whether measurements of water quality were used to calibrate model parameters related to dissolved oxygen, nutrients, and algae;
- The number of years of data used for calibration of nutrients, DO, and algae; and
- Whether calibration data included measurements of water quality processes⁵ and, if yes, which ones.

⁵ Process measurements include those that go beyond measurements of constituent concentrations (e.g., collection of chamber measurements of sediment oxygen demand versus reliance only on water column dissolved oxygen concentrations).

4. Summary of Available Information

This section summarizes the information obtained from the literature search. For each of the four models, a similar sequence of information is provided:

- Discussion of literature search process;
- Literature table summarizing the studies obtained in the search, including author(s), year, waterbody name, geographic area and climate, and watershed/waterbody characteristics;
- Data table with summary statistics for model rates and constants;
- Discussion of calibration data and approaches; and
- Discussion of information gaps.

It should be noted that there is overlap in some of the eutrophication kinetics employed in WASP, CE-QUAL-W2, QUAL2K/QUAL2Kw, and HSPF. In some cases, it may be possible for a user of the data tables to investigate parameters across all models in cases where the underlying kinetic processes in each model are similar. However, a preliminary evaluation of governing equations across models identified numerous issues associated with a cross-model comparison of parameters. A discussion of this evaluation, barriers encountered, and suggested future research is included in Section 6 of this report. Before assuming that parameter values reported for one model will meet the needs for what appear to be similar parameters used in a second model, users should review the kinetic formulations employed in each of the models to be sure that the associated rates and coefficients are used in a consistent kinetic formulation across the models. Detailed information on the theoretical underpinnings of each model are available either in the model user's manual or associated documentation. It may also be important for the user to compare the underlying model code in situations where they are considering comparing RCK parameters across models.

4.1 WASP

Summary of Sources

Summary of Literature sources for WASP applications found via the Google Scholar and U.S. EPA AskWaters search engines were reviewed following the methods described in Section 3. Initial screening activities identified approximately 150 papers. These papers were then reviewed in more detail, with the review focusing on the following items:

- Peer-reviewed journal papers vs. grey literature – As described in Section 3, literature selection depended on thorough documentation of model setup, calibration, and verification. Peer, reviewed journal papers were considered high value (in terms of acceptability for this effort), since they were reviewed by impartial and knowledgeable practitioners. Additionally, reports prepared for states and federal agencies were included if model documentation was sufficient or if the report was reviewed by a technical advisory committee.
- Multi-year or multi-season data sets – Modeling efforts that included calibration/validation data sets that included more than one year or one season of data were considered to be of higher value compared to data sets that consisted of just one year or season of data. The principal reason for this is that it is easier to over-calibrate a model to one year (or season) of data than it

is to calibrate to multi-year (or multi-season) data sets. A model that can reproduce the major features of multi-year data sets can be considered more robust. However, models that appeared to adjust model constants and coefficients from year to year, unless justifiable, were considered to be of lesser value as compared to models that used a consistent set of constants and coefficients throughout the calibration/validation period.

- Quantitative skill assessment – Papers that presented quantitative skill assessment metrics and results were considered of higher value, assuming that the model skill could be quantified as being good or acceptable (see Arhonditsis and Brett, 2004; Fitzpatrick, 2009), than papers that presented just qualitative skill, i.e., time-series or spatial profiles of model versus data. Papers that presented only qualitative skill assessment were not necessarily rejected, but required additional review to determine their acceptability.
- Rate and coefficient values – Model rates and coefficients presented in the papers were also reviewed as to their reasonableness and consistency with the range of values reported in the modeling literature, previous WASP applications and the range of coefficients reported in WASP documentation and EPA’s 1985 Rates Manual. Sources reporting RCK values that deviated significantly from acceptable ranges were eliminated from further consideration.

The tables developed for WASP were supplemented with additional information drawn from eutrophication-based studies performed by HydroQual (now HDR), and the USACE ERDC. The reason for including these grey-literature sources is that the sediment diagenesis/nutrient flux model (SFM) is a recent addition to WASP and only two peer-reviewed papers were found that used the SFM (Brady et al., 2013, Testa et al., 2013). However, since the version of SFM that is incorporated in WASP is virtually identical to that used by HDR and the USACE ERDC, the Project Team believed that incorporating this information was appropriate for this effort. The non-WASP models that incorporate the SFM are HDR’s RCA model code, the USACE’s CE-QUAL-ICM (Cercio and Cole, 1994) model code, and CE-QUAL-W2 and QUAL2Kw.

After detailed screening, 47 papers passed relevance and criteria checks, including eight HydroQual, HDR and USACE ERDC reports that provided information concerning the application of the SFM and associated RCK values for eutrophication (Table 6). Of these 47 papers, 28 were peer-reviewed journal articles, eight were TMDL reports (prepared by EPA, states, or consulting firms under contract to EPA or states), six were reports prepared by HydroQual or HDR, two by USACE ERDC, one by USGS, one by Tetra Tech, and one was a doctoral thesis. WASP has been used in many other TMDL studies, but the team was not successful in locating those studies via Google, Google Scholar, or the EPA AskWATERS TMDL search engine. For additional resources regarding WASP, see Section 9 of this report. Detailed examples of application of the WASP model to nutrient and DO problems, along with extensive tables of relevant rates and constants are also available in U.S. EPA (1995).

While a few of the papers used data sets of a limited time frame (i.e., a few weeks to a summer season) for model calibration, the team decided to include them because the model appeared well-calibrated and the model coefficients were reasonable. While several papers modeled only BOD/DO, the majority simulated water column phytoplankton and/or attached algae or periphyton.

Table 6. WASP Literature Sources

| Citation | Study Location | Type of Water body | Watershed Characteristics | Calibration period |
|--|---|--------------------|--|-------------------------------------|
| Camacho, R., J. Martin, B. Watson, M. Paul, L. Zheng, and J. Stribling, 2014. Modeling the Factors Controlling Phytoplankton in the St. Louis Bay Estuary, Mississippi and Evaluating Estuarine Responses to Nutrient Load Modifications. <i>Journal of Environmental Engineering</i> . 1943-7870.0000892. | St. Louis Bay, Mississippi | Estuary | 1,840 km ² drainage; avg depth = 1.4m; surface area = 39.8 km ² ; watershed undeveloped (52%-forest, 23%-timber, 15%-anthropogenic uses) | January 27, 2011-December 31, 2011. |
| Canu, D., C. Solidoro, and G. Umgiesser, 2004. Modelling the Responses of the Lagoon of Venice Ecosystem to Variations in Physical Forcings. <i>Ecological Modelling</i> . 174(2). | The Lagoon of Venice | Lagoon | avg. depth = 1 m; surface area = 550 km ² | 1987, 2000 |
| Cerucci, M., G. Jalgama, and R. Ambrose, 2010. Comparison of the Monod and Droop Methods for Dynamic Water Quality Simulations. <i>Journal of Environmental Engineering</i> . 1943-7870.0000257. | Raritan River, New Jersey | River | 2,850 km ² drainage. | 2003-2005 |
| Chen, C., W. Lung, S. Li, and C. Lin, 2012. Technical Challenges with BOD/DO Modeling of Rivers in Taiwan. <i>Journal of Hydro-environmental Research</i> . 3(8). | The Danshui River and the Chungkang River, Taiwan | River | Danshui River (watershed 2726 km ²); Chungkang River (watershed area of 446 km ²). | October-November 2006 |
| Dilks, D., and T. James, 2011. Parameter Uncertainty in a Highly Parameterized Model of Lake Okeechobee. <i>Lake and Reservoir Management</i> . 27(4). | Lake Okeechobee, Florida | Lake | surface area = 1800 km ² ; avg depth = 2.7 m; eutrophic | 1983–2000 |
| Dongil, S., and K. Minae, 2011. Application of EFDC and WASP7 in Series for Water Quality Modeling of the Yongdam Lake, Korea. <i>Journal of Korea Water Resources Association</i> . 44(6). | The Yongdam Lake, South Korea | Lake | Withdrawal facilities for water supply; natural flow through spillways; hydropower generation discharge to Geum River | 2005 |
| Gin, K., Q. Zhang, E. Chan, and L. Chou, 2001. Three-Dimensional Ecological-Eutrophication Model for Singapore. <i>Journal of environmental Engineering</i> . 10(928). | Southwest Monsoon, Singapore | River | Increased loading from treated industrial and domestic effluents, urban runoff, and sedimentation | August 1998 (14 days) |
| Gu, R., and M. Don, 1998. Water Quality Modeling in the Watershed-based Approach for waste Load Allocations. <i>Water Science Technology</i> . 38(10). | Des Moines River, Iowa, USA | River | 4600 km ² drainage area; annual mean discharges = 1000 m ³ /s; 7Q10=2.8 m ³ /s | 1975-1977 |

| Citation | Study Location | Type of Water body | Watershed Characteristics | Calibration period |
|--|---------------------------------|--------------------|--|---|
| Huang, Y., C. Yang, and P. Tang, 2010. Water Quality Management Scenarios for the Love River in Taiwan. International Conference on Challenges in Environmental Science and Computer Engineering. | The Love River, Taiwan | Stream | Catchment area of 62 km ² , an urban-type tidal stream | May 18 – October 13, 2009 |
| James, R.T., J. Martin, T. Wool, and P.F. Wang, 1997. A Sediment Resuspension and Water Quality Model of Lake Okeechobee. 33(3). | Lake Okeechobee, Florida | Lake | Lake Okeechobee is a large (surface area 1,732 km ²) shallow (mean depth 2.7 m) lake | January 1, 1990- December 31, 1991 |
| Jia, H., Y. Zhang, and Y. Guo, 2010. The Development of a Multi-Species Algal Ecodynamic Model for Urban Surface Water Systems and its Application. Ecological Modelling. 221(15). | Urban river system, Beijing | River | Urban area | March - October 2004 |
| Kardos, J., and C. Obropta, 2011. Water Quality Model Uncertainty Analysis of a Point-Point Source Phosphorus Trading Program. Journal of the American Water Resources Association. 47(6). | Passaic River Basin, New Jersey | River Basin | 1733 km ² and 347 km ² watershed area in New Jersey and New York | 2007 |
| Kim, T., and Y. Sheng, 2009. Estimation of Water Quality Model Parameters. KSCE Journal of Civil Engineering. 14(3). | Indian River Lagoon, Florida | Lagoon estuary | Narrow except the Inter-Coastal Waterway (0.5-7 km); extends 255 km | |
| Kish, S., J. Barlett, J. Warwick, A. McKay, and C. Fritsen, 2006. Long-Term Dynamic Modeling Approach to Quantifying Attached Algal Growth and Associated Impacts on Dissolved Oxygen in the Lower Truckee River, Nevada. 132(10). | Truckee River, Nevada | River | The Truckee River Basin comprises an area of about 7,925 km ² . Mostly agricultural area. 195 km long Truckee River. | August 2000– December 2001 |
| Lai, Y., C. Yang, C. Hsieh, C. Wu, and C. Kao, 2011. Evaluation of Non-Point Source Pollution and River Water Quality Using a Multimedia Two-Model System. Journal of Hydrology. 409(3-4). | The Kaoping River, Taiwan | River | The Kaoping River Basin: 3625 km ² Forest-56%, BrdIf evergreen-7.7%, Farms-15.5%, Marsh-5.3%, Shrub+Grassland-7.5%, Resid+commerce-2.6% River length=171 km, Mean Flow=239 m ³ /s. | 2008-2009 |
| Lindenschmidt, K.E., I. Pech, and M. Baborowski, 2009. Environmental Risk of Dissolved Oxygen Depletion of Diverted Flood Waters in River Polder Systems--A Quasi-2D Flood Modelling Approach. Science of the Total Environment. 407(5). | Elbe River, Germany | River | Mean Q=153 m ³ /s (1998) Mean Q=228 m ³ /s (1999) Mean Q=194 m ³ /s (2000) Mean Q=2743 m ³ /s (2002) | 12 - 21 August of 2002, and Apr-Aug of 1998, 1999, 2000 |

| Citation | Study Location | Type of Water body | Watershed Characteristics | Calibration period |
|--|--|--------------------|---|--|
| Liu, Z., W. Kingery, D. Huddleston, F. Hossain, W. Chen, N. Hashim, and J. Kieffer, 2007. Modeling Nutrient Dynamics Under Critical Flow Conditions in Three Tributaries of St. Louis Bay. <i>Journal of Environmental Science and Health, Part A</i> . 43(6). | St. Louis Bay, Mississippi | Bay | The drainage area is approximately 1,840 km ² with two major tributaries, Jourdan River and Wolf River | March 16 to July 23, 1998, January 1 to April 30, 1999 |
| Lundgren, R., and R. Nustad, 2008. Calibration of a Water-Quality Model for Low-Flow Conditions on the Red River of the North at Fargo, North Dakota, and Moorhead, Minnesota, 2003. USGS. Scientific Investigations Report. | Red River, North Dakota, and Moorhead, Minnesota | River | 19.2-mi reach of the Red River | Sept. 24-27, 2003 |
| Lung, W., and A. Nice, 2007. Eutrophication Model for the Patuxent Estuary: Advances in Predictive Capabilities. <i>Journal of Environmental Engineering</i> . 133(9). | The Patuxent Estuary | Estuary | | 1997-1999 |
| Lung, W., and H. Paerl, 1988. Modeling Blue-green Algal Blooms in the Lower Neuse River. <i>Water Research</i> . 22(7). | Neuse River, North Carolina | River | Neuse River drains approx. 25% of North Carolina's land area, flowing through the Piedmont and Coastal Plain regions. | 1983-1985 |
| Lung, W., 1986. Assessing Phosphorus Control in the James River Basin. <i>Journal of Environmental engineering</i> . 112(1). | James River Estuary, Virginia | Estuary | | Summer 1983 |
| Melendez, W., M. Settles, J. Pauer, and K. Rygwelski, 2009. LM3: A High-resolution Lake Michigan Mass Balance Water Quality Model. Grosse Ile, Michigan: U.S. EPA. | Lake Michigan | Lake | | 1994-1995 |
| Narasimhan, B., R. Srinivasan, S. Bednarz, M. Ernst, and P. Allen, 2010. A Comprehensive Modeling Approach for Reservoir Water Quality Assessment and Management Due to Point and Nonpoint Source Pollution. <i>Transactions of ASABE</i> . 53(5). | Cedar Creek reservoir, Texas | Reservoir | Reservoir surface area of 13,350 ha and a volume of 795 million m ³ . | 1991-2001 |
| Pauer, J., A. Anstead, W. Melendez, and R. Kreis, 2008. The Lake Michigan Eutrophication Model, LM3 - Eutro: Model Development and Calibration. <i>Water Environment Research</i> 80(9). | Lake Michigan | Lake | | 1994-1995 |

| Citation | Study Location | Type of Water body | Watershed Characteristics | Calibration period |
|--|---|-----------------------|---|-----------------------------|
| Sangsurasak, C., H. Hsieh, W. Wongphathanakul, and W. Wirojanagud, 2006. Water Quality Modeling in the Nam Pong River, Northeast Thailand. ScienceAsia. 32. | Nam Pong River, Thailand | River | Mostly agricultural land DO= 3.1 $\mu\text{mol/L}$ | 1999-2000 |
| Simachaya, W., 1999. Integrated Approaches to Water Quality Management Using Geographic Information Systems and the WASP5 Simulation Model: Application to the Tha Chin River Basin, Thailand. University of Guelph. | Tha Chin River Basin, Thailand | River | Depth: 3-12m; Width: 100-600m; avg freshwater inflow: 32 m^3/s predominantly agriculture (83%) | 1995, 2014 |
| Soyupak, S., L. Mukhallalati, D. Yemisen, A. Bayar, and C. Yurteri, 1996. Evaluation of Eutrophication Control Strategies for the Keban Dam Reservoir. Ecological Modelling. 97. | Keban Dam Reservoir (KDR), Anatolia, Turkey | Reservoir | Surface Area=675 km^2 , Volume=30.6E9 m^3 . | 1992 |
| Tetra Tech, Inc., 2009. TMDLs for Dissolved Oxygen and Nutrients in Selected Subsegments in the Mississippi River Basin, Louisiana. | Capitol Lake, Baton Rouge, Louisiana | Lake | 60-acre freshwater lake drainage area: 1.731 acres predominant land use is developed (96.76%) | August 30-September 1, 2007 |
| Tetra Tech, Inc., 2008. Nutrient and Sediment TMDLs for the Indian Creek Watershed, Pennsylvania: Established by the U.S. Environmental Protection Agency. | Indian Creek, Pennsylvania | third-order stream | drainage area = 7 mi^2 , flows 6.1 miles, various degrees of residential development scattered throughout watershed. Middle portion of watershed is predominantly pastures | 1997-2004 |
| Tufford, D., and H. McKellar, 1999. Spatial and Temporal Hydrodynamic and Water Quality Modeling Analysis of a Large Reservoir on the South Carolina (USA) Coastal Plain. Ecological Modelling. 114. | Lake Marion, South Carolina | Lake | Surface area: 330.7 km^2 ; drainage area: 25,433.8 km^2 ; mean depth: 4 m; maximum depth: 23.4 m | 1985-1990 |
| U.S. EPA, 2000. Total Maximum Daily Load (TMDL) Development for Dissolved Oxygen in the Taylors Creek in the Ogeechee River Basin. | Taylors Creek, Georgia | Creek | Stream Flow=4.35cfs, DO=5.0 mg/L, BOD=2.5 mg/L, Temp=26 $^{\circ}\text{C}$ | |
| U.S. EPA, 2003. Modeling Report for Wissahickon Creek, Pennsylvania Nutrient TMDL Development, including Appendix F: Technical Memo for the Wissahickon Creek Model. | Wissahickon Creek, Pennsylvania | Creek and Tributaries | | 2002 |

| Citation | Study Location | Type of Water body | Watershed Characteristics | Calibration period |
|---|----------------------------------|--------------------|---|----------------------------|
| U.S. EPA, 2005. Total Maximum Daily Load (TMDL) for Dissolved Oxygen and Nutrients in Butcher Pen Creek (2322) Lower St. Johns River Basin, Florida. | Butcher Pen Creek, Florida | Creek | St. Johns River Basin drainage = 9500 mi ² Butcher Pen is tributary to Cedar River. Urban and residential area-80% of land use. | 1995-2002 |
| U.S. EPA, 2006. Total Maximum Daily Load (TMDL) for Dissolved Oxygen in Hogan Creek (WBID 2252) Lower St. Johns River Basin, Florida. | Hogan Creek, Florida | Creek | St. Johns River Basin drainage = 9500 mi ² Hogan Creek area = 3.4 mi ² . Urban and residential area-98% | 1996-2003 |
| U.S. EPA Region 4, 2013. Appendix A Modeling Report Cedar Creek (WBID 1926): Nutrients, BOD, and Dissolved Oxygen. | Cedar Creek, Florida | Tributary | Tributary basin to the Braden River; 5 km ² ; 76% Urban, | 2003-2007 |
| U.S. EPA, 2013. Model Setup and Calibration for McKay Bay. | McKay Bay, Florida | Bay | | January 2003-December 2007 |
| U.S. EPA Region 4, 2013. Modeling Report Camp Branch (WBID:251) Nutrients and Dissolved Oxygen. | Camp Branch, Florida | Creek | In the Choctawhatchee River Basin; flows 5.4 mi; drainage area = 7.7 mi ² 7.7 mi ² , predominately agricultural and forest land | 2000-2002 |
| U.S. EPA Region 4, 2013. Modeling Report Owen Creek and Myakka River Dissolved Oxygen Nutrients. | Owen Creek Myakka River, Florida | Creek | 60% agriculture 16% wetlands, 15% forest, | 1999-2009 |
| Wang, J., Y. Shen, H. Zhen, Y. Feng, Z. Wang, and X. Yang, 2011. Three-dimensional numerical modelling of water quality in Dahuofang Reservoir in China. Science China Physics, Mechanics & Astronomy. 54(7). | Dahuofang Reservoir | Reservoir | length=35 km; width=max 4 km, min=0.3 km; initial design capacity=21.87E8 m ³ ; drainage area=5437 km ² ; mean depth=12 m | April 1 - November 1, 2006 |
| Warwick, J.J., D. Cockrum, and M. Horvath, 1997. Estimating Non-Point-Source Loads and Associated Water Quality Impacts. Journal of water Resources Planning and Management. | Carson River, Nevada | River | Terminates at Lahontan Reservoir | Jul-90 |

| Citation | Study Location | Type of Water body | Watershed Characteristics | Calibration period |
|---|---------------------------------|--------------------|--|---|
| Warwick, J.J., D. Cockrum, and A. McKay, 1999. Modeling the Impact of Subsurface Nutrient Flux on Water Quality in the Lower Truckee River, Nevada. <i>Journal of the American Water Resources Association</i> . 35(4). | Lower Truckee River, Nevada | River | Portion of river below Derby Dam; derives runoff from melting snow in Sierra Nevada Mountains | July 27-30, 1993; August 17-20, 1993 |
| Wool, T.A., S.R. Davie, and H.N. Rodriguez, 2003. Development of Three-Dimensional Hydrodynamic and Water Quality Models to Support Total Maximum Daily Load Decision Process for the Neuse River Estuary, North Carolina. <i>Journal of Water Resources Planning and Management</i> . Vol. 129, Issue 4. | Neuse River, North Carolina | Estuary | Neuse River drains approx. 25% of North Carolina's land area, flowing through the Piedmont and Coastal Plain regions. | 1998 - 2000 |
| Yang, C., W. Lung, J.T. Kuo, and J.H. Liu, 2010. Water Quality Modeling of a Hypoxic Stream. <i>Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management</i> . | NanZiGuop Stream, Taiwan | Stream | length: 3.4 km, catchment area: 1.9E7 m ² , outlet for significant amount of domestic sewage and industrial waste | October 27-28, 2005 |
| Yenilmez, F., and A. Aksoy, 2013. Comparison of Phosphorus Reduction Alternatives in Control of Nutrient concentrations in Lake Uluabat (Bursa, Turkey): Partial versus Full Sediment Dredging. <i>Limnologica</i> . 43. | Lake Uluabat, Turkey | Lake | surface area=116-155 km ² ; average depth=3 m; min depth=0.8 m; eutrophic | June 1999 - June 2000 |
| Zheng L., C. Chen, and F. Zhang, 2004. Development of Water Quality Model in the Satilla River Estuary, Georgia. <i>Ecological Modelling</i> . 178. | Satilla River Estuary, Georgia | Estuary | Intertidal salt marsh "blackwater" high conc. humic and tannic acids mean depth=4 km; max depth=23 m; width=1-4 km | April 8 and 16, 1995; October 1996; July 1997 |
| Zou, R., S. Carter, L. Shoemaker, A. Parker, and T. Henry, 2006 Integrated Hydrodynamic and Water Quality Modeling System to Support Nutrient Total Maximum Daily Load Development for Wissahickon Creek, Pennsylvania. <i>Journal of Environmental Engineering</i> . 132(4). | Wissahickon Creek, Pennsylvania | Creek | drains 164 km ² , extends 38.6 miles | 2002 |
| Zouiten, H., C. Alvarez Diaz, A. Garcia Gomez, J. Revilla Cortezon, and J. Garcia Alba, 2013. An Advanced Tool for Eutrophication Modeling in Coastal Lagoons: Application to the Victoria Lagoon in the North of Spain. <i>Ecological Modelling</i> . 265. | Victoria Lagoon, Spain | Lagoon | Wetlands, natural reserve, freshwater coastal lagoon periodically becomes saline area= 61ha: 39.5 ha marsh, 21.5 ha dunes | May 1 – November 1, 2009 |

As a model capable of being applied in one, two or three dimensions, WASP applications reported in the tables included lakes, reservoirs, creeks, streams, rivers, lagoons, tidal embayments, and estuaries. In many the earlier papers, the gross transport features of the waterbody were assumed to be at steady state and/or were estimated via calibration to observed temperature and salinity profiles using procedures developed by Pritchard (1964) or Lung and O'Connor (1984), while in more recent papers, the waterbody transport was computed by hydrodynamic models such as DYNHYD (Ambrose et al., 1993), DYRESM (Imberger and Patterson, 1981), or EFDC (Hamrick, 1996). In the case of the RCA model applications, either the ECOM (Blumberg and Mellor, 1987) or EFDC (Hamrick, 1996) hydrodynamic models have been used to provide transport information, while in the case of the CE-QUAL-ICM application, the CH3D hydrodynamic model (Sheng, 1989) has been used.

Several more recent papers also have some discussion of linkages between WASP and watershed models such as HSPF (Bicknell et al., 2014), SWAT (Neitsch et al., 2011), and LSPC (Tetra Tech, 2009) to provide estimates of nutrient loadings to the waterbody under investigation. The basin sizes involved in these applications have ranged from as small as < 10 km² to as large as 166,000 km². Land use has varied from almost exclusively urban settings to largely agricultural or largely forested/timberland. Information, where available, concerning the watershed characteristics for each included study are contained within the RCK tables.

Climatologically, the study areas include embayments and estuaries in the Atlantic Northeast (Massachusetts, New York, and Connecticut), humid subtropical regions (Florida, Mississippi, Alabama, Georgia, Texas, Turkey), temperate subtropical region (Virginia and Maryland), humid continental cool summer (Vermont), warm/hot summer continental/hemiboreal climates (North Dakota, Iowa), mixed subtropical/tropical climate (Thailand), the Mediterranean (Italy), and semi-arid areas (Nevada).

Tabulating rates and constants values for WASP from the literature is difficult because of the many recent changes in the model, notably including the addition of benthic algae (2006), multiple-algae (2011), and sediment diagenesis (2017) components. These updates added many new kinetic equations and variables and change the number of parameters, and in some cases their interpretation. As a result, published modeling reports from one generation of WASP may not be fully applicable to the current version, and some important parameters—such as internal half-saturation constants for nutrients in algal cells—were not retrieved in the search process for this report.

Results of the survey of rates found in the literature on WASP are provided in Table 7 through 10. Unlike CE-QUAL-W2, for example, the current version of WASP does not have a comprehensive user's guide containing tables of default parameter values. Instead, default and/or example values are spread throughout the many update reports, and are lacking for many parameters. For some rates, there are conflicting default value recommendations among different user updates. Therefore, the tables provide a column of "representative" values, which are intentionally not characterized as defaults. It should be noted, however, that the WASP benthic algae representation is largely consistent with QUAL2K/QUAL2Kw, while the multi-algae and sediment diagenesis routines share many kinetic representations with both QUAL2K/QUAL2Kw and CE-QUAL-W2. Therefore, the WASP user may gain additional insight on rates and constants for WASP applications by consulting the rate tables for CE-QUAL-WQ (Table 12) and QUAL2K/QUAL2Kw (Tables 17–20).

Summary Statistics for Rates and Constants

Table 7. WASP Rates and Constants: Nutrient Parameters

| Nutrient Parameter | Count | Min | Max | Mean | Median | Representative Values | Units |
|---|-------|--------|------|-------|--------|-----------------------|----------------------|
| Denitrification rate at 20 °C | 20 | 0 | 1.05 | 0.199 | 0.09 | 0.09 | day ⁻¹ |
| Denitrification temperature coefficient | 14 | 1.04 | 1.08 | 1.060 | 1.08 | 1.045 | – |
| Dissolved organic nitrogen decay in sediment temperature coefficient | 1 | 1.08 | 1.08 | 1.08 | 1.08 | – | – |
| Fraction of dissolved organic nitrogen | 2 | 1 | 1 | 1 | 1 | 1.0 | – |
| Fraction of dissolved organic phosphorous | 3 | 0.5 | 1 | 0.833 | 1 | 0.85 | – |
| Fraction of non-recycled organic nitrogen | 2 | 0.15 | 0.4 | 0.275 | 0.275 | 0.5 | – |
| Fraction of non-recycled organic phosphorus | 1 | 0.2 | 0.2 | 0.2 | 0.2 | 0.5 | – |
| Half saturation constant for denitrification oxygen limitation | 16 | 0.01 | 10 | 0.867 | 0.1 | 0.1 | mg O ₂ /L |
| Half saturation constant for nitrification oxygen limitation | 17 | 0.01 | 2 | 1.183 | 1 | 2 | mg O ₂ /L |
| Nitrification rate | 26 | 0.001 | 2.5 | 0.317 | 0.1 | 0.09 -0.013 | day ⁻¹ |
| Nitrification rate temperature correction coefficient | 17 | 1.04 | 1.08 | 1.071 | 1.08 | 1.08 | – |
| Organic carbon mineralization rate | 1 | 0.02 | 0.02 | 0.02 | 0.02 | – | day ⁻¹ |
| Organic N mineralization rate at 20 °C | 18 | 0.0033 | 0.5 | 0.096 | 0.065 | 0.075 | day ⁻¹ |
| Organic N mineralization temperature correction coefficient | 14 | 1.04 | 1.08 | 1.072 | 1.08 | 1.08 | – |
| Organic P mineralization rate at 20 °C | 16 | 0.02 | 0.75 | 0.156 | 0.125 | 0.22 | day ⁻¹ |
| Organic P mineralization temperature correction coefficient | 12 | 1.02 | 1.08 | 1.067 | 1.08 | 1.08 | – |
| Sediment bed organic N decomposition rate at 20 °C | 4 | 0.0004 | 0.1 | 0.033 | 0.0152 | 0.0004 | day ⁻¹ |
| Sediment bed organic N decomposition temperature correction coefficient | 4 | 1.07 | 1.08 | 1.078 | 1.08 | 1.08 | – |
| Sediment bed organic P decomposition rate at 20 °C | 4 | 0 | 0.27 | 0.068 | 0.0002 | 0.0004 | day ⁻¹ |
| Sediment bed organic P decomposition temperature correction coefficient | 4 | 0 | 1.08 | 0.808 | 1.075 | 1.08 | – |
| Settling velocity of particulate inorganic P | 1 | 18 | 18 | 18 | 18 | – | m/d |
| Settling velocity of particulate organic N | 2 | 0.3 | 0.5 | 0.4 | 0.4 | – | m/d |
| Settling velocity of particulate organic P | 2 | 0.3 | 0.5 | 0.4 | 0.4 | – | m/d |

Table 8. WASP Rates and Constants: Oxygen Parameters

| Oxygen parameter | Count | Min | Max | Mean | Median | Representative Values | Units |
|---|-------|---------|--------|--------|--------|-----------------------|-----------------------|
| BOD decay rate | 20 | 0.01 | 0.3 | 0.131 | 0.125 | 0.16 – 0.21- | day ⁻¹ |
| BOD decay rate temperature correction coefficient | 12 | 1.04 | 1.08 | 1.047 | 1.047 | 1.047 | day ⁻¹ |
| CBOD decay | 1 | 0.05 | 0.05 | 0.05 | 0.050 | – | day ⁻¹ |
| CBOD sediment decomposition rate at 20 °C | 1 | 0.0001 | 0.0001 | 0.0001 | 0.000 | – | day ⁻¹ |
| CBOD sediment decomposition rate temperature correction coefficient | 1 | 1.08 | 1.08 | 1.08 | 1.080 | – | – |
| Fraction of BOD carbon source for denitrification | 1 | 0.1 | 0.1 | 0.1 | 0.100 | – | – |
| Fraction of detritus to BOD | 1 | 1 | 1 | 1 | 1.000 | – | – |
| Fraction of dissolved CBOD | 2 | 0.5 | 1 | 0.75 | 0.750 | 0.5 | – |
| Half-saturation constant for oxygen limitation | 9 | 0 | 0.5 | 0.34 | 0.500 | 0.5 | mg O ₂ /L |
| Oxygen to Carbon stoichiometric ratio | 4 | 2.67 | 2.67 | 2.67 | 2.670 | – | G O ₂ /gC |
| Reaeration coefficient at 20 °C | 6 | 0.00005 | 2 | 0.74 | 0.500 | 0.125 | day ⁻¹ |
| Reaeration temperature correction coefficient | 6 | 1.024 | 1.048 | 1.036 | 1.035 | 1.045 | day ⁻¹ |
| Respiration | 1 | 0.1 | 0.1 | 0.1 | 0.100 | – | day ⁻¹ |
| Sediment oxygen demand | 4 | 0 | 1 | 0.45 | 0.350 | 0.2 – 4.0 | g/m ² /day |
| Settling velocity of CBOD and organic matter | 2 | 0.05 | 0.5 | 0.28 | 0.275 | – | m/d |
| Settling rate for particulate CBOD | 1 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | – | m/d |
| SOD temperature correction coefficient | 3 | 1.06 | 1.08 | 1.073 | 1.080 | 1.08 | – |
| Temperature adjustment for reaeration rate | 2 | 1.028 | 1.028 | 1.028 | 1.028 | – | – |

Table 9. WASP Rates and Constants: Algae Parameters

| Algae Group | Parameter | Count | Min | Max | Median | Representative Values | Units |
|-------------------------|------------------------------------|-------|---------|-----|--------|-----------------------|-------------------|
| Phytoplankton (generic) | Growth rate | 30 | 0 | 4 | 2 | 2 | day ⁻¹ |
| Phytoplankton (generic) | Growth rate temperature correction | 19 | 0 | 10 | 1.068 | 1.068 | – |
| Phytoplankton (generic) | Death rate | 19 | 3.5E-07 | 0.2 | 0.1 | 0.02 | day ⁻¹ |
| Phytoplankton (generic) | Death rate temperature factor | 2 | 1 | 1 | 1 | – | – |
| Phytoplankton (generic) | Grazing rate | 6 | 0 | 1.2 | 0.245 | 0 | L/mgC/d |

| Algae Group | Parameter | Count | Min | Max | Median | Representative Values | Units |
|-------------------------|--|-------|---------|------|--------|-----------------------|-------------------|
| Phytoplankton (generic) | Respiration rate | 21 | 0.01 | 0.2 | 0.1 | 0.125 | day ⁻¹ |
| Phytoplankton (generic) | Respiration rate temperature factor | 13 | 1.045 | 1.08 | 1.068 | 1.045 | – |
| Phytoplankton (generic) | Extinction coefficient | 2 | 0 | 2 | 1 | 0.1 5 | m ⁻¹ |
| Phytoplankton (generic) | N:Chl-a | 2 | 0.007 | 7 | 3.5035 | 7.2 | – |
| Phytoplankton (generic) | P:Chl-a | 2 | 0.001 | 1 | 0.5005 | 1 | – |
| Phytoplankton (generic) | C:Chl-a | 20 | 0.025 | 80 | 35 | 40 | – |
| Phytoplankton (generic) | P:C | 14 | 0.01 | 0.24 | 0.025 | 0.025 | – |
| Phytoplankton (generic) | N:C | 17 | 0.1 | 0.3 | 0.2 | 0.18 | – |
| Phytoplankton (generic) | Si:C | 2 | 0.8 | 0.8 | 0.8 | – | – |
| Phytoplankton (generic) | C:O | 4 | 2.67 | 2.67 | 2.67 | – | – |
| Phytoplankton (generic) | Half-saturation for nutrient recycling | 2 | 0 | 1 | 0.5 | – | mg Phyt C/L |
| Phytoplankton (generic) | Half-saturation constant for nitrogen uptake | 7 | 2.5E-05 | 25 | 0.025 | – | mgN/L |
| Phytoplankton (generic) | Half-saturation constant for silica uptake | 2 | 0.03 | 0.05 | 0.04 | – | mgSi/L |
| Phytoplankton (generic) | Half-saturation for phosphorus uptake | 7 | 1.0E-06 | 1 | 0.001 | – | mgP/L |
| Phytoplankton (generic) | Half-saturation for nitrogen limited growth | 11 | 0.005 | 0.4 | 0.025 | 0.025 | mgN/L |
| Phytoplankton (generic) | Half-saturation for phosphorus limited growth | 14 | 0.0005 | 0.01 | 0.0025 | 0.001 | mgP/L |
| Phytoplankton (generic) | Half saturation constant for phytoplankton limitation of phosphorus mineralization | 2 | 0 | 1 | 0.5 | – | mgC/L |
| Phytoplankton (generic) | Organic phosphorus mineralization rate | 2 | 0.06 | 0.22 | 0.14 | – | day ⁻¹ |
| Phytoplankton (generic) | Fraction recycled to organic nitrogen pool | 9 | 0.3 | 0.8 | 0.5 | – | – |
| Phytoplankton (generic) | Fraction recycled to organic phosphorus pool | 9 | 0.1 | 0.65 | 0.45 | – | – |
| Phytoplankton (generic) | Saturation light intensity | 8 | 120 | 720 | 275 | 200 – 500 | ly/d |

| Algae Group | Parameter | Count | Min | Max | Median | Representative Values | Units |
|-------------------------|--|-------|---------|-------|--------|-----------------------|----------------------|
| Phytoplankton (generic) | Light extinction coefficient | 13 | 0 | 5 | 0.35 | – | m ⁻¹ |
| Phytoplankton (generic) | Phytoplankton optimal light saturation | 4 | 200 | 350 | 260 | – | ly/d |
| Phytoplankton (generic) | Algal settling rate | 6 | 2.3E-07 | 0.5 | 0.04 | 0.1 | m/d |
| Phytoplankton (generic) | Mortality ratio of phytoplankton and zooplankton for PON | 2 | 0 | 0.5 | 0.25 | – | – |
| Phytoplankton (generic) | Phytoplankton optimal light saturation | 4 | 200 | 350 | 260 | – | ly/d |
| Phytoplankton (generic) | Phytoplankton Temperature Coefficient for Sediment Decay | 2 | 1.08 | 1.08 | 1.08 | – | – |
| Phytoplankton (generic) | Phytoplankton Phosphorus:Carbon Ratio | 3 | 0.025 | 0.025 | 0.025 | – | – |
| Phytoplankton (generic) | DOP mineralization rate | 3 | 0.026 | 0.43 | 0.22 | – | day ⁻¹ |
| Phytoplankton (generic) | DOP mineralization rate | 3 | 0.026 | 0.43 | 0.22 | – | day ⁻¹ |
| Phytoplankton (generic) | Organic phosphorus mineralization rate | 2 | 0.06 | 0.22 | 0.14 | – | day ⁻¹ |
| Benthic algae | P:C | 2 | 0.015 | 0.02 | 0.018 | 0.025 | mgP/mgC |
| Benthic algae | Growth rate | 2 | 2 | 25 | 13.5 | 9 | gD/m ² /d |
| Benthic algae | Respiration rate | 2 | 0 | 0.1 | 0.05 | 0.03 | day ⁻¹ |
| Benthic algae | Ammonia preference | 2 | 0.025 | 0.1 | 0.063 | 0.025 | mgN/L |
| Blue green algae | Algal settling rate | 3 | 1.2E-06 | 0.19 | 0.05 | – | m/d |
| Blue green algae | Growth rate | 2 | 1.3 | 2.32 | 1.81 | – | day ⁻¹ |
| Blue green algae | Half-saturation for nitrogen limited growth | 3 | 0 | 0.4 | 0.015 | – | mgN/L |
| Diatoms | Growth rate | 2 | 2 | 2.5 | 2.25 | – | day ⁻¹ |
| Diatoms | Growth rate temperature correction | 2 | 0.2 | 20 | 10.1 | – | °C |
| Periphyton | Growth rate | 7 | 0.6 | 1.52 | 0.85 | – | day ⁻¹ |
| Periphyton | Growth rate temperature correction | 5 | 1.055 | 1.06 | 1.06 | 1.07 | – |
| Periphyton | Death rate | 3 | 0.009 | 0.05 | 0.02 | 0.05 | day ⁻¹ |
| Periphyton | Respiration rate | 6 | 0.015 | 0.15 | 0.063 | 0.10 | day ⁻¹ |

| Algae Group | Parameter | Count | Min | Max | Median | Representative Values | Units |
|-------------|---|-------|-------|-------|--------|-----------------------|-------------------|
| Periphyton | Respiration rate temperature factor | 3 | 0.069 | 0.078 | 0.078 | 1.07 | – |
| Periphyton | P:C | 3 | 0.01 | 0.03 | 0.025 | 0.025 | – |
| Periphyton | N:C | 4 | 0.12 | 0.21 | 0.18 | 0.18 | – |
| Periphyton | C:O | 2 | 2.67 | 3.6 | 3.135 | 2.69 | – |
| Periphyton | Half-saturation for nitrogen limited growth | 3 | 0.01 | 0.025 | 0.025 | 0.02 | mg/L |
| Periphyton | Half-saturation for phosphorus limited growth | 2 | 0.005 | 0.005 | 0.005 | 0.001 | mg/L |
| Periphyton | Half-saturation for periphyton density | 3 | 6.5 | 6.5 | 6.5 | – | gC/m ² |
| Periphyton | Periphyton Velocity Half Saturation | 2 | 0.25 | 0.25 | 0.25 | – | m/s |
| Periphyton | Periphyton Velocity Limitation Minimum | 2 | 0.15 | 0.15 | 0.15 | – | m/s |
| Periphyton | Carrying capacity | 2 | 10 | 30 | 20 | – | gC/m ² |

Table 10. WASP Rates and Constants: Sediment and Detritus Parameters

| Sediment/Detritus Parameter | Count | Min | Max | Mean | Median | Representative Values | Units |
|---|-------|--------|--------|-------|--------|-----------------------|----------------------|
| Active aerobic layer depth for phosphate flux model (top layer) | 1 | 0.1 | 0.1 | 0.1 | 0.1 | – | cm |
| Active anaerobic layer depth for phosphate flux model (bottom layer) | 1 | 9.9 | 9.9 | 9.9 | 9.9 | – | cm |
| Active sediment layer depth for diagenesis and SOD/ammonia flux model | 1 | 10 | 10 | 10 | 10 | – | cm |
| Ammonia oxidation normalization constant | 8 | 0.37 | 0.74 | 0.509 | 0.37 | – | mg O ₂ /L |
| Burial velocity for layer 2 to inactive sediments | 8 | 0.2 | 1 | 0.338 | 0.25 | 0.25 | cm/yr |
| Carbon-Nitrogen ratio | 8 | 5.68 | 5.68 | 5.68 | 5.68 | – | G C/g N |
| Carbon-Phosphorus ratio | 8 | 41 | 41 | 41 | 41 | – | G C/g P |
| Carbon-Silica ratio | 8 | 2 | 2 | 2 | 2 | – | G C/g Si |
| Coefficient for calculation of partition coefficient for phosphate in aerobic layer | 1 | 300 | 300 | 300 | 300 | – | – |
| Critical Oxygen concentration for phosphate sorption | 9 | 2 | 2 | 2 | 2 | 2 | mg O ₂ /L |
| Critical Oxygen concentration for silica sorption | 8 | 2 | 2 | 2 | 2 | 1 | mg/L |
| Decay constant for benthic stress | 8 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | day ⁻¹ |
| Diagenesis rate for POC, PON, POP G1 | 8 | 0.035 | 0.035 | 0.035 | 0.035 | 0.035 | day ⁻¹ |
| Diagenesis rate for POC, PON, POP G2 | 8 | 0.0018 | 0.0018 | 0.002 | 0.0018 | 0.0018 | day ⁻¹ |

| Sediment/Detritus Parameter | Count | Min | Max | Mean | Median | Representative Values | Units |
|---|-------|-------|-------|-------|--------|-----------------------|----------------------|
| Diagenesis rate for Si | 8 | 0.5 | 0.5 | 0.5 | 0.5 | – | day ⁻¹ |
| Diffusion coefficient for dissolved mixing | 8 | 5 | 25 | 13.44 | 8.75 | – | cm ² /d |
| Diffusion coefficient for particle mixing | 9 | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | cm ² /d |
| Dissolution rate of particulate biogenic silica at 20 °C | 8 | 0.5 | 0.75 | 0.531 | 0.5 | 0.5 | day ⁻¹ |
| Fraction of POM in G1 reactivity class | 1 | 0.65 | 0.65 | 0.65 | 0.65 | – | – |
| Fraction of POM in G2 reactivity class | 1 | 0.2 | 0.2 | 0.2 | 0.2 | – | – |
| Fraction of POM in G3 reactivity class | 1 | 0.15 | 0.15 | 0.15 | 0.15 | – | – |
| Fraction POC to G2 | 8 | 0.2 | 0.25 | 0.206 | 0.2 | – | – |
| Fraction POC to G3 | 8 | 0.1 | 0.15 | 0.144 | 0.15 | – | – |
| Fraction POC, PON, POP to G1 | 8 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | – |
| Fraction PON to G2 | 8 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | – |
| Fraction PON to G3 | 8 | 0.1 | 0.1 | 0.1 | 0.1 | – | – |
| Fraction POP to G2 | 8 | 0.2 | 0.25 | 0.206 | 0.2 | 0.2 | – |
| Fraction POP to G3 | 8 | 0.05 | 0.15 | 0.138 | 0.15 | – | – |
| Half-saturation coefficient for ammonia in the nitrification reaction | 8 | 728 | 728 | 728 | 728 | 0.728 | mgN/m ³ |
| Half-saturation constant of Dissolved Silica in dissolution reaction | 8 | 50 | 100 | 62.5 | 50 | – | gSi/L |
| Mineralization rate of POM in G1 reactivity class at 20°C | 1 | 0.035 | 0.035 | 0.035 | 0.035 | – | day ⁻¹ |
| Mineralization rate of POM in G2 reactivity class at 20°C | 1 | 0 | 0 | 0 | 0 | – | day ⁻¹ |
| Mineralization rate of POM in G3 reactivity class at 20°C | 1 | 0 | 0 | 0 | 0 | – | day ⁻¹ |
| Particle mixing half-saturation constant for oxygen | 8 | 4 | 4 | 4 | 4 | 4 | mg O ₂ /L |
| Partition coefficient between Dissolved/Sorbed phosphate in Layer 1 | 8 | 20 | 300 | 79.4 | 37.5 | – | L/kg |
| Partition coefficient between Dissolved/Sorbed phosphate in Layer 2 | 9 | 20 | 1000 | 171.1 | 100 | 20 | L/kg |
| Partition coefficient between Dissolved/Sorbed silica in Layer 1 | 8 | 5 | 10 | 9.063 | 10 | – | L/kg |
| Partition coefficient between Dissolved/Sorbed silica in Layer 2 | 8 | 15 | 100 | 83.1 | 100 | 100 | L/kg |
| Reaction velocity for dissolved ammonia oxidation | 9 | 0.09 | 0.16 | 0.130 | 0.131 | 0.1313 | m/d |
| Reaction velocity for dissolved nitrate oxidation in Layer 1 | 7 | 0.085 | 0.125 | 0.101 | 0.1 | 0.1 | m/d |
| Reaction velocity for dissolved nitrate oxidation in Layer 2 | 7 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | m/d |
| Reaction velocity for dissolved sulfide oxidation in Layer 1 | 8 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | m/d |

| Sediment/Detritus Parameter | Count | Min | Max | Mean | Median | Representative Values | Units |
|---|-------|-------|-------|-------|--------|-----------------------|----------------------|
| Reaction velocity for dissolved sulfide oxidation in Layer 2 | 8 | 0.4 | 0.4 | 0.4 | 0.4 | – | m/d |
| Reaction velocity for methane oxidation | 1 | 1.25 | 1.25 | 1.25 | 1.25 | 0.7 | m/day |
| Reference concentration of POC in reactivity class G1 for particle mixing calculation in phosphate flux model | 1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.2667 | mgC/g |
| Silica detritus flux | 8 | 0.1 | 100 | 73.8 | 100 | – | g/m ³ /d- |
| Silica saturation concentration in porewater | 8 | 40 | 40 | 40 | 40 | 40 | mgSi/L |
| Solids concentration in Layer 1 | 7 | 0.5 | 0.95 | 0.56 | 0.5 | – | kg/L |
| Solids concentration in Layer 2 | 6 | 0.5 | 1.09 | 0.60 | 0.5 | – | kg/L |
| Sulfide oxidation normalization constant | 8 | 4 | 4 | 4 | 4 | 4 | mg O ₂ /L |
| Sulfide partition coefficient | 8 | 1 | 1 | 1 | 1 | – | – |
| Sulfide partition coefficient in Layer 1 | 8 | 100 | 100 | 100 | 100 | 100 | L/kg |
| Sulfide partition coefficient in Layer 2 | 8 | 100 | 100 | 100 | 100 | 100 | L/kg |
| Temperature coefficient for ammonia oxidation | 16 | 1.123 | 1.125 | 1.124 | 1.124 | 1.123 | – |
| Temperature coefficient for Dd | 8 | 1.08 | 1.15 | 1.096 | 1.09 | 1.08 | – |
| Temperature coefficient for diagenesis of POC, PON, POP G1 | 8 | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 | – |
| Temperature coefficient for diagenesis of POC, PON, POP G2 | 8 | 1.15 | 1.15 | 1.15 | 1.15 | 1.15 | – |
| Temperature coefficient for diagenesis of Si | 8 | 1.1 | 1.1 | 1.1 | 1.1 | – | – |
| Temperature coefficient for Dp | 8 | 1.08 | 1.15 | 1.107 | 1.117 | 1.117 | – |
| Temperature coefficient for methane and ammonia oxidation | 1 | 1.079 | 1.079 | 1.079 | 1.079 | 1.079 | – |
| Temperature coefficient for nitrate oxidation | 8 | 1.08 | 1.1 | 1.083 | 1.08 | 1.08 | – |
| Temperature coefficient for POM in G1 reactivity class | 1 | 1.1 | 1.1 | 1.1 | 1.1 | – | – |
| Temperature coefficient for POM in G2 reactivity class | 1 | 1.15 | 1.15 | 1.15 | 1.15 | – | – |
| Temperature coefficient for POM in G3 reactivity class | 1 | 0 | 0 | 0 | 0 | – | – |
| Temperature coefficient for sulfide oxidation | 8 | 1.08 | 1.08 | 1.08 | 1.08 | 1.079 | – |
| Temperature correction coefficient for diffusion coefficient for dissolved phase mixing | 1 | 1.08 | 1.08 | 1.08 | 1.08 | – | – |
| Temperature correction coefficient for diffusion coefficient for particle mixing | 1 | 1.117 | 1.117 | 1.117 | 1.117 | – | – |
| Temperature Effect on Silica dissolution | 8 | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 | – |
| Thickness of active sediment layer | 8 | 10 | 10 | 10 | 10 | 0.1 | cm |

Calibration Data and Approaches

As is the case for the other models contained within this report, a primary concern with calibration of WASP is collecting enough high-quality data, to both describe the pollutant inputs to the system as well as make qualitative model versus data comparisons and/or perform quantitative skill assessment.

Generally, input data consists of:

- Pollutant loadings to the system, including point and non-point sources and if the surface area of the waterbody under investigation is large enough, atmospheric sources as well;
- Boundary conditions, either at the upstream end of streams, rivers or inflows to lakes and reservoirs, or at the downstream ends of estuaries, tidal embayments, or coastal waterbodies; and
- Exogenous inputs such as solar radiation, winds, and light attenuation.

Although not traditionally thought of as an “input” to a water quality model, transport information provided by a companion or coupled hydrodynamic model is an important input to a water quality model. If the hydrodynamic model fails to reproduce the major features of transport within a waterbody, in particular, vertical stratification due to thermal heating in lakes and reservoirs, density driven circulation in estuarine, tidal embayments, and coastal systems, destratification due to wind-mixing, and fall decreases in air temperatures, then the accompanying water quality model will likely not calibrate well to the water quality variables of interest such as dissolved oxygen and phytoplankton biomass.

As was mentioned earlier, it is generally desirable to have multiple or multi-year datasets for model calibration. In the case of BOD/DO models, year-long data sets are generally not necessary because the models are generally being applied to worst-case conditions, such as the “7Q10” or the lowest 7-day average flow that occurs on average once every 10 years. However, it is good modeling practice to calibrate and confirm model performance with a few DO surveys. In the case of more complicated eutrophication models, especially as applied to lakes, reservoirs, and estuarine applications, model calibration/confirmation to a few year-long or seasonal surveys or multi-year data sets is preferable, to avoid over-calibrating a model using a dataset that is not representative of more typical or average environmental conditions.

Most, but not all, of the WASP studies met these conditions. However, not meeting these conditions was not sufficient to rule out a study if the calibration and the RCK values used in the model calibration appeared reasonable based on expert judgment. Most of the phytoplankton or eutrophication modeling studies used multi-year studies. Available datasets within these studies generally included monthly sampling and in some cases bi-weekly sampling that occurred during the critical spring and summer periods. Generally, these datasets also included multiple monitoring or sampling stations within the waterbody, and qualitative and quantitative skill assessment results were presented for a subset of these stations.

The addition of SFM capabilities to WASP and other water quality modeling programs, such as Q2K, Q2Kw, and CE-QUAL-W2, has both removed a degree of freedom in model calibration and improved model capability in projecting changes in future water quality in response to a management scenario. Prior to the SFM, sediment oxygen demand (SOD) and nutrient fluxes were effectively another boundary condition to the water column that had to be parameterized by the user. While sometimes supported by

field measurements of SOD and nutrient fluxes, the sediments were generally treated as an adjustable parameter in model calibration. The problem, however, was to predict the change in SOD and nutrient flux that would result from implementing a management action to reduce organic matter or nutrient inputs to the waterbody. Use of the SFM has largely removed this degree of freedom in model calibration, since now there is a direct coupling and mass balance between the water column and the sediment bed. SFM tracks the deposition of phytoplankton and detrital organic matter to the sediment, its decomposition or diagenesis within the bed, and the flux of resultant end-products (SOD and nutrients) back to the overlying water column, all within a mass balance framework. This capability is likely most useful to systems having an abundance of fine sediments and may be less applicable to cobble or gravel dominated river systems.

Of interest is the fact that, with a very few exceptions, the RCK values arrived at through the original development and calibration of the SFM to Chesapeake Bay (DiToro and Fitzpatrick, 1993) and as documented in DiToro (2001) have not changed in the various applications to different waterbodies. Generally, the only SFM coefficients that have varied from site to site are the phosphorus partition coefficients and the particle mixing coefficients. These values may change from model application to model application or from site to site based on the quantities of iron that are contained in local sediments that effect phosphorus partitioning to iron oxides, and the types and numbers of biota and sediments that are present in the waterbody, which can affect particle mixing in the sediment bed. In the case of the latter, sites that are dominated by the presence of combined sewer overflows (CSO) and a limited pollution-tolerant benthic community would be expected to have less bioturbation or particle mixing as compared to an oligotrophic or mesotrophic waterbody with a more diverse benthic community, which could include a greater population of burrowing organisms. Given the consistent use of the original defaults in numerous applications, potential users of the SFM should carefully consider deviations from the reported SFM values presented in the RCK tables.

Overall, many WASP parameters in recent literature were determined through manual calibration using default or literature starting values (from the scientific literature, site specific studies, from the EPA 1985 Rates Manual, etc.). Values for individual parameters were sometimes altered slightly, but remained within ranges suggested in the literature and the EPA 1985 Rates Manual, and in the WASP model manual as applicable in an effort to improve model skill (i.e., reduce relative or mean differences and RMSE of the modeled values against observed data). For most parameters, the default values remained unchanged during calibration. For the studies where parameters were manually calibrated, the researchers or model practitioners followed a generally consistent procedure to achieve good agreement between modeled and observed data, first calibrating hydrodynamics then water quality. Generally, within each RCK category, model coefficients or parameters were manipulated in a logical way and were not changed at random to increase model fit. There were a few cases, however, where reaeration rates or SOD appear to have been adjusted slightly by model segment/distance or season, the reason(s) for which were not explained in the paper. There were also a few cases where a specific model coefficient fell outside of the range of generally acceptable bounds, but may not have affected the calibration directly. These occurrences are documented in the RCK tables.

4.2 CE-QUAL-W2

The CE-QUAL-W2 (W2) model is a 2D laterally averaged model that has been applied in a variety of systems where longitudinal and vertical gradients are likely to exist. Because of consistent model updates and use, there is a large body of literature that presents hydrodynamics and water quality studies using W2. [See section 2.2 for more details.]

Summary of Sources

Literature searches returned thousands of documents that reference W2, although many were not applications of the model. As discussed above, the methodology for identifying relevant literature was composed of multiple culling steps that eventually resulted in a relatively small subset of papers and reports that met all relevance criteria. From an initial pool of thousands of search results, more than 100 were pulled from searches for initial assessment, resulting in 57 papers being selected for detailed review (Table 11). The screening process used for this task disqualified papers without electronic access, making it likely that some papers with relevant, documented RCK values were removed from consideration due to lack of availability. Throughout the literature evaluation process, preference was given to documents with thorough model documentation, as described in Section 3.

Of the 57 papers and reports that were reviewed, 31 passed relevance and criteria checks. These consisted of: 12 U.S. Geological Survey (USGS) reports; seven peer-reviewed journal articles; five Portland State University (PSU) reports (prepared for the States of Washington and Idaho); four USACE modeling reports; one report each by the USDA, the State of Washington, and Tetra Tech (prepared for the State of Ohio). Many of the W2 reported model applications were led by a relatively small group of model practitioners associated with USGS, USACE, and PSU. The remaining body of literature was not useful for the purposes of this study (i.e., no parameter values were provided), but does show the breadth of W2 application. For example, PSU reports more than 100 current projects utilizing W2 as a hydrodynamic and/or water quality model and a history of more than 2,300 documented applications worldwide. Many of these studies do not have publicly accessible calibration reports or results at this time.

For additional resources regarding CE-QUAL-W2, see also Section 9 of this report.

Table 11. CE-QUAL-W2 Literature Sources

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|---|--------------------------------------|-------------------|--|---|--|
| Afshar, A., and M. Saadatpour, 2009. Reservoir Eutrophication Modeling, Sensitivity Analysis, and Assessment: Application to Karkheh Reservoir, Iran. Environmental Engineering Science. 26(7). | Karkheh Reservoir, Iran (southwest) | Reservoir | 50,000 km ² drainage; avg depth = 61.8 m; active storage = 3500 Mm ³ ; primarily arid landcover with minimal agriculture | May-December 2005 (monthly data) | |
| Annear R., S. Wells, and C. Berger, 2005. Upper Spokane River Model in Idaho: Boundary Conditions and Model Setup and Calibration for 2001 and 2004. Portland State University Technical Report EWR-02-05. Prepared for the Washington Department of Ecology. | Upper Spoke River, Idaho | River | 15,540 km ² drainage; avg Q =100 m ³ /s; primarily forested with urban influence in City of Coeur d' Alene; 3 WWTP discharges | January-December 2001 | Updated model from Wells, 2003 with additional data. |
| Annear, R., C. Berger, and S. Wells, 2006. Pend Oreille River Model: Model Development and Calibration. Portland State University Technical Report EWR-02-06. Prepared for the Idaho Department of Environmental Quality. | Pend Oreille River, Oregon | River | avg Q =600 m ³ /s; primarily forested with some agriculture and urban cover; 3 WWTP discharges | Summer 2004, 2005 (continuous T; variable WQ sampling intervals) | |
| Bales, J., K. Sarver, and M. Giorgino, 2001. Mountain Island lake, North Carolina: Analysis of Ambient Conditions and Simulation of Hydrodynamics, Constituent Transport, and Water-Quality Characteristics, 1996-1997. USGS Water Resources Investigations Report 01-4138. | Mountain Island Lake, North Carolina | Reservoir | 4,820 km ² drainage; avg depth = 4.9 m; primarily forested watershed with minor residential and agricultural use; water level controlled by very large upstream reservoir | April 1996-September 1997 (continuous T, DO, SC; periodic WQ vertical profiles; bi-monthly WQ grab samples) | |
| Berger, C., R. Annear, and S. Wells, 2001. Lower Willamette River Model: Model Calibration. Portland State University Department of Civil Engineering Technical Report EWR-2-01. | Lower Willamette River, Oregon | River | 29,785km ² drainage; mixed forest, agriculture, and developed land (includes Portland); known WWTP point discharges; tidally influenced at lower reaches | May-October 1993, '94, '97, '98, '99 | |
| Berger, C., R. Annear, and S. Wells, 2003. Upper Spokane River Model: Model Calibration, 2001. Portland State University Department of Civil Engineering Technical Report EWR-1-03. Prepared for the City of Spokane. | Upper Spokane River, Washington | River | avg Q =150 m ³ /s; mixed forested, agriculture, clearcut; 4 point source discharges in City of Spokane; other details in Annear et al, 2001 background data report | March-September 2001 (continuous Q; periodic WQ) | Update to Berger et al. 2002 model (above). |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|--|---|-------------------|---|---|---|
| Berger, C., R. Annear, S. Wells, and T. Cole, 2002. Upper Spokane River Model: Model Calibration, 1991 and 2000. Portland State University Department of Civil Engineering Technical Report EWR-01-02. Prepared for the Washington Department of Ecology. | Upper Spokane River, Washington | River | avg Q =150 m ³ /s; mixed forested, agriculture, clearcut; 4 point source discharges in City of Spokane; other details in Annear et al, 2001 background data report | February-September 1991 and January-September 2000 (continuous Q and water level; periodic WQ) | |
| Cole, T., and D. Tillman, 2001. Water Quality Model of Allatoona and West Point Reservoirs using CE-QUAL-W2. ERDC/EL SR-01-3, U.S. Army Engineer Research and Development Center. | Allatoona Lake and West Point Lake, Georgia | Reservoirs | Allatoona Lake: 2,845 km ² drainage; some municipal and agricultural input West Point Lake: 8,754 km ² drainage; abundant municipal (Atlanta) and agricultural influence | Allatoona Lake: 1992, 1993, 1996, 1997 (hourly inflows, daily outflows; very limited WQ data) West Point Lake: 1979, 1996, 1997 (hourly inflows, daily outflows; very limited WQ data) | Some boundary parameters calculated from other available data (inflow T calculated from meteorological data; WQ data set to upstream sample). |
| Cole, T.M., and D.H. Tillman, 1997. "Water Quality Modeling of Lake Monroe Using CE-QUAL-W2," Miscellaneous Paper EL-99-1, U.S. Army Engineer Waterways Experiment Station, Vicksburg, Mississippi. | Lake Monroe, Indiana | Reservoir | 1,142 km ² drainage; avg depth=5.5-7m; residence time=180-410 days; active storage=300-430 Mm ³ ; primarily forested, minor agriculture | First calibrated to 1994 (most WQ data, low water year); 1992, 1995, 1996 added after (more normal water years); WQ data available only for 1994 | Relatively limited WQ data. Some calculations used to estimate specific WQ concentrations. |
| Debele, B., R. Srinivasan, and J. Parlange, 2006. Coupling upland watershed and downstream waterbody hydrodynamic and water quality models (SWAT and CE-QUAL-W2) for better water resources management in complex river basins. <i>Environmental Model Assessment</i> . 13. 135-153. | Cedar Creek Reservoir (and upland watershed), Texas | Reservoir | 5,244 km ² drainage; active storage = 698 Mm ³ ; avg depth=6.5 m; primarily agricultural (64%) with mixed forest (12%) and residential (11%); 2 WWTP inflows | SWAT output used as CE-QUAL-W2 input; W2 simulation for 1997 to 2001 with hourly boundary data (from SWAT) | Coupled watershed (SWAT) and waterbody (CE-QUAL-W2) model. |
| Flowers, J., L. Hauck, and R. Kiesling, 2001 Water Quality Modeling of Lake Waco Using CE-QUAL-W2 for Assessment of Phosphorus Control Strategies. Prepared for the USDA: Lake Waco-Bosque River Initiative. TR0114. | Lake Waco and Bosque River, Texas | Reservoir | 4,300 km ² drainage; avg depth - 6m; active storage = 179 Mm ³ ; primarily forested with 29% agriculture and known non-point source contamination issues | June 1996 - July 1998 (monthly data) | Coupled SWAT/CE-QUAL-W2; independent calibration. |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|---|-------------------------------|-------------------|--|---|---|
| Galloway, J., and W. Green, 2002. Simulation of Hydrodynamics, Temperature, and Dissolved Oxygen in Norfolk Lake, Arkansas, 1994-1995. USGS Water Resources Investigations Report 02-4250. | Norfolk Lake, Arkansas | Reservoir | 4,683 km ² drainage; active storage = 1,540 Mm ³ ; avg depth=17 m; retention time=0.9 years; mixed forested and agricultural | January 1994 - December 1995 (daily T; periodic vertical profiles and boundary values for chemical data) | |
| Galloway, J., and W. Green, 2006. Analysis of Ambient Conditions and Simulation of Hydrodynamics and Water Quality Characteristics in Beaver Lake, Arkansas, 2001 through 2003. USGS Scientific Investigations Report 2006-5003. | Beaver Lake, Arkansas | Reservoir | 3087 km ² drainage; avg depth = 18m; active storage = 2040 Mm ³ ; mixed forest and agriculture; 3 cities with point source discharges in watershed | April 2001-April 2003 (continuous Q; monthly WQ only during well-mixed conditions) | |
| Galloway, J., and W. Green, 2003. Simulation of Hydrodynamics, Temperature, and Dissolved Oxygen in Bull Shoals Lake, Arkansas, 1994-1995. USGS Water Resources Investigation Report 03-4077. | Bull Shoals Lake, Arkansas | Reservoir | 15,675 km ² drainage; avg min. outflow = 4.6 m ³ /s; active storage = 4194 Mm ³ ; avg depth = 23 m; reservoir retention time = 0.75 years (avg); mixed forested and agricultural, minor municipal input | January 1994 - December 1995 (daily T; periodic vertical profiles and boundary values for chemical data) | DO concentrations at inflow set to concentration for 100% saturation at a given T. |
| Galloway, J., R. Ortiz, J. Bales, and D. Mau, 2008. Simulation of Hydrodynamics and Water Quality in Pueblo Reservoir, Southeastern Colorado, for 1985 through 1987 and 1999 through 2002. USGS Scientific Investigations Report 2008-5056. | Pueblo Reservoir, Colorado | Reservoir | active storage = 441 Mm ³ ; avg inflow discharge = 22 m ³ /s; primarily plains landcover with some agriculture and minor developed land | October 1985 to September 1987 = water years 1986 and 1987; daily inflow/outflow T and hydrodynamic data; period WQ data, regression model used to interpolate loads) | Some recomputation done to convert daily inflow/outflow data to hourly for use in model. Some WQ data interpolated from discrete samples. |
| Giorgino, M., and J. Bales, 1997. Rhodhiss Lake, North Carolina: Analysis of Ambient Conditions and Simulation of Hydrodynamics, Constituent Transport, and Water-Quality Characteristics, 1993-1994. USGS Water Resources Investigations Report 97-4131. | Rhodhiss Lake, North Carolina | Reservoir | avg depth = 8 m; mixed-use watershed (managed forest, agriculture, urban/industrial, textile mills, machinery and dye plants, furniture manufacturing) | April 1993-March 1994 (continuous Q and water level; monthly WQ) | |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|--|---|-------------------|---|--|--|
| Green, W., J. Galloway, J. Richards, and E. Wesolowski, 2003. Simulation of Hydrodynamics, Temperature, and Dissolved Oxygen in Table Rock Lake, Missouri, 1996-1997. USGS Water Resources Investigations Report 03-4237. | Table Rock Lake, Missouri | Reservoir | 10,412 km ² drainage; avg min. outflow = 4.4 m ³ /s; active storage = 3330 Mm ³ ; avg depth = 19 m; reservoir retention time = 0.8 years (avg); mixed agriculture and forest, some municipal input | January 1996 - December 1997 (hourly or daily T; hourly or daily inflow WQ; periodic vertical profiles) | DO concentrations at non-measured inflows set to concentration for 80% saturation at a given T. |
| Gunduz, O., S. Soyupak, and C. Yurteri, 1998. Development of Water Quality Management Strategies for the Proposed Isikli Reservoir. <i>Water Science Technology</i> . 37(2): 369-376. | Proposed Isikli Reservoir, Turkey | Reservoir | active storage = 25 Mm ³ ; max depth=24 m; mixed agricultural, developed, and arid landcover | Initial conditions from March 1995 upstream river WQ data; simulation period March to October 1995 | Modeling of a proposed reservoir, so no model validation. All coefficients are default or literature values. |
| Ha, S., and J. Lee, 2008. Application of CE-QUAL-W2 Model to Eutrophication Simulation in Daecheong Reservoir Stratified by Turbidity Storms. Proceedings of TAAL2007: The 12 th World Lake Conference. 824-833. | Daecheong Reservoir, South Korea | Reservoir | 4,166 km ² drainage; avg depth - 20 m; active storage = 790 Mm ³ ; primarily forested with 20% agriculture | 2003 (wet year) and 2005 (dry year) | |
| Hart, R., W. Green, D. Westerman, J. Peterson, and J. De Lanoi, 2013. Simulated Effects of Hydrologic, Water Quality, and Land-Use Changes of the Lake Maumelle Watershed, Arkansas, 2004-2010. USGS Scientific Investigations Report 2012-5246. | Lake Maumelle, Arkansas | Reservoir | 355 km ² drainage; avg depth =7.6 m; active storage = 270 Mm ³ ; primarily forested with minor clearcut and agriculture; no point source discharges | 2004-2010 | Coupled HSPF/CE-QUAL-W2. Outputs from HSPF used as input to CE-QUAL following independent calibration. |
| Kuo, J., W. Lung, C. Yang, W. Liu, M. Yang, and T. Tang, 2006. Eutrophication modeling of reservoirs in Taiwan. <i>Environmental Modelling & Software</i> . 21(6): 829-844. | Te-Chi and Tseng-Wen Reservoirs, Taiwan | Reservoir | Te-Chi: 592 km ² drainage; active storage = 183 Mm ³ Tseng-Wen: 481 km ² drainage; active storage = 659 Mm ³ ; numerous nonpoint nutrient sources in both reservoirs (agricultural) | 1998-1999 (monthly WQ and vertical T profiles; continuous outflow T and hydrodynamics) | |
| Liu, W, W. Chen, and N. Kimura, 2009. Impact of phosphorus load reduction on water quality in a stratified reservoir-eutrophication modeling study. <i>Environmental Monitoring Assessment</i> . 159:393-406. | Mingder Reservoir, Taiwan | Reservoir | 61 km ² drainage; active storage = 165 Mm ³ ; mixed forest, agricultural, residential; significant nonpoint nutrient sources; regular algae blooms in reservoir | 2003-2004 (seasonal WQ samples including vertical profiles; continuous inflow/outflow T and hydrodynamic data) | |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|--|---|-------------------|--|---|--|
| Lung, W. and S. Bai, 2003. A Water Quality Model for the Patuxent Estuary: Current Conditions and Predictions under Changing Land-use Scenarios. <i>Estuaries</i> . 26(2A):267-279. | Patuxent River estuary, Maryland | Estuary | 2,401 km ² drainage; mixed forest, urban, and agricultural; heavily influenced by point and nonpoint nutrient sources; downstream of DC and Baltimore | August 1997 - July 1998 (details on data collection in Weller et al. 2003) | |
| Pickett, P. and S. Hood, 2008. Lake Whatcom Watershed Total Phosphorus and Bacteria Total Maximum Daily Loads. Volume 1. Water Quality Study Findings. Department of Ecology State of Washington. Publication No. 08-03-024, App B-F. | Lake Whatcom, Washington | Lake | Volume: 921 Mm ³ cubic meters Mean depth: 46 m Surface area: 20.3 km ² Land uses are predominantly urban, rural residential, and forestry. Pollution sources: manure, fertilizers, septic systems, soil particles, and dust particles. | Jan 2002 - Dec 2003 | Coupled HSPF/CE-QUAL-W2. Outputs from HSPF used as input to CE-QUAL following independent calibration. Calibration years: 2002 - dry year 2003 - average year |
| Rounds, S., and T. Wood, 2001. Modeling Water Quality in the Tualatin River, Oregon, 1991-1997. USGS Water-Resources Investigations Report 01-4041; original model: Rounds, S.A., Wood, T.M., and Lynch, D.D., 1999, Modeling discharge, temperature, and water quality in the Tualatin River, Oregon: U.S. Geological Survey Water-Supply Paper 2465-B. | Tualatin River, Oregon | River | Details on watershed in Rounds, et al., 1999 | Original model calibrated to May-October 1991-1993 Updated with May-October 1994-1997 | Expansion on a previous model to include additional data. |
| Smith, D., T. Threadgill, and C. Larson, 2012. Modeling the Hydrodynamics and water Quality of the Lower Minnesota River using CE-QUAL-W2. USACE Technical Report ERDC/EL TR-12-12. | Minnesota River (lower 40 miles), Minnesota | River | 43,771 km ² drainage; avg discharge = 4,414 cfs; primarily agricultural (70%) with increasing development at river outlet (Twin Cities); 4 large point source discharges; lower 15 miles used as shipping channel | First calibrated to water year 2006; recalibrated to 1988 data (low flow year); validated to 1988 and 2001-2006 | |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|---|---|-------------------|---|--|--|
| Smith, E., R. Kiesling, J. Galloway, and J. Ziegeweid,. 2014. Water Quality and Algal Community Dynamics of Three Sentinel Deepwater Lake in Minnesota Utilizing CE-QUAL-W2 Models. USGS Scientific Investigations Report 2014-5066. | Carlos (a), Elk (b), Trout (c) lakes, Minnesota | Lake | Carlos: 634 km ² drainage; primarily forested Elk: 8 km ² drainage; mixed forest/prairie Trout: 3.6 km ² drainage; dimictic; primarily forested | Carlos: April-November 2011; Elk: April-November 2011; Trout: April-October, 2010 | 3 separate models in 3 sentinel deepwater lakes; Non-traditional morphology for CE-QUAL-W2. |
| Sullivan, A., and S. Rounds, 2004. Modeling Hydrodynamics, Temperature, and Water Quality in Henry Hagg Lake, Oregon, 2000-2003. USGS Scientific Investigations Report 2004-5261. | Henry Hagg Lake, Oregon | Lake | 105 km ² drainage; active storage = 76 Mm ³ ; primarily forested with few (if any) contaminant sources; high extraction demand | 2000-2001 (continuous water T and meteorology; monthly WQ) | |
| Sullivan, A., and S. Rounds, 2011. Modeling Hydrodynamics, Water Temperature, and Water Quality in the Klamath River Upstream of Keno Dam, Oregon, 2006-2009. USGS Scientific Investigations Report 2011-5105. | Klamath River, Oregon | River | Channel width =100-300 m; depth = <1-6 m; 3 large WWTP inputs; flow-controlled river with irrigation diversions | April-November 2006-2009 (continuous monitoring; intermittent grab samples) | |
| Tetra Tech, 2008. TMDLs for the Black River Watershed, Ohio. Prepared for the State of Ohio Environmental Protection Agency. | Lower Black River, Ohio | River | 1,217 km ² drainage; avg Q=333 cfs; mixed agricultural and highly urbanized land uses; numerous point source discharges and abundant nonpoint influence; highly impaired river | Jan 2002 - Dec 2003 | Coupled HSPF/CE-QUAL-W2. Outputs from HSPF used as input to CE-QUAL following independent calibration. |
| Tillman, D., T. Cole, and B. Bunch, 1999. Detailed Reservoir Water Quality Modeling (CE-QUAL-W2), Alabama-Coosa-Tallapoosa/Apalachicola-Chattahoochee-Flint (ACT/ACF) Comprehensive Water Resource Study. USACE ERDC Technical Report EL-99-15. | Weiss, Neely Henry, and Walter George Reservoirs, Alabama | Reservoirs | Report includes engineering characteristics of each reservoir (water elevation, embankment and spillway size, powerhouse capacity, etc.) | January 1991 - November 1994 (discontinuous historical records across reservoirs; monthly samples where available; primarily summer/fall sampling dates) | Model calibrated to 3 separate reservoirs. Post-calibration parameters identical for all. |

As a 2-D laterally averaged model capable of simulating vertical and longitudinal hydrodynamics and water quality, W2 can be applied for a variety of purposes. The studies examined during this project reflected the range of possible applications of W2, with the main trend across all studies being the desire to model in two dimensions for both hydrodynamics (such as velocities, water level, outflow discharge, thermal stratification, etc.) and water quality (such as nutrient loads, DO, and pH). W2 can be used to simulate reservoir conditions under changing watershed conditions. In some cases, this can be accomplished by coupling a separate watershed model (e.g., SWAT, HSPF) with W2 and using the output from watershed models as the upstream boundary condition for W2. Two of the sources of RCK values included in the data table used this coupled model method.

W2 has been applied nationwide and globally. Nationally, the studies are clustered in certain regions, with many W2 applications in the Pacific Northwest (Washington, Oregon, Idaho) and South/Southeast (Arkansas, Missouri, Alabama, Georgia). There were additional studies performed elsewhere in the United States including North Carolina, Minnesota, Indiana, Texas, and Colorado. The peer-reviewed journal articles provide the remaining geographic range, both nationally and globally, with model applications in: Texas, Maryland, Taiwan, Turkey, Korea, and Iran. It is clear from the geographic distribution of the W2 applications, both by government agencies and academic researchers, that the model can be applied in many geographic regions. The only area not represented in the selected papers was the Northeast.

As discussed above, W2 was developed and optimized for use in relatively long and narrow waterbodies, and has been applied in reservoirs, lakes, estuaries, and linked waterbody systems (multiple reservoirs). Most of the applications have been to reservoirs, in part due to the needs of the agency that originally developed W2 (USACE) and since the original model was not applicable to rivers (or systems with significant bottom slope). The W2 model was updated in 2007 (Version 3 and higher) to allow simulation of free-flowing rivers. As a result, W2 can model linked rivers and reservoirs, which is reflected in the literature, with many studies simulating the upstream and/or downstream water body in addition to the reservoir. W2 has also been used in systems with non-ideal geomorphologies (e.g., small, deep lakes with very small surface area to volume ratios) to assess its capabilities to model vertical gradients in those systems.

Basin sizes ranged from <10 to tens of thousands of km² with a wide range of lake/reservoir volumes and surface areas. Land use within these basins ranged from heavily forested to agricultural and urban, with many rivers and reservoirs impacted by nonpoint and point source pollution. Nearly all the modeled waterbodies were influenced by some degree of runoff or WWTP pollution. Details on the watershed characteristics for each included study are contained within Table 11. The resulting distributions of rate values are summarized in Table 12. Note that the current release of CE-QUAL-W2 also includes separate rates for macroalgae, but none of the selected examples includes that module. Default rates are shown as provided in Cole and Wells (2018).

Summary Statistics for Rates and Constants

Table 12. CE-QUAL-W2 Rates and Constants

| Group | Parameter | Description | Default | Count | Min | Max | Median | Units |
|------------|-----------|--|---------|-------|--------|---------|--------|-------------------|
| ALGAL RATE | AG | Maximum algal growth rate | 2 | 28 | 0.34 | 6.5 | 1.9 | day ⁻¹ |
| ALGAL RATE | AR | Maximum algal respiration rate | 0.04 | 28 | 0.005 | 0.4 | 0.04 | day ⁻¹ |
| ALGAL RATE | AE | Maximum algal excretion rate | 0.04 | 28 | 0.005 | 0.15 | 0.04 | day ⁻¹ |
| ALGAL RATE | AM | Maximum algal mortality rate | 0.1 | 28 | 0 | 0.41 | 0.08 | day ⁻¹ |
| ALGAL RATE | AS | Algal settling rate | 0.1 | 28 | 0 | 0.8 | 0.1 | day ⁻¹ |
| ALGAL RATE | AHSP | Algal half-saturation for phosphorus limited growth | 0.003 | 28 | 0.0005 | 0.042 | 0.003 | g m ⁻³ |
| ALGAL RATE | AHSN | Algal half-saturation for nitrogen limited growth | 0.014 | 28 | 0 | 0.2 | 0.014 | g m ⁻³ |
| ALGAL RATE | AHSSI | Algal half-saturation for silica limited growth | 0 | 7 | 0 | 0.003 | 0 | g m ⁻³ |
| ALGAL RATE | ASAT | Light saturation intensity at maximum photosynthetic rate | 100 | 25 | 40 | 500 | 90 | W m ⁻² |
| ALGAL TEMP | AT1 | Lower temperature for algal growth | 5 | 23 | 0 | 16 | 5 | °C |
| ALGAL TEMP | AT2 | Lower temperature for maximum algal growth | 25 | 23 | 5 | 30 | 16.5 | °C |
| ALGAL TEMP | AT3 | Upper temperature for maximum algal growth | 35 | 24 | 10 | 35.1 | 25 | °C |
| ALGAL TEMP | AT4 | Upper temperature for algal growth | 40 | 24 | 20 | 40 | 35 | °C |
| ALGAL TEMP | AK1 | Fraction of algal growth rate at AT1 | 0.1 | 23 | 0.1 | 0.2 | 0.1 | |
| ALGAL TEMP | AK2 | Fraction of maximum algal growth rate at AT2 | 0.99 | 23 | 0.6 | 0.99 | 0.99 | |
| ALGAL TEMP | AK3 | Fraction of maximum algal growth rate at AT3 | 0.99 | 23 | 0.95 | 0.99 | 0.99 | |
| ALGAL TEMP | AK4 | Fraction of algal growth rate at AT4 | 0.1 | 22 | 0.01 | 0.3 | 0.1 | |
| ALG STOICH | AP | Stoichiometric equivalent between algal biomass and phosphorus, fraction | 0.005 | 15 | 0.0015 | 0.02268 | 0.005 | |
| ALG STOICH | AN | Stoichiometric equivalent between algal biomass and nitrogen, fraction | 0.08 | 15 | 0.059 | 0.0825 | 0.08 | |
| ALG STOICH | AC | Stoichiometric equivalent between algal biomass and carbon, fraction | 0.45 | 15 | 0.45 | 0.55 | 0.45 | |

| Group | Parameter | Description | Default | Count | Min | Max | Median | Units |
|------------|-----------|--|---------|-------|-------|-------|--------|-------------------------------|
| ALG STOICH | ASI | Stoichiometric equivalent between algal biomass and silica, fraction | 0.18 | 3 | 0.18 | 0.18 | 0.18 | |
| ALG STOICH | ACHLA | Ratio between algal biomass and chlorophyll a in terms of mg algae/ μg chl-a | 0.05 | 11 | 0.031 | 0.4 | 0.094 | mg algae/ μg chl-a |
| ALG STOICH | APOM | Fraction of algal biomass that is converted to particulate organic matter when algae die | 0.8 | 18 | 0.5 | 0.8 | 0.8 | |
| ALG STOICH | ANPR | Algal half saturation constant for ammonium preference | 0.001 | 3 | 0.001 | 0.003 | 0.001 | |
| EPI RATE | EG | maximum epiphyton/periphyton growth rate | 2 | 5 | 1.2 | 2 | 1.5 | day ⁻¹ |
| EPI RATE | ER | maximum epiphyton/periphyton respiration rate | 0.04 | 5 | 0.04 | 0.15 | 0.04 | day ⁻¹ |
| EPI RATE | EE | maximum epiphyton/periphyton excretion rate | 0.04 | 5 | 0.04 | 0.04 | 0.04 | day ⁻¹ |
| EPI RATE | EM | maximum epiphyton/periphyton mortality rate | 0.1 | 5 | 0.1 | 0.1 | 0.1 | day ⁻¹ |
| EPI RATE | EB | epiphyton/periphyton burial rate | 0.001 | 4 | 0.001 | 0.1 | 0.001 | |
| EPI RATE | EHSP | epiphyton half-saturation for phosphorus limited growth | 0.003 | 0 | N/A | N/A | N/A | g m ⁻³ |
| EPI RATE | EHSN | epiphyton half-saturation for nitrogen limited growth | 0.014 | 0 | N/A | N/A | N/A | g m ⁻³ |
| EPI RATE | EHSSI | epiphyton half-saturation for silica limited growth | - | 0 | N/A | N/A | N/A | g m ⁻³ |
| EPI HALF | ESAT | light saturation intensity at maximum photosynthetic rate | 75 | 5 | 75 | 150 | 150 | W m ⁻² |
| EPI HALF | EHS | biomass limitation factor | 35 | 1 | 20 | 20 | 20 | g m ⁻² |
| TEMP | ET1 | Lower temperature for periphyton growth | 5 | 5 | 1 | 5 | 1 | °C |
| TEMP | ET2 | Lower temperature for maximum periphyton growth | 25 | 5 | 3 | 25 | 3 | °C |
| TEMP | ET3 | Upper temperature for maximum periphyton growth | 35 | 5 | 16 | 35 | 20 | °C |
| TEMP | ET4 | Upper temperature for periphyton growth | 40 | 5 | 30 | 40 | 30 | °C |
| TEMP | EK1 | Fraction of periphyton growth rate at ET1 | 0.1 | 5 | 0.1 | 0.3 | 0.1 | |
| TEMP | EK2 | Fraction of maximum periphyton growth rate at ET2 | 0.99 | 5 | 0.6 | 0.99 | 0.99 | |
| TEMP | EK3 | Fraction of maximum periphyton growth rate at ET3 | 0.99 | 5 | 0.99 | 0.99 | 0.99 | |
| TEMP | EK4 | Fraction of periphyton growth rate at ET4 | 0.1 | 5 | 0.1 | 0.1 | 0.1 | |
| EPI STOICH | EP | Stoichiometric equivalent between epiphyton/periphyton biomass and phosphorus | 0.005 | 4 | 0.003 | 0.005 | 0.0045 | |

| Group | Parameter | Description | Default | Count | Min | Max | Median | Units |
|------------|-----------|--|---------|-------|--------|---------|---------|-------------------|
| EPI STOICH | EN | Stoichiometric equivalent between epiphyton/periphyton biomass and nitrogen | 0.08 | 4 | 0.06 | 0.08 | 0.08 | |
| EPI STOICH | EC | Stoichiometric equivalent between epiphyton/periphyton biomass and carbon | 0.45 | 4 | 0.45 | 0.45 | 0.45 | |
| EPI STOICH | ESI | Stoichiometric equivalent between epiphyton/periphyton biomass and silica | 0.18 | 1 | 145 | 145 | 145 | |
| EPI STOICH | EPOM | Fraction of epiphyton/periphyton biomass that is converted to particulate organic matter when epiphyton/periphyton die | 0.8 | 4 | 0.8 | 0.8 | 0.8 | |
| DOM | LDOMDK | Labile DOM decay rate | 0.1 | 24 | 0.03 | 0.5 | 0.1 | day ⁻¹ |
| DOM | RDOMDK | Refractory DOM decay rate | 0.001 | 23 | 0.0005 | 0.015 | 0.001 | day ⁻¹ |
| DOM | LRDDK | Labile to refractory DOM decay rate | 0.01 | 22 | 0.001 | 0.01 | 0.001 | day ⁻¹ |
| POM | LPOMDK | Labile POM decay rate | 0.08 | 23 | 0.002 | 0.101 | 0.08 | day ⁻¹ |
| POM | RPOMDK | Refractory POM decay rate | 0.001 | 16 | 0.0005 | 0.01 | 0.001 | day ⁻¹ |
| POM | LRPDK | Labile to refractory POM decay rate | 0.01 | 8 | 0.001 | 0.02 | 0.0015 | day ⁻¹ |
| POM | POMS | POM settling rate | 0.45 | 22 | 0 | 2.5 | 0.165 | day ⁻¹ |
| OM STOICH | ORGP | Stoichiometric equivalent between organic matter and phosphorus | 0.005 | 20 | 0.0005 | 0.02268 | 0.005 | |
| OM STOICH | ORGN | Stoichiometric equivalent between organic matter and nitrogen | 0.08 | 19 | 0.01 | 0.0825 | 0.08 | |
| OM STOICH | ORGC | Stoichiometric equivalent between organic matter and carbon | 0.45 | 16 | 0.45 | 0.6 | 0.45 | |
| OM STOICH | ORGSi | Stoichiometric equivalent between organic matter and silica | 0.18 | 2 | 0.18 | 0.18 | 0.18 | |
| OM RATE | OMT1 | Lower temperature for organic matter decay | 4 | 21 | 2 | 5 | 4 | °C |
| OM RATE | OMT2 | Upper temperature for organic matter decay | 25 | 21 | 20 | 30 | 30 | °C |
| OM RATE | OMK1 | Fraction of organic matter decay rate at OMT1 | 0.1 | 21 | 0.05 | 0.2 | 0.1 | |
| OM RATE | OMK2 | Fraction of organic matter decay rate at OMT2 | 0.99 | 21 | 0.9 | 0.99 | 0.99 | |
| CBOD | KBOD | 5-day decay rate @ 20 °C | 0.1 | 11 | 0.0186 | 2 | 0.07475 | day ⁻¹ |

| Group | Parameter | Description | Default | Count | Min | Max | Median | Units |
|-------------|-----------|--|---------|-------|--------|-------|---------|------------------------|
| CBOD | TBOD | Arrhenius Temperature coefficient | 1.02 | 9 | 1.0147 | 1.047 | 1.02 | |
| CBOD | RBOD | Ratio of CBOD5 to ultimate CBOD | 1.85 | 9 | 1 | 1.85 | 1 | |
| CBOD | CBODS | CBOD settling rate | 0 | 1 | 0 | 0 | 0 | day ⁻¹ |
| CBOD STOICH | CBODP | P stoichiometry for CBOD decay (mg P/mg O ₂) | 0.004 | 7 | 0.002 | 2 | 0.083 | mg P/mg O ₂ |
| CBOD STOICH | CBODN | N stoichiometry for CBOD decay (mg N/mg O ₂) | 0.06 | 6 | 0.06 | 1.047 | 0.08 | mg N/mg O ₂ |
| CBOD STOICH | CBODC | C stoichiometry for CBOD decay (mg C/mg O ₂) | 0.32 | 6 | 0.32 | 1.85 | 0.825 | mg C/mg O ₂ |
| PHOSPHOR | PO4R | Sediment release rate of phosphorus, fraction of SOD | 0.001 | 22 | 0.0001 | 0.05 | 0.00204 | |
| PHOSPHOR | PARTP | Phosphorus partitioning coefficient for suspended solids | 0 | 18 | 0 | 3 | 0 | |
| AMMONIUM | NH4REL | Sediment release rate of ammonium, fraction of SOD | 0.001 | 20 | 0.001 | 0.2 | 0.02 | |
| AMMONIUM | NH4DK | Ammonium decay rate | 0.12 | 27 | 0.01 | 0.4 | 0.12 | day ⁻¹ |
| NH4 RATE | NH4T1 | Lower temperature for ammonia decay | 5 | 22 | 4 | 10 | 5 | °C |
| NH4 RATE | NH4T2 | Lower temperature for maximum ammonia decay | 25 | 22 | 20 | 35 | 25 | °C |
| NH4 RATE | NH4K1 | Fraction of nitrification rate at NH4T1 | 0.1 | 22 | 0.1 | 0.2 | 0.1 | |
| NH4 RATE | NH4K2 | Fraction of nitrification rate at NH4T2 | 0.99 | 22 | 0.99 | 0.99 | 0.99 | |
| NITRATE | NO3DK | Water column denitrification rate or nitrate decay rate | 0.03 | 26 | 0.01 | 2.6 | 0.1 | day ⁻¹ |
| NITRATE | NO3S | Nitrate loss velocity to the sediments because of sediment denitrification | 0.001 | 5 | 0 | 0.5 | 0.2 | m day ⁻¹ |
| NO3 RATE | NO3T1 | Lower temperature for nitrate decay | 5 | 21 | 4 | 5 | 5 | °C |
| NO3 RATE | NO3T2 | Lower temperature for maximum nitrate decay | 25 | 21 | 20 | 30 | 25 | °C |
| NO3 RATE | NO3K1 | Fraction of denitrification rate at NO3T1 | 0.1 | 21 | 0.1 | 0.1 | 0.1 | |
| NO3 RATE | NO3K2 | Fraction of denitrification rate at NO3T2 | 0.99 | 21 | 0.99 | 0.99 | 0.99 | |
| SILICA | DSIR | Dissolved silica sediment release rate, fraction of SOD | 0.1 | 3 | 0.1 | 0.1 | 0.1 | |
| SILICA | PSIS | Particulate biogenic settling rate | 1 | 3 | 0.04 | 1 | 0.1 | m sec ⁻¹ |
| SILICA | PSIDK | Particulate biogenic silica decay rate | 0.3 | 3 | 0.1 | 0.3 | 0.3 | day ⁻¹ |
| SILICA | PARTSI | Dissolved silica partitioning coefficient | 0 | 2 | 0 | 0.2 | 0.1 | |

Calibration Data and Approaches

The primary concern with calibration of the W2 model is collecting enough high-quality input data, both boundary conditions and in-pool conditions. W2 will not produce a well-calibrated model using only in-pool measurements and requires boundary conditions for inflow, outflow, and tributaries to model hydrodynamics and water quality. As described in the model manual, meteorological and inflow/outflow hydrodynamic data should ideally be continuous for the calibration year with hourly to daily measurements. W2 is capable of modeling diel fluctuations, which require hourly data at least for successful calibration and simulation. Monthly in-pool sampling may be appropriate, although storm events may warrant additional sampling attention. For this task, the length of calibration period and spatiotemporal sampling frequency were not considered as disqualifying characteristics during literature review, although multiple studies did mention the potential shortcomings of a limited dataset. Nearly all the studies using W2 had sufficient input data and/or took steps to address data limitations. Details on calibration periods for each RCK parameter source are included in Table 6.

All the W2 studies used at least a single water year for calibration, and many used multiple water years with varying hydrologic conditions (wet/dry). In some cases, additional calibration years were added to previously calibrated models in the same system to increase model confidence. During model evaluation, most of the studies used multiple water years to make sure that the calibrated model could accurately simulate a wide range of hydrologic conditions. Most of the studies had continuous inflow/outflow temperature and hydrodynamic data (such as discharge and water level) at an hourly to daily interval. For studies with insufficient data, nearby meteorological stations and available hydrologic data were correlated to generate hourly to daily inflow values. Most of the studies also calibrated using vertical profiles in addition to in-pool point samples, both of which were collected monthly with additional storm samples. In some cases, the in-pool measurements were taken only seasonally, although the studies included a discussion of potential issues associated with limited data. For all studies, whenever possible, the calibration was conducted using the water year(s) with the largest amount of available data. Generally, errors in prediction of temperatures, stratification, and transport were commonly attributable to inadequate bathymetric data or poorly defined boundary conditions.

Many parameters in the RCK tables were determined through manual calibration using default or literature starting values. Initial values came from other studies of similar systems, including the EPA 1985 Rates Manual, extensive tables of values included in the W2 manuals, and other literature. Calibration strategies varied, but most commonly involved systematic variation of individual parameters within ranges suggested in the literature and model manual to obtain the best graphical “fit” of model predictions and observations (qualitative) and/or quantitatively reduce RMSE of the modeled values against observed data. In many cases, the default values or literature values remained unchanged during calibration. For the studies where parameters were manually calibrated, the researchers followed a generally consistent procedure to achieve good agreement between modeled and observed data, calibrating first hydrodynamics and then water quality. Within each category parameters were manipulated in a logical way and were not changed at random to increase model fit.

4.3 HSPF

As a starting point, the methods for literature searches and study selection described in Section 3 were used for HSPF. However, the project team was aware from the onset that locating relevant values by means of keyword-based searching would be more challenging for HSPF than for the other models. Several factors contribute to the challenge:

- HSPF is different from the other three models in that it simulates both land surface runoff and washoff processes and receiving water processes. Only receiving water parameters are relevant to this update of EPA's Rates Manual. Many (likely most) search results lead to studies that utilize HSPF's surface module PERLND as opposed to its receiving water module RCHRES.
- The majority of the RCHRES module code was created prior to 1985, and has therefore not been treated as novel in the published literature. Within the scope of the current effort, only post-1985 information was being sought. The HSPF model has been extensively applied since 1985, with substantial additional experience in model calibration; however, these results are present primarily in regulatory gray literature (e.g., TMDL reports) rather than in the peer-reviewed journal literature, making them more difficult to find.
- RCHRES offers numerous alternatives for modeling the current project's Group 1 water quality constituents. Each of the post-1985 enhancements is structured as a modeling option; hence, even carefully designed keyword combinations rarely guarantee that studies that are being identified utilize the specific enhancements/options that are sought by this project.

Because of these challenges, the HSPF data table that accompanies this report has relatively few parameter values compared with the other models, given the focus of this project on model applications in surface water systems since 1985. Additional parameter values are available in the HSPFParm database described under Summary of Sources.

Summary of Sources

The automated literature searches resulted in 22 pieces of literature that were deemed to be potentially relevant to HSPF. More careful examination of these documents substantiated the weaknesses of using a keyword-based approach to meet the needs specific to HSPF. Many of the reports documented studies that used HSPF to simulate runoff and washoff to receiving waters (i.e., used HSPF PERLND), and subsequently used another water quality model to simulate receiving water processes (e.g., EFDC [Hamrick, 1996], WASP [Section 4.1], QUAL2K [Section 4.4], or CE-QUAL-W2 [Section 4.2]).

In parallel to evaluating the documents that were identified by means of automated literature search, a supplemental approach to mining relevant parameter values was pursued. The approach relied on: 1) mining HSPF parameter values that EPA had already collected and distributed in a published tool (HSPFParm); and 2) accessing and mining values from studies that were known to utilize the code enhancements of interest and were also known to have been performed by well-qualified HSPF modelers.

The first source of relevant parameter values was U.S. EPA's HSPFParm (Donigian et al., 1999), an interactive database of HSPF model parameters. To support an expanding community of HSPF modelers

that needed a readily available source of model parameter values that can provide the best possible starting point for developing new watershed applications, EPA funded AQUA TERRA Consultants to collect available HSPF parameter values from applications across North America, assimilate the parameter values into a single database, and develop an interactive interface that enables modelers to access and utilize the database. The resulting product, named HSPFParm, contains parameter values for model applications in more than 70 watersheds in 14 states. The parameter values that are contained in the database characterize a broad variety of physical settings, land use practices and water quality constituents.

The Minnesota Pollution Control Agency has subsequently funded the expansion of HSPFParm to include input sequences that represent the State's HUC-8 watersheds and are the basis for developing the State's TMDLs.

The studies (Table 13) that yielded relevant parameter values were the following:

- A study prepared at Portland State University entailing a model application in Oregon;
- A study prepared at Memphis State University entailing a model application in Tennessee;
- A study prepared by Maryland Department of the Environment that included parameter values for five separate watersheds primarily in Maryland;
- A study prepared for U.S. EPA ORD detailing a model application in Pennsylvania;
- A study prepared for Minnesota Pollution Control Agency;
- The parameter values established by U.S. EPA's Chesapeake Bay program for the Phase IV Chesapeake Bay Watershed Model;⁶ and
- Model input representing 19 HUC-8 watersheds in Minnesota developed by three different contractors to Minnesota Pollution Control Agency: AQUA TERRA (9 watersheds); Tetra Tech (10 watersheds);

The second type of source for relevant parameter values was any study known to utilize the code enhancements of interest and known to have been performed by well qualified HSPF modelers. Two additional collections of parameter values were obtained as follows:

- Parameter values for post-1985 nutrient enhancements were mined for 14 watersheds contained in the Puget Sound drainage.
- Parameter values for post-1985 benthic algae enhancements were mined from an application in the Truckee River (Nevada) watershed for the Cities of Sparks and Reno.

⁶ Values are reported for 19 sub-watersheds within the Chesapeake drainage. This is a pivotal body of data since HSPF's post-1985 nutrient enhancements were designed to support this effort.

Table 13. HSPF Literature Sources

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|---|--|-----------------------------|--|-------------------------|---|
| <p>Aqua Terra and King County, 2003. King County Watershed Modeling Services – Green River Water Quality Assessment, and Sammamish-Washington Analysis and Modeling Program Watershed Modeling Report. Prepared for King County Department of Natural Resources and Parks, Water and Land Resources Division. Seattle, WA. Prepared by Aqua Terra Consultants, Everett, Washington and Mountain View, California in conjunction with King County.</p> | <p>Puget Sound Drainage, Washington</p> | <p>Rivers & Streams</p> | <p>Forest, pasture/agriculture, low density residential, high density residential, commercial/industrial (on till soil, outwash soil, saturated soil, and rock)</p> | <p>1/1991 - 12/2004</p> | <p>14 models - each shown separately in RCK table</p> |
| <p>Bicknell B.R., A.S. Donigian Jr., T.H. Jobes, and R.V. Chinnaswamy, 1996. Modeling Nitrogen Cycling and Export in Forested Watersheds using HSPF. Prepared for U.S. EPA; Athens, Georgia.</p> | <p>Young Woman's Creek - an 11.3-mile creek in the West Branch Susquehanna River, Pennsylvania</p> | <p>River</p> | <p>Forest</p> | <p>1/1984 - 12/1991</p> | |
| <p>Donigian, A.S., Jr., 1997. Preliminary Calibration Results for Blue Earth, Watonwan, Redwood, Yellow Medicine, Cottonwood and Hawk Watersheds. Prepared for Minnesota Pollution Control Agency; St. Paul, Minnesota.</p> | <p>Minnesota</p> | <p>Rivers</p> | <p>Forest, cropland; pasture; marsh/wetland; animal waste application area; impervious urban/residential</p> | <p>1/1986 - 12/1992</p> | <p>6 models developed in study (main stem river and tributary). Each included separately in RCK table.</p> |
| <p>LimnoTech, 2008. Final Draft Calibration of the Truckee River HSPF Water Quality Model. Prepared for the Cities of Reno and Sparks, Nevada, January 2008.</p> | <p>Truckee River Drainage, Nevada & California</p> | <p>River</p> | <p>Coniferous forest; deciduous forest; shrub; grassland; pasture; golf courses; farm; marsh; barren; low/high density residential; commercial; industrial; confined feeding</p> | <p>1/2000 - 12/2002</p> | <p>A total of 43 segments were used for this application, Segments range in length from 0.13 miles to 3.24 miles.</p> |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|---|---|----------------------|--|--------------------|---|
| MDE, 1991. Patuxent Watershed Model - Final Report. Maryland Department of the Environment; Baltimore, Maryland. | Patuxent River, Maryland | Rivers & 1 Reservoir | 19 separate land use categories: forest; tillage; hay; pasture; wetlands; residential; commercial; industrial; major roads; animal areas | 1/1986 - 12/1990 | 5 separate models in this study (Upper Patuxent, Middle Patuxent, Lower Patuxent, North Patuxent, South Patuxent). Each included separately in RCK table. |
| Mishra, A., A.S. Donigian, Jr., and B.R. Bicknell, 2014. HSPF Watershed Modeling Phase 3 for the Crow Wing, Redeye, and Long Prairie Rivers Watersheds: Calibration and Validation of Hydrology, Sediment, and Water Quality Constituents. Final Report. AQUA TERRA Consultants, Mountain View, CA. Prepared for Minnesota Pollution Control Agency, St. Paul, Minnesota. | Minnesota | Rivers | Forest; cropland; pasture; marsh/wetland; animal waste application area; impervious urban/residential | 1/2003 - 12/2009 | 3 models developed in study (main stem river and tributary). Each included separately in RCK table. |
| Moore, L.W., et al., 1992. Feasibility of an Integrated Geographic Information/Nonpoint Modeling System. Memphis State University; Memphis; Tennessee. | West Sandy Creek, Kentucky Lake watershed, Henry County, TN | River | 11% cropland; 33% pasture and hay; 50% forest; 6% other (urban, quarries, gullies) | 1/1987 - 12/1987 | |
| Patwardhan, A.S., R.M. Jacobson, A.S. Donigian Jr., and R.V. Chinnaswamy, 1996. HSPF Model Application to the LeSueur Watershed Preliminary Findings and Recommendations. Minnesota Pollution Control Agency; St. Paul, Minnesota. | LeSueur River, Minnesota | River | Forest; cropland; pasture; marsh/wetland; animal waste application area; impervious urban/residential | 1/1986 - 12/1992 | |
| Tang, F., 1993. Calibration and Verification of HSPF Model for Tualatin River Basin Water Quality. Technical Report EWR-003-93; Dept. Civil Eng.; Portland State University; Portland, Oregon. | Tualatin River, western Oregon | River | Mixed land use segments simulated including urban, crops, forest, limited range & wetland | 1/1991 - 12/1991 | |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period | Notes |
|--|---|----------------------|--|--------------------|--|
| Tetra Tech, 2009. Minnesota River Basin Turbidity TMDL and Lake Pepin Excessive Nutrient TMDL. Prepared for Minnesota Pollution Control Agency; St. Paul, Minnesota. | Minnesota River Basin, Minnesota | Rivers & 1 Reservoir | Forest; cropland; feedlots; pasture; urban; marsh/wetlands | 1/1993 - 12/2006 | 10 separate models in this study. Each included separately in RCK table. |
| U.S. EPA, 1998. Chesapeake Bay Watershed Model Application and Calculation of Nutrient and Sediment Loadings. Phase IV Model Documentation and Results. Prepared by Modeling Subcommittee of CBP. February 1998. | Chesapeake Bay Watershed, North Central United States | Rivers & 1 Reservoir | Forest; conventional tillage (high till); cropland; conservation tillage (low till); cropland; hay; pasture; urban/residential; animal waste/feedlot areas; impervious urban/residential | 1/1984 - 12/1991 | 19 separate models in this study. Each included separately in RCK table. |

Studies selected to provide parameter values for HSPF nutrient routines represent the Pacific Northwest, Mid-Atlantic and the Upper Midwest. These regions are characterized by streams that can transport a significant fraction of inorganic nutrient washoff associated with inorganic sediment. Generally, the climatic distribution of the current collection of parameter values is skewed towards northern latitudes that experience coastal or large lake influences. The formulations in the post-1985 HSPF benthic algae enhancement are uniquely relevant to relatively shallow and clear Western streams. Applications of the DSSAMt model (from which the formulations were adopted) also appears to be limited to this geographic area and stream type. Hundreds of HSPF applications have occurred throughout the United States that have not been captured by the literature search or by the alternative effort made for this project. Relevant parameter values exist for applications in other regions, but the materials were not identified by the search strategy used for this report and would need to be retrieved from the gray literature such as TMDL model calibration reports. For additional resources regarding HSPF, see also Section 9 of this report. Details on the watershed characteristics for each included study were contained within Table 13. The resulting distributions of rates and constants values are summarized in Table 14.

Summary Statistics for Rates and Constants

Table 14. HSPF Rates and Constants

| Block | Name | Description | Count | Min | Max | Mean | Median | Default | Units |
|--------------|--------|--|-------|-------|------|--------|--------|---------|----------|
| CONV-VAL1 | CVBO | Conversion from mg biomass to mg oxygen | 49 | 1.63 | 5 | 1.65 | 1.63 | 1.98 | mg/mg |
| CONV-VAL1 | CVBPC | Conversion from biomass expressed as P to C | 49 | 106 | 200 | 106.24 | 106 | 106 | mols/mol |
| CONV-VAL1 | CVBPN | Conversion from biomass expressed as P to N | 49 | 10 | 16 | 15.98 | 16 | 16 | mols/mol |
| CONV-VAL1 | BPCNTC | Percentage of biomass that is carbon (by weight) | 49 | 10 | 49 | 48.90 | 49 | 49 | – |
| NUT-BENPARM | BRTAM1 | Benthic release rate of ammonia under aerobic conditions | 41 | 0 | 4 | 0.0777 | 0 | 0 | mg/m2.hr |
| NUT-BENPARM | BRTAM2 | Benthic release rate of ammonia under anaerobic conditions | 41 | 0 | 33 | 0.4082 | 0 | 0 | mg/m2.hr |
| NUT-BENPARM | BRPO41 | Benthic release rate orthoP under aerobic conditions | 41 | 0 | 2.7 | 0.0354 | 0 | 0 | mg/m2.hr |
| NUT-BENPARM | BRPO42 | Benthic release rate of orthoP under anaerobic conditions | 41 | 0 | 2.7 | 0.0332 | 0 | 0 | mg/m2.hr |
| NUT-BENPARM | ANAER | Concentration of DO below which anaerobic conditions exist | 41 | 0.001 | 1 | 0.0428 | 0.001 | 0.005 | mg/L |
| NUT-NITDENIT | KTAM20 | Nitrification rate of ammonia at 20 °C | 60 | 0.001 | 0.6 | 0.0401 | 0.002 | – | 1/hr |
| NUT-NITDENIT | KNO220 | Nitrification rate of nitrite at 20 °C | 50 | 0.001 | 0.05 | 0.0081 | 0.012 | – | 1/hr |
| NUT-NITDENIT | TCNIT | Temperature correction coefficient for nitrification | 60 | 1 | 1.07 | 1.0647 | 1.04 | 1.07 | – |
| NUT-NITDENIT | KNO320 | Nitrate denitrification rate | 50 | 0.001 | 3.5 | 0.0333 | 0.002 | – | 1/hr |
| NUT-NITDENIT | TCDEN | Temperature correction coefficient for denitrification | 50 | 1 | 1.07 | 1.0404 | 1.04 | 1.07 | – |
| NUT-NITDENIT | DENOXT | Threshold value for DO above which denit. ceases | 60 | 1 | 100 | 5.5860 | 5 | 2 | mg/L |

| Block | Name | Description | Count | Min | Max | Mean | Median | Default | Units |
|--------------|-----------|--|-------|---------|--------|--------|--------|---------|-------|
| NUT-NH3VOLAT | EXPNVG | Exponent in gas layer mass transfer equation for NH3 volatilization | 5 | 0.5 | 0.5 | 0.5000 | 0.5 | 0.5 | – |
| NUT-NH3VOLAT | EXPNVL | Exponent in liquid layer mass transfer equation for NH3 volatilization | 5 | 0.667 | 0.667 | 0.6670 | 0.667 | 0.6667 | – |
| NUT-BEDCONC | BRTAM(1) | Constant bed concentrations of ammonia-N adsorbed to clay | 45 | 0.0001 | 300 | 39.2 | 40 | 0 | mg/kg |
| NUT-BEDCONC | BRTAM(2) | Constant bed concentrations of ammonia-N adsorbed to sand | 45 | 0.0002 | 600 | 103.8 | 100 | 0 | mg/kg |
| NUT-BEDCONC | BRTAM(3) | Constant bed concentrations of ammonia-N adsorbed to silt | 45 | 0.0003 | 550 | 102.3 | 100 | 0 | mg/kg |
| NUT-BEDCONC | BRPO4(1) | Constant bed concentrations of ortho-phosphorus-P adsorbed to clay | 45 | 0.00005 | 200 | 84.4 | 100 | 0 | mg/kg |
| NUT-BEDCONC | BRPO4(2) | Constant bed concentrations of ortho-phosphorus-P adsorbed to sand | 45 | 0.0003 | 3500 | 457.2 | 250 | 0 | mg/kg |
| NUT-BEDCONC | BRPO4(3) | Constant bed concentrations of ortho-phosphorus-P adsorbed to silt | 45 | 0.0004 | 1000 | 256.8 | 250 | 0 | mg/kg |
| NUT-ADSPARM | ADNHPM(1) | Adsorption coefficients (Kd) for ammonia-N adsorbed to clay | 35 | 10 | 300 | 30.2 | 150 | – | ml/g |
| NUT-ADSPARM | ADNHPM(2) | Adsorption coefficients (Kd) for ammonia-N adsorbed to sand | 20 | 100 | 4000 | 257.1 | 100 | – | ml/g |
| NUT-ADSPARM | ADNHPM(3) | Adsorption coefficients (Kd) for ammonia-N adsorbed to silt | 35 | 100 | 4000 | 329.0 | 150 | – | ml/g |
| NUT-ADSPARM | ADPOPM(1) | Adsorption coefficients for ortho-phosphorus-P adsorbed to clay | 20 | 100 | 9500 | 371.9 | 100 | – | ml/g |
| NUT-ADSPARM | ADPOPM(2) | Adsorption coefficients for ortho-phosphorus-P adsorbed to sand | 20 | 1000 | 30000 | 2360.7 | 1000 | – | ml/g |
| NUT-ADSPARM | ADPOPM(3) | Adsorption coefficients for ortho-phosphorus-P adsorbed to silt | 20 | 1000 | 100000 | 2607.9 | 1000 | – | ml/g |
| PLNK-PARM1 | RATCLP | Ratio of chl-a content of biomass to P content | 50 | 0.6 | 0.68 | 0.6769 | 0.68 | 0.6 | – |
| PLNK-PARM1 | NONREF | Non-refractory fraction of algal biomass | 50 | 0.2 | 0.6 | 0.4713 | 0.5 | 0.5 | – |

| Block | Name | Description | Count | Min | Max | Mean | Median | Default | Units |
|------------|--------|--|-------|----------|--------|--------|--------|---------|---------|
| PLNK-PARM1 | LITSED | Multiplication factor to total sediment concentration to determine sediment contribution to light extinction | 50 | 0 | 1 | 0.0032 | 0 | 0 | 1/mg.ft |
| PLNK-PARM1 | ALNPR | Fraction of N requirements for phytoplankton growth that is satisfied by nitrate | 50 | 0.1 | 0.7 | 0.2560 | 0.25 | 1 | - |
| PLNK-PARM1 | EXTB | Base extinction coefficient for light | 50 | 0.01 | 0.6 | 0.1865 | 0.12 | - | 1/ft |
| PLNK-PARM1 | MALGR | Maximum unit algal growth rate | 50 | 0.001 | 0.32 | 0.0878 | 0.075 | 0.3 | 1/hr |
| PLNK-PARM2 | CMMLT | Michaelis-Menten constant for light-limited algal growth | 49 | 0.000001 | 0.04 | 0.0258 | 0.033 | 0.033 | ly/min |
| PLNK-PARM2 | CMMN | Nitrate Michaelis-Menten constant for N-limited algal growth | 49 | 0.000001 | 0.045 | 0.0348 | 0.045 | 0.045 | mg/L |
| PLNK-PARM2 | CMMNP | Nitrate Michaelis-Menten constant for P-limited algal growth | 49 | 0.000001 | 0.0284 | 0.0041 | 0.0001 | 0.0284 | mg/L |
| PLNK-PARM2 | CMMP | Michaelis-Menten constant for P-limited algal growth | 49 | 0.000001 | 0.05 | 0.0110 | 0.015 | 0.015 | mg/L |
| PLNK-PARM2 | TALGRH | Temperature above which phytoplankton growth ceases | 49 | 50 | 95 | 94.4 | 95 | 95 | °F |
| PLNK-PARM2 | TALGRL | Temperature below which phytoplankton growth ceases | 49 | -110 | 50 | -15.0 | -10 | 43 | °F |
| PLNK-PARM2 | TALGRM | Temperature below which phytoplankton growth is retarded | 49 | 50 | 86 | 79.8 | 77 | 77 | °F |
| PLNK-PARM3 | ALR20 | Phytoplankton respiration rate at 20 °C | 49 | 0.000001 | 0.007 | 0.0049 | 0.005 | 0.004 | 1/hr |
| PLNK-PARM3 | ALDH | High phytoplankton unit death rate | 49 | 0.000001 | 0.02 | 0.0156 | 0.02 | 0.01 | 1/hr |
| PLNK-PARM3 | ALDL | Low phytoplankton unit death rate | 49 | 0.000001 | 0.003 | 0.0011 | 0.001 | 0.001 | 1/hr |
| PLNK-PARM3 | OXALD | Increment to phytoplankton unit death rate due to anaerobic conditions | 49 | 0.000001 | 0.03 | 0.0295 | 0.03 | 0.03 | 1/hr |
| PLNK-PARM3 | NALDH | Inorganic N concentration below which high phytoplankton death rate occurs | 49 | 0 | 0.025 | 0.0120 | 0.01 | 0 | mg/L |

| Block | Name | Description | Count | Min | Max | Mean | Median | Default | Units |
|------------|--------|--|-------|-------|--------|--------|--------|---------|-------|
| PLNK-PARM3 | PALDH | Inorganic P concentration below which high phytoplankton death rate occurs | 49 | 0 | 0.005 | 0.0025 | 0.002 | 0 | mg/L |
| PHYTO-PARM | SEED | Minimum concentration of phytoplankton not subject to advection | 38 | 0.018 | 10 | 1.0272 | 1 | – | mg/L |
| PHYTO-PARM | MXSTAY | Concentration of phytoplankton not subject to advection at low flow | 48 | 0.05 | 25 | 2.8424 | 2 | – | mg/L |
| PHYTO-PARM | OREF | Flow at which concentration of phytoplankton not subject to advection is between SEED and MXSTAY | 48 | 2 | 6000 | 202.5 | 100 | – | cfs |
| PHYTO-PARM | CLALDH | Chl-a concentration above which high algal death rate occurs | 49 | 15 | 9999 | 139.6 | 20 | 50 | µg/L |
| PHYTO-PARM | PHYSET | Phytoplankton settling rate | 49 | 0 | 0.15 | 0.0176 | 0.015 | 0 | ft/hr |
| PHYTO-PARM | REFSET | Settling rate for dead refractory organics | 49 | 0 | 1 | 0.0357 | 0.021 | – | ft/hr |
| BENAL-PARM | MBAL | Maximum benthic algal biomass | 45 | 60 | 800000 | 49904 | 2500 | 600 | mg/m2 |
| BENAL-PARM | CFBALR | Ratio of benthic algal to phytoplankton respiration | 45 | 0.1 | 1 | 0.3525 | 0.35 | 1 | – |
| BENAL-PARM | CFBALG | Ratio of benthic algal to phytoplankton growth rate | 45 | 0.08 | 1 | 0.9305 | 1 | 1 | – |

For the advanced benthic algae parameters, the literature search resulted in only a single study (LimnoTech, 2008. Final Draft Calibration of the Truckee River HSPF Water Quality Model). The benthic algae parameters from this study are listed in Table 15.

Table 15. Advanced Benthic Algae Parameters

| Parameter | Module | Description | Value | Units |
|-----------|--------------|--|---------|---------|
| MINBAL | BENAL-PARM | Minimum benthic algae density (as biomass) | 1000.0 | mgDW/m2 |
| CAMPR | BENAL-PARM | Coefficient in the alternative nitrogen preference equation for benthic algae | 20.0 | – |
| FRAVL | BENAL-PARM | Fraction of nonrefractory nutrients resulting from benthic algae death/removal that are assumed to be immediately available as inorganic nutrients, plus refractory organic carbon | 0.250 | – |
| NMAXFX | BENAL-PARM | Concentration of available inorganic nitrogen in the water column (TAM + NO ₃ + NO ₂) above which nitrogen-fixation by benthic algae is suppressed | 0.20 | mg/L |
| MBALGR | BENAL-GROW | Maximum benthic algae base growth rate for each benthic algae species | 0.120 | /hr |
| TCBALG | BENAL-GROW | Temperature correction coefficient for growth for each species | 1.067 | – |
| CMMNB | BENAL-GROW | Half-saturation constant for nitrogen-limited growth for each species. If the value is zero, then growth is not limited (i.e., this species fixes nitrogen) | 0.0250 | mg/L |
| CMMPB | BENAL-GROW | Half-saturation constant for phosphorus-limited growth for each species | 0.0050 | mg/L |
| CMMD1 | BENAL-GROW | Coefficient for total benthic algae density in the density-limited growth equation for each species | 0.010 | – |
| CMMD2 | BENAL-GROW | Half-saturation constant for density-limited growth for each species | 16000.0 | mg/m2 |
| CSLIT | BENAL-GROW | Saturation light level for each species | 0.2780 | ly/min |
| BALR20 | BENAL-RESSCR | Benthic algae respiration rate at 20 C for each species | 0.00550 | /hr |
| TCBALR | BENAL-RESSCR | Temperature correction coefficient for respiration for each species | 1.0670 | – |
| CSLOF1 | BENAL-RESSCR | Rate coefficient in the benthic algae scour equation for each species | 0.00010 | /hr |
| CSLOF2 | BENAL-RESSCR | Multiplier of velocity in the exponent in the benthic algae scour equation for each species | 4.50 | – |
| GRORES | BENAL-RESSCR | Fraction of photorespiration needed to support growth/photosynthesis for each species | 0.0750 | – |

| Parameter | Module | Description | Value | Units |
|-----------|-------------|--|---------------|-------------------|
| CREMVL | BENAL-GRAZE | Annual benthic algae grazing (removal) rate by invertebrates | 34.660 | mg/mg/yr |
| CMMBI | BENAL-GRAZE | Half-saturation constant for grazing by invertebrates | 10000.0 | mg/m ² |
| BINV | BENAL-GRAZE | Biomass (density) of grazing invertebrates in the reach | (2400 - 4150) | mg/m ² |
| TCGRAZ | BENAL-GRAZE | Temperature correction coefficient for macroinvertebrate grazing | 1.060 | – |
| FRRIF | BENAL-RIFF1 | Fraction of the reach that is composed of riffles where benthic algae can grow | (0.5 - 1.0) | – |
| CMMV | BENAL-RIFF1 | Half-saturation constant for riffle velocity in the nutrient availability equation for benthic algae | 0.20010 | ft/s |
| RIFCQ1 | BENAL-RIFF1 | Critical flow levels for riffle velocity and average depth | 105.9 | cfs |
| RIFCQ2 | BENAL-RIFF1 | Critical flow levels for riffle velocity and average depth | 211.9 | cfs |
| RIFCQ3 | BENAL-RIFF1 | Critical flow levels for riffle velocity and average depth | 317.8 | cfs |
| RIFVEL(1) | BENAL-RIFF2 | Riffle velocity multipliers corresponding to the critical flow values (RIFCQ) | 1.80 | – |
| RIFVEL(2) | BENAL-RIFF2 | Riffle velocity multipliers corresponding to the critical flow values (RIFCQ) | 1.50 | – |
| RIFVEL(3) | BENAL-RIFF2 | Riffle velocity multipliers corresponding to the critical flow values (RIFCQ) | 1.20 | – |
| RIFVEL(4) | BENAL-RIFF2 | Riffle velocity multipliers corresponding to the critical flow values (RIFCQ) | 1.00 | – |
| RIFDEP(1) | BENAL-RIFF2 | Depth multipliers corresponding to the critical flow values (RIFCQ) | 0.550 | – |
| RIFDEP(2) | BENAL-RIFF2 | Depth multipliers corresponding to the critical flow values (RIFCQ) | 0.650 | – |
| RIFDEP(3) | BENAL-RIFF2 | Depth multipliers corresponding to the critical flow values (RIFCQ) | 0.750 | – |
| RIFDEP(4) | BENAL-RIFF2 | Depth multipliers corresponding to the critical flow values (RIFCQ) | 0.850 | – |

Calibration Data and Approaches

The predominant procedure for calibration is adjustment of default values (default values are not available for all the parameters of interest) using a systematic approach to vary parameter values individually to increase similarity between modeled and observed data. A detailed summary of HSPF model use and calibration is provided in Duda et al. (2012). Guidance on HSPF calibration for flow and sediment is provided in U.S. EPA (2000) and (2006), respectively. Comprehensive national guidance on nutrient parameters and rates for HSPF has not been developed; however, RESPEC (2018) provides information on acceptable ranges of kinetic coefficients for application in Minnesota.

Since the enhancement of HSPF related to nutrient-sediment interactions is very dependent on sediment scour/deposition phenomena, calibration requires comparison to monitored data for variable flow conditions. Ideally the monitored data record extends at least over the period of several years. Likewise, calibration of the benthic algae enhancement is best supported with monitored data for an annual cycle of population growth/decline.

Results of the rates and constants search for nutrient-related parameters in HSPF are shown in Table 14. Default values shown in this table are from Bicknell et al. (2014). These are the defaults that HSPF assumes when user data are not provided and in some cases, represent nominal values that will prevent code crashes rather than physically realistic estimates.

An advantage of utilizing the alternative method of obtaining parameter values for HSPF enhancements that is described above (i.e., mining them from complete model input sequences) is that a full set of parameter values can be provided for each model application. However, this data mining is resource-intensive; it was pursued for HSPF to compensate for the limited information on parameter values for this model in journal articles and readily discoverable technical reports.

4.4 QUAL2K and QUAL2Kw

The initial literature search for Q2K and/or Q2Kw returned more than 50 papers and reports that discussed a modeling study using Q2K or Q2Kw and addressed nutrients, dissolved oxygen, or algae. Of these studies, 17 (Table 16) were deemed to be appropriate for inclusion in this survey based on the criteria noted above (tabulation of parameters; identification of parameter sources, calibration data, and calibration procedures; evaluation of model performance).

Summary of Sources

Eight of the studies were published in peer-reviewed journals, eight were reports by state environmental agencies or boards (California, Washington, Oregon, and Montana), and one was a Tetra Tech report for EPA and the State of California. These selected studies contained thorough documentation of modeling activities and calibration parameters as described in Section 3.

Studies were generally geared towards regulatory goals, with more than half undertaken to support development of TMDLs or numeric nutrient criteria in the United States. Four studies are from outside of the United States and are geared towards evaluating the impacts of waste discharges on river water quality.

All the Q2K applications selected from the United States were conducted in western states (California, Montana, Oregon, Utah, and Washington). The four studies from outside of the United States were done in China, Portugal, Nepal, and India. Climatologically, the study areas include rivers in the Pacific Northwest (Oregon and Washington), tropical and humid subtropical regions (Deccan Plateau in India and Zhejiang Province in China, respectively), a warm temperate region (Kathmandu Valley, Nepal), the Mediterranean (Portugal), and subhumid (Utah) and semi-arid (southern California, Montana) areas.

The waterbodies studied are rivers and streams in a variety of basin types and sizes. For example, some of the Q2K applications are in systems fed by snowmelt (Yellowstone River, Wenatchee River, Jordan River); in a contrasting example, most of the flow of the New River in southern California consists of tributary/agricultural drain and wastewater inputs. For additional resources regarding QUAL2K/QUAL2Kw, see also Section 9 of this report. Detailed examples of application of the older QUAL2E model along with extensive tables of relevant rates and constants are also available in U.S. EPA (1995).

Table 16. QUAL2K and QUAL2Kw Literature Sources

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period |
|--|--|---|---|---|
| Butkus, S., 2011. Dissolved Oxygen Model Development and Evaluation. Memorandum for California Regional Water Quality Control Board North Coast Region. | Santa Rosa Creek and Lake Jonvie, Santa Rosa, California | River (a) and lake (b) (separate models) | Details on watershed contained in Butkus, S., 2011. Water Quality Model Development History for the Laguna de Santa Rosa TMDL. Memorandum for California Regional Water Quality Control Board North Coast Region. | Calibrated to 3 diel sampling events in August 2009 |
| Carroll, J., S. O'Neal, and S. Golding, 2006. Wenatchee River Basin Dissolved Oxygen, pH, and Phosphorus Total Maximum Daily Load Study. Prepared for Washington State Department of Ecology Environmental Assessment Program. | Wenatchee River, northwest Washington (east flank of Cascades) | River (a) and tributary (b) (separate models) | 3555 km ² drainage; primarily forested watershed with relatively pristine headwaters; some agricultural and municipal runoff in lower river reaches (two small cities) | Calibrated to 2 synoptic surveys in 09/2002 and 10/2002 |
| Fang, X., J. Zhang, C. Mei, and M. Wong, 2014. The assimilative capacity of Qiantang River watershed, China. <i>Water and Environment Journal</i> . 28, 192-202. | Zhejiang Province, China (eastern coastal China) | River | Heavily populated and agricultural watershed with thousands of point sources. 41700 km ² drainage; 14.08 million people in watershed | Calibrated to seasonal water quality surveys from 01/2000 to 06/2005 |
| Flynn, K., and M.W. Suplee, 2011. Using a computer water quality model to derive 20 numeric nutrient criteria: Lower Yellowstone River. WQPBDMSTECH-22. Helena, MT: Montana Dept. of Environmental Quality. | A 232.9 km (144.7 mile) segment of the lower Yellowstone River in eastern Montana. | River | Study area was a 232.9 km (144.7 mile) segment of the lower Yellowstone River in eastern Montana. | Two synoptic surveys: August 17-26, 2007, for calibration. September 11-20, 2007, for validation. |
| Flynn, K., M. Suplee, S. Chapra, and H. Tao, 2015. Model-based Nitrogen and Phosphorus (Nutrient) Criteria for Large Temperate Rivers: 1. Model Development and Application. <i>Journal of the American Water Resources Association</i> . 51(2). | Segment of the lower Yellowstone River, Montana | River | River segment runs from Billings to Sidney, Montana (536 km). Flow is unregulated. Water yield is 334 m ³ /s annually and base flow is 177 m ³ /s | August 17-26, 2007 and August 23-30, 2000 |
| Kannel, P.R., and S. Lee. 2007. Application of QUAL2Kw for Water Quality Modeling and Dissolved Oxygen Control in the River Bagmati. <i>Environmental Monitoring Assess.</i> 125:201-207. | Bagmati River, Kathmandu Valley of Nepal | River | Study area is about 20 km of the Bagmati between Atterkhel village and Chovar | 19-20 June, 2004 (pre-monsoon) 2-3 December, 2004 (post-monsoon) |
| Kannel, P.R., Y.-S. Lee, S.R. Kannel, and G.J. Pelletier, 2007. Application of automated QUAL2Kw for water quality modeling and management in the Bagmati River, Nepal. <i>Ecological Modelling</i> , 202, 503-517. | Bagmati River in Kathmandu. Study area was the upper 25 km of the river. | River | Bagmati River basin in central part of Nepal. Study covered the upper 25 km length of the Bagmati River. Drainage area = 651 sq. km within the Kathmandu Valley. | January 2-6 (winter) Year uncertain - likely 2005 or 2006 based on 2007 publication date |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period |
|---|---|-------------------|--|--|
| Kori, B., T. Shashidhar, and S. Mise, 2013. Application of automated Qual2kw for water quality modeling in the River Karanja, India. <i>Global Journal of Bio-Science and Biotechnology</i> , 2(2): 193-203. | Karanja River, Pradesh state, India. Deccan Plateau. Stretch of river between Karanja Reservoir and Bhalki pump station (21.85 km). | River | Karanja River is a tributary to the Godavari River, in Pradesh state of India. River has a dam and a pumping station about 21.85 km downstream of the reservoir. Catchment area of river at proposed dam site is 2,025.4 km ² . | June 30, 2010 (pre-monsoon season). |
| Mohamedali, T., and S. Lee, 2008. Bear-Evans Watershed Temperature and Dissolved Oxygen Total Maximum Daily Load: Water Quality Improvement Report. Prepared for State of Washington Department of Ecology. | Bear Creek (a), Evans Creek (b), Cottage Lake Creek (c), northwest Washington | River | 57.8 km ² drainage (main stem of 132 km ² basin); mixed-use watershed with 3 cities and ~50% developed land (primarily residential) | Calibrated to continuous and grab samples from 06/2006 to 10/2006 |
| Oliveira, B., J. Bola, P. Quinteiro, H. Nadais, and L. Arroja, 2012. Application of Qual2Kw model as a tool for water quality management: Certima River as a case study. <i>Environ Monit Assess.</i> 184. 6197-6210. | Certima River, Portugal (west-central) | River | Mixed-use watershed with numerous diffuse contaminant sources. | Calibrated to full sampling season in 2008 |
| Pelletier, G., S. Chapra, and H. Tao, 2006. QUAL2Kw - A Framework for Modeling Water Quality in Streams and Rivers Using a Genetic Algorithm for Calibration. <i>Environmental Modelling & Software.</i> 21:419-425. | NA | NA | NA | NA |
| Sargeant, D., B. Carey, M. Roberts, and S. Brock, 2006. Henderson Inlet Watershed Fecal Coliform Bacteria, Dissolved Oxygen, pH, and Temperature Total Maximum Daily Load Study. Environmental Assessment Program, Washington State Department of Ecology. | Woodland Creek, near Olympia, Washington (south Puget Sound) | River | 76.8 km ² drainage; mixed urban/suburban and forested watershed, minor agriculture. Drains into southern Puget Sound (some tidal influence) | Calibrated to 8 storm events and 4 dry season events in 2003; also used data from previous studies in Henderson Inlet. |
| Snouwaert, E., and T. Stuart, 2015. North Fork Palouse River Dissolved Oxygen and pH Total Maximum Daily Load Water Quality Improvement Report and Implementation Plan. Department of Ecology State of Washington. Publication No. 15-10-029 Part 1 (July). | North Fork Palouse River, Washington | River | The North Fork Palouse River lies north of the confluence with the South Fork Palouse River at Colfax, in southeastern Washington. The upper part of the watershed lies in western Idaho, beyond Potlatch, Idaho. | July 1 – August 31, 2007; September 1 – September 19, 2012; September 20 – September 30, 1987. |
| Tetra Tech, 2009. New River QUAL2K Water Quality Model for the New River Dissolved Oxygen TMDL. Prepared for U.S. EPA Region 9 and California Regional Water Quality Control Board Colorado River Basin Region. | New River, southern California/Mexico border (drains into Salton Sea) | River | Heavily polluted (unnatural) river composed primarily of agricultural runoff, industrial wastewater, and municipal discharge. | Calibrated to single 07/16/2006 sampling event (1 headwater and 17 tributary/WWTP sites). |

| Citation | Study Location | Type of Waterbody | Watershed Characteristics | Calibration period |
|--|--|-------------------------------|---|--|
| Turner, D., B. Kasper, P. Heberling, B. Lindberg, M. Wiltsey, G. Arnold, and R. Michie, 2006. Umpqua Basin Total Maximum Daily Load (TMDL) and Water Quality Management Plan (WQMP). Oregon Department of Environmental Quality. | Impaired streams in the Umpqua Basin in southwestern Oregon: Calapooya, Elk, Jackson, and Steamboat creeks | Streams in forested watershed | Basin is about 3.24 million acres. It is 90% forestland. Includes fisheries, recreational uses, and forestry. | Calibrated to synoptic surveys: Calapooya: July 24, 2002. Elk: September 25, 2002 Jackson: August 26-29, 2002 Steamboat: August 9, 2000. |
| Turner, D., G. Pelletier, and B. Kasper, 2009. Dissolved Oxygen and pH Modeling of a Periphyton Dominated, Nutrient Enriched River. <i>Journal of Environmental Engineering</i> . 135(8). 645-655. | South Umpqua River, southwestern Oregon | River | High elevation forest/mountains; lowland agriculture and urban development | Two models calibrated and compared for 1991 and 2004 sampling seasons. |
| von Stackelberg, N. O., and B. T. Neilson, 2012. Collaborative Approach to Calibration of a Riverine Water Quality Model. <i>Journal of Water Resources Planning and Management</i> . 140.3: 393-405. | Jordan River, Utah | River | 83 km from Utah Lake to Great Salt Lake. | Water surveys were performed for 3-day periods in October 2006, February 2007, September 2007, August 2009. |

Basin sizes range from about 58 km² to thousands of km². One study (Turner et al., 2006; citation in Table 16) developed models for four waterways within a larger basin (13,112 km²). Land uses range from heavily forested to more varied land uses, and the rivers in these sources receive inputs from nonpoint (e.g., agricultural runoff) and point (e.g., wastewater treatment plant effluents) sources. Details on study locations, watershed characteristics, and environmental conditions were provided in Table 16. The resulting ranges of rates and constants are shown in Table 17 through 20. Default rates and constants shown in Tables 17 through 20 were provided directly to the project team by Greg Pelletier, developer of the QUAL2Kw model.

Summary Statistics for Rates and Constants

Table 17. QUAL2K and QUAL2Kw Rates and Constants: Nutrient Parameters

| Nutrient Parameter | Count | Min | Max | Median | Units | Default Value |
|--|-------|-------|------|--------|---------------------------------------|---------------|
| C:N:P | 19 | N/A | N/A | N/A | gC:gN:gP | 40:7.2:1 |
| Denitrification rate | 23 | 0 | 1.9 | 1 | day ⁻¹ | 0.1 |
| Denitrification rate T correction | 15 | 1.044 | 1.07 | 1.07 | – | 1.07 |
| Inorganic P sediment oxygen attenuation half saturation constant | 3 | 1.56 | 1.97 | 1.77 | Mg O ₂ /L | 1 |
| Inorganic P settling velocity | 16 | 0 | 2 | 0.8855 | m/d | 0.8 |
| Nitrification rate | 23 | 0.01 | 10 | 2.5 | day ⁻¹ | 0.08 |
| Nitrification rate T correction | 15 | 1.01 | 1.08 | 1.07 | – | 1.07 |
| Organic N hydrolysis | 20 | 0.001 | 4.3 | 0.2 | day ⁻¹ | 0.015 |
| Organic N hydrolysis T correction | 15 | 1.05 | 1.08 | 1.07 | – | 1.07 |
| Organic N settling velocity | 16 | 0 | 1.8 | 0.11 | m/d | 0.0005 |
| Organic P hydrolysis | 23 | 0.001 | 4.2 | 0.43 | day ⁻¹ | 0.03 |
| Organic P hydrolysis T correction | 15 | 1 | 1.07 | 1.07 | – | 1.07 |
| Organic P settling velocity | 14 | 0.003 | 1.8 | 0.1 | m/d | 0.001 |
| Prescribed inorganic phosphorus flux | 2 | 0 | 100 | 50 | mg P/m ² /d | – |
| Prescribed NH ₄ flux | 2 | 0 | 500 | 250 | mg NH ₄ /m ² /d | – |

Table 18. QUAL2K and QUAL2Kw Rates and Constants: Oxygen Parameters

| Oxygen Parameter | Count | Min | Max | Median | Units | Default Value |
|---|-------|----------|--------|--------|-----------------------|---------------|
| Slow CBOD oxidation rate | 2 | 0.000001 | 0.001 | 0.001 | day ⁻¹ | – |
| Slow CBOD oxidation rate T correction | 2 | 1.014 | 1.047 | 1.031 | – | 1.024 |
| Fast CBOD oxidation rate | 20 | 0.016 | 4.3 | 2.5 | day ⁻¹ | 0.05 – 0.3 |
| Fast CBOD oxidation rate T correction | 12 | 1.047 | 1.05 | 1.047 | – | 1.047 |
| Oxygen enhance parameter bottom algae respiration | 10 | 0.6 | 0.6 | 0.6 | L/mg O ₂ | 0.6 |
| Oxygen enhance parameter denitrification | 10 | 0.6 | 0.6 | 0.6 | L/mg O ₂ | 0.6 |
| Oxygen for carbon oxidation | 10 | 2.67 | 2.69 | 2.69 | g O ₂ /g C | 2.69 |
| Oxygen for nitrification | 9 | 4.57 | 4.57 | 4.57 | g O ₂ /g N | 4.57 |
| Oxygen inhibition parameter CBOD oxidation | 10 | 0.6 | 0.6 | 0.6 | L/mg O ₂ | 0.6 |
| Oxygen inhibition parameter nitrification | 10 | 0.6 | 0.6 | 0.6 | L/mg O ₂ | 0.6 |
| Oxygen inhibition parameter phytoplankton respiration | 9 | 0.6 | 0.6 | 0.6 | L/mg O ₂ | 0.6 |
| Reaeration model T correction | 10 | 1.024 | 1.05 | 1.024 | – | 1.024 |
| Slow CBOD hydrolysis rate | 16 | 0 | 3.9988 | 0.817 | day ⁻¹ | 0 |
| Slow CBOD hydrolysis rate T correction | 12 | 1 | 1.07 | 1.047 | – | 1.047 |
| Slow CBOD oxidation rate | 14 | 0 | 5 | 0.200 | day ⁻¹ | 0 |
| Slow CBOD oxidation rate T correction | 6 | 1.047 | 1.047 | 1.047 | – | 1.047 |

Table 19. QUAL2K and QUAL2Kw Rates and Constants: Algae Parameters

| Group | Algae Parameter | Count | Min | Max | Median | Units* | Default Value |
|--------------|---------------------------------------|-------|---------|---------|----------|------------------------|---------------|
| Bottom algae | Ammonia preference | 20 | 1.2 | 84 | 25 | µg N/L | 25 |
| Bottom algae | Basal respiration rate | 22 | 0.007 | 1.2 | 0.2 | day ⁻¹ | 0.2 |
| Bottom algae | Bottom algae coverage | 2 | 0 | 100 | 50 | % | – |
| Bottom algae | C:Chl-a | 5 | N/A | N/A | N/A | gC:gChl-a | 40:1 |
| Bottom algae | C:N:P | 4 | N/A | N/A | N/A | gC:gN:gP | 40:7.2:1 |
| Bottom algae | Death rate | 22 | 0.00095 | 1 | 0.3 | day ⁻¹ | 0.1 |
| Bottom algae | Death rate T correction | 8 | 1.05 | 1.07 | 1.07 | – | 1.07 |
| Bottom algae | Dry Weight | 4 | 100 | 100 | 100 | mg D | 100 |
| Bottom algae | Excretion rate | 20 | 0 | 0.48 | 0.20 | day ⁻¹ | 0.02 |
| Bottom algae | Excretion rate T correction | 8 | 1 | 1.07 | 1.07 | – | 1.07 |
| Bottom algae | External nitrogen half sat constant | 24 | 15 | 493 | 206 | µg N/L | 300 |
| Bottom algae | External phosphorus half sat constant | 24 | 2.9 | 178 | 74 | µg P/L | 100 |
| Bottom algae | First-order model carrying capacity | 3 | 77 | 300 | 200 | g D/m ² | – |
| Bottom algae | First-order model carrying capacity | 8 | 1000 | 1000 | 1000 | mg A/m ² | 1000 |
| Bottom algae | Growth rate temperature correction | 10 | 1.004 | 1.08 | 1.07 | – | 1.07 |
| Bottom algae | Inorganic carbon half sat constant | 20 | 0 | 0.00013 | 0.000013 | moles/L | 0.000013 |
| Bottom algae | Internal nitrogen half sat ratio | 20 | 0.9 | 9 | 2.2 | – | 0.9 |
| Bottom algae | Internal phosphorus half sat ratio | 20 | 0.09 | 4.6 | 1.4 | – | 0.13 |
| Bottom algae | Light constant | 20 | 1.7 | 100 | 59 | langleys/d | 100 |
| Bottom algae | Maximum growth rate | 11 | 1.3 | 100 | 15 | g D/m ² /d | – |
| Bottom algae | Maximum growth rate | 13 | 50 | 500 | 350 | mg A/m ² /d | 200 |

| Group | Algae Parameter | Count | Min | Max | Median | Units* | Default Value |
|---------------|---|-------|-------|------|--------|-------------------|---------------|
| Bottom algae | Maximum uptake rate for nitrogen | 9 | 100 | 720 | 364 | mg N/gD/d | – |
| Bottom algae | Maximum uptake rate for nitrogen | 13 | 2.8 | 226 | 72 | mg N/mg A/d | 72 |
| Bottom algae | Maximum uptake rate for phosphorus | 9 | 50 | 200 | 100 | mg P/gD/d | – |
| Bottom algae | Maximum uptake rate for phosphorus | 13 | 0.4 | 490 | 10 | mg P/mg A/d | 5 |
| Bottom algae | Nitrogen uptake water column fraction | 4 | 1 | 1 | 1 | – | 1 |
| Bottom algae | Phosphorus uptake water column fraction | 4 | 1 | 1 | 1 | – | 1 |
| Bottom algae | Photo-respiration rate parameter | 3 | 0.3 | 0.6 | 0.6 | – | – |
| Bottom algae | Respiration rate temperature correction | 10 | 1 | 1.07 | 1.07 | – | 1.07 |
| Bottom algae | Subsistence quota for nitrogen | 8 | 7.2 | 72 | 7.4 | mg N/g D | – |
| Bottom algae | Subsistence quota for nitrogen | 14 | 0.3 | 7.0 | 2.9 | mg N/mg A | 0.72 |
| Bottom algae | Subsistence quota for phosphorus | 8 | 1 | 10 | 2.9 | mg P/g D | – |
| Bottom algae | Subsistence quota for phosphorus | 14 | 0.013 | 7.2 | 0.37 | mg P/mg A | 0.1 |
| Phytoplankton | Ammonia preference | 16 | 20 | 80 | 25 | μg N/L | 25 |
| Phytoplankton | C:Chl-a | 21 | N/A | N/A | N/A | gC:gChl-a | 40:1 |
| Phytoplankton | C:N:P | 5 | N/A | N/A | N/A | gC:gN:gP | 40:7.2:1 |
| Phytoplankton | Death rate | 19 | 0 | 0.59 | 0.05 | day ⁻¹ | 0 |
| Phytoplankton | Death rate temperature correction | 14 | 1 | 1.07 | 1.07 | – | 1.07 |
| Phytoplankton | Dry weight | 1 | 107 | 107 | 107 | g D | 100 |
| Phytoplankton | Excretion rate | 5 | 0 | 0.1 | 0.05 | day ⁻¹ | 0.3 |
| Phytoplankton | Excretion rate temperature correction | 5 | 1.07 | 1.07 | 1.07 | – | 1.07 |
| Phytoplankton | External nitrogen half sat constant | 16 | 13 | 50 | 15 | μg N/L | 15 |
| Phytoplankton | Phosphorus half sat constant | 17 | 0 | 30 | 2 | μg P/L | 2 |

| Group | Algae Parameter | Count | Min | Max | Median | Units* | Default Value |
|---------------|---|-------|-------|--------|----------|-------------------|---------------|
| Phytoplankton | Growth rate temperature correction | 14 | 1.001 | 1.07 | 1.07 | – | 1.07 |
| Phytoplankton | Inorganic carbon half sat constant | 16 | 0 | 0.0011 | 0.000013 | moles/L | 0.000013 |
| Phytoplankton | Internal nitrogen half sat ratio | 7 | 2.5 | 9 | 9 | – | 9 |
| Phytoplankton | Internal phosphorus half sat ratio | 7 | 0.05 | 4.4 | 1.3 | – | 1.3 |
| Phytoplankton | Light constant | 18 | 35 | 100 | 58 | langleys/d | 57.6 |
| Phytoplankton | Maximum growth rate | 19 | 0.2 | 4.1 | 2.5 | day ⁻¹ | 2.5 |
| Phytoplankton | Maximum uptake rate for nitrogen | 6 | 447 | 1333 | 720 | mg N/g D/d | 720 |
| Phytoplankton | Maximum uptake rate for nitrogen | 2 | 40 | 40 | 40 | mg N/mg A/d | – |
| Phytoplankton | Maximum uptake rate for phosphorus | 6 | 100 | 169 | 100 | mg P/g D/d | 100 |
| Phytoplankton | Maximum uptake rate for phosphorus | 2 | 27 | 27 | 27 | mg P/mg A/d | – |
| Phytoplankton | Respiration rate | 19 | 0.015 | 0.7 | 0.1 | day ⁻¹ | 0.1 |
| Phytoplankton | Respiration rate temperature correction | 15 | 1 | 1.07 | 1.07 | – | 1.07 |
| Phytoplankton | Settling velocity | 19 | 0 | 2 | 0.15 | m/d | 0.15 |
| Phytoplankton | Subsistence quota for nitrogen | 2 | 2.5 | 2.5 | 2.5 | mg N/mg A | 0 |
| Phytoplankton | Subsistence quota for phosphorus | 2 | 0.1 | 0.1 | 0.1 | mg P/mg A | 0 |
| Phytoplankton | Subsistence Quota of Intracellular N | 4 | 7.2 | 7.2 | 7.2 | mg N/g D | 7.2 |
| Phytoplankton | Subsistence Quota of Intracellular P | 4 | 1 | 1 | 1 | mg P/g D | 1 |

* Depending on the model version, algal parameters and rates may be expressed relative to grams of dry weight biomass (g D) or relative to mg of chlorophyll a (mg A).

Table 20. QUAL2K and QUAL2Kw Rates and Constants: Sediment, Detritus, and Biofilm Parameters

| Sediment/Detritus/Biofilm Parameter | Count | Min | Max | Median | Units | Default Value |
|---|-------|----------|-------|--------|-------------------------------------|---------------|
| Ammonia preference | 1 | 25 | 25 | 25 | µg N/L | – |
| Biofilm growth rate temperature correction | 1 | 1.047 | 1.047 | 1.047 | – | – |
| Carrying capacity | 1 | 100 | 100 | 100 | g D/m ² | – |
| Death rate | 1 | 0.05 | 0.05 | 0.05 | day ⁻¹ | – |
| Death rate T correction | 1 | 1.07 | 1.07 | 1.07 | – | – |
| Detritus dissolution rate | 22 | 0.001 | 5 | 0.63 | day ⁻¹ | 0.23 |
| Detritus settling velocity | 21 | 0 | 4.8 | 0.5 | m/d | 1 |
| Detritus dissolution rate T correction | 14 | 1 | 1.07 | 1.07 | – | 1.07 |
| External nitrogen half sat constant | 1 | 15 | 15 | 15 | µg N/L | – |
| External phosphorus half sat constant | 1 | 2 | 2 | 2 | µg P/L | – |
| Fast CBOD half sat | 1 | 0.5 | 0.5 | 0.5 | mg O ₂ /L | – |
| Fraction of dissolution to fast CBOD | 1 | 1 | 1 | 1 | – | 1 |
| Inorganic suspended sediment settling velocity | 15 | 0.000001 | 1.9 | 0.61 | m/d | 0.1 |
| Max biofilm growth rate | 1 | 5 | 5 | 5 | g O ₂ /m ² /d | – |
| Oxygen inhibition parameter | 1 | 0.6 | 0.6 | 0.6 | L/mg O ₂ | 0.6 |
| Prescribed SOD | 2 | 0 | 0 | 0 | g O ₂ /m ² /d | – |
| Respiration rate | 1 | 0.2 | 0.2 | 0.2 | day ⁻¹ | – |
| Respiration rate T correction | 1 | 1.07 | 1.07 | 1.07 | – | – |
| Sed denitrification transfer coefficient | 20 | 0 | 0.95 | 0.21 | m/d | – |
| Sed denitrification transfer coefficient T correction | 14 | 1.042 | 1.07 | 1.07 | – | – |
| Sed P oxygen attenuation half sat constant | 15 | 0 | 2.0 | 1.4 | mg O ₂ /L | 1 |

| Sediment/Detritus/Biofilm Parameter | Count | Min | Max | Median | Units | Default Value |
|-------------------------------------|-------|------|------|--------|-------------------------------------|---------------|
| Sediment N flux | 2 | 0.8 | 100 | 50 | mg N/m ² /d | – |
| Sediment oxygen demand | 4 | 0 | 10 | 2.3 | g O ₂ /m ² /d | – |
| Sediment P flux | 2 | 0 | 0.9 | 0.45 | mg P/m ² /d | – |
| Temp correction | 1 | 1.05 | 1.05 | 1.05 | – | – |

Calibration Data and Approaches

There was a wide range of calibration periods for the Q2K applications, with some studies utilizing one or two sampling events, and others utilizing more than 10. Generally, the timing of sampling events appears to be most often targeted towards the dry or low flow season, which is consistent with the application of Q2K as a steady-state model. No distinctions were made between Q2K and Q2Kw in the parameter value tables that accompany this report. In some cases, applications of Q2Kw are likely to apply the non-uniform kinematic wave function that distinguishes Q2Kw from Q2K, as well as the autocalibration feature in Q2Kw. Calibration is most accurate when using data collected during the most likely steady-state condition (i.e., baseflow).

Autocalibration of parameters using the genetic algorithm in QUALK2Kw was used by eight studies. Three studies followed autocalibration with manual calibration for at least some parameters. Others began with the model default or literature values and used the autocalibration process to generate final parameters. Manual calibration starting with model default or literature values was done by five studies. Three studies used experimental or literature values for calibration. Some studies used more than one calibration approach for the various parameters.

5. Variation in Model Coefficients

The biggest variations in model coefficients can be found in phytoplankton growth rates and nutrient recycle rates. Certainly, there is much information in the literature concerning algal growth rates, both for individual species (often related to harmful algal blooms such as freshwater *Microcystis*, *Anabaena*, and other cyanobacteria or blue-greens, and marine dinoflagellates such as *Alexandrium*, *Prorocentrum*, etc.) and taxonomic groups (such as diatoms, greens, dinoflagellates, cyanobacteria, etc.). However, it is important to recognize that individual phytoplankton taxonomic groups, as well as individual species, may be present on an episodic basis; i.e., residing for several days to several weeks, and the reasons for these short-term blooms and crashes are not fully understood. Furthermore, phytoplankton spatial and temporal heterogeneity or patchiness in large lake, reservoir, or estuarine systems can be related to flood or storm events, vertical velocities associated with wind-induced stress or Ekman-type upwelling, aggregation of phytoplankton along tidal fronts when river flow and tides are in opposite direction, or lake seiche driven upwelling or coastal upwelling of nutrient-rich waters associated with local-winds or mesoscale eddies. This patchy behavior is extremely difficult to simulate with current hydrodynamic and water quality models.

It is also important to recognize that monitoring or sampling programs are often at temporal and spatial scales that are inconsistent with patch dynamics as opposed to more region-wide algal growth. Furthermore, in attempting to model phytoplankton biomass, modelers are often limited to datasets that contain only chlorophyll a as an indicator of biomass. As has been shown in the literature, phytoplankton carbon to chlorophyll a ratios vary as a function of temperature, light, and nutrient limitation (Chalup and Laws, 1990, Geider et al., 1997, Finenko et al., 2003). Therefore, given these factors that can contribute to the spatial and temporal variability of phytoplankton biomass, it is not surprising that phytoplankton growth rates used in modeling studies can vary so much from site to site and from application to application. This natural variability is also the reason that it is recommended to

use multi-year data sets to calibrate eutrophication models when data are available and this level of model development is feasible under a project budget and schedule.

The other set of model coefficients that show considerable variation are nutrient recycle rates. While the project team was able to find and report on the range of RCK values used in the modeling studies, it was difficult to find information in the literature that described empirical studies where rates of reaction were reported for nutrient hydrolysis (particulate organic matter conversion to dissolved organic matter) or mineralization (dissolved organic matter conversion to its inorganic form). Therefore, these rate coefficients tend to be treated as a “freely tunable” calibration parameter. It is also important to recognize that there is a wide range in the “reactivity” of organic matter (Eckenfelder, 1970, Middleburg, 1989, Ogawa et al., 2011). Discharges from CSOs tend to have very high reaction rates, while oceanic organic matter has very low reaction rates; organic matter associated with phytoplankton production has intermediate reaction rates. Therefore, it is not surprising that these coefficients vary across sites and model applications. In addition, with the development of the SFM, water quality modeling codes (CE-QUAL-W2 [Section 4.2], CE-QUAL-ICM [Cerco and Cole, 1994], RCA [HydroQual, 2004]) have started to differentiate between different forms of organic matter (particulate versus dissolved) and various pools of reactivity (labile and refractory) (Cole and Wells, 2015; Cerco, 1994, 2004; HydroQual, 1991, 2000). Although the current version of WASP does not consider various pools of reactivity for organic nitrogen and phosphorus, WASP does permit the modeler to utilize up to three pools of CBOD. Since it is possible that future releases of WASP will be expanded to include labile and refractory organic nutrient pools, the project team decided to include RCK values from model applications where labile and refractory organic matter (C, N, P) were used in conjunction with the SFM.

6. Conclusions

Significant improvements have been made to the water quality models WASP, CE-QUAL-W2, HSPF, Q2K and Q2Kw since 1985 including additional simulation capacity for multiple algal groups (both suspended and benthic), and changes in the way the models represent interactions between the water column and bed sediments. WASP, CE-QUAL-W2, and Q2Kw have incorporated complete sediment diagenesis models that account for deposition of organic matter, diagenesis of organic matter in sediments, and flux of end-products back to the water column. HSPF and Q2K have implemented more robust simulations of sediment–nutrient interactions and sediment–water fluxes without adding a complete sediment diagenesis module. There have also been major improvements to the models’ treatment of anoxic/hypoxic conditions, with all models incorporating nitrification and denitrification in the water column and sediments as a function of oxygenation.

Model updates have generally focused on increasing the ability of the models to differentiate between reactive and recalcitrant forms of organic matter, in particular organic nitrogen and organic phosphorus, and incorporating this differentiation into algal growth, respiration, and mortality calculations. The addition of multiple phytoplankton groups requires RCK parameters related to growth and respiration as a function of temperature, nutrient limitation, stoichiometry, and settling. Therefore, the models were updated to allow the user to specify temperature optimum curves for algal growth, respiration, excretion, and death rates, or at a minimum, to specify temperature corrections that include upper and lower temperature limits. The incorporation of more robust sediment–nutrient interaction simulations

or full sediment diagenesis nutrient flux models allows the water quality models to simulate the impact of sediment flux on algal growth and water quality in general.

Other more general model changes include computational improvements since 1985, such as the addition of a genetic algorithm for auto-calibration of RCK parameters available in Q2Kw. Specific model additions and changes post-1985 are presented in Table 21.

Table 21. Model Additions and Changes since 1985

| Model | Water Quality State Variables | Sediment Simulation | Other Changes |
|------------|--|--|--|
| WASP | <ul style="list-style-type: none"> Multiple phytoplankton groups Dissolved organic nitrogen Detrital organic carbon 3 types of CBOD Biogenic and dissolved silica Benthic algal model Macrophytes pH-alkalinity model Water temperature | Sediment diagenesis nutrient flux model (SFM) | <ul style="list-style-type: none"> User-defined temperature optimum curves for algal rates Stream/River Transport Algorithms (kinematic and dynamic wave) Hydraulics of weirs Predictive water column light model |
| CE-QUAL-W2 | <ul style="list-style-type: none"> Multiple phytoplankton groups Multiple macrophyte, epiphyte, and zooplankton groups Nitrification and denitrification Decay of sediments, DOM, POM CBOD, BOD-N, BOD-P New reaeration formulations specific to rivers, lakes and reservoirs, estuaries, and aeration over spillways Photo-degradation N₂ gas for TDG simulation CH₄, SO₄, H₂S, reduced and oxidized forms of Fe and Mn Non-conservative alkalinity | Sediment diagenesis nutrient flux model (SFM) in production (in current beta version) | <ul style="list-style-type: none"> Variable stoichiometry allowed (previously fixed stoichiometric constants for C:N:P) Fish habitat analysis Particle transport Hypolimnetic aeration Dynamic shading computation |
| QUAL2K(w) | <ul style="list-style-type: none"> CBOD speciation Explicit simulation of attached bottom algae Light extinction parameter pH simulation (as a function of alkalinity and TOC simulations) Pathogens Denitrification at low DO Reach-specific kinetic parameters | Sediment–water fluxes of DO and nutrients simulated internally (Q2K); Sediment diagenesis nutrient flux model (SFM) (Q2Kw) | <ul style="list-style-type: none"> Hydraulics of weirs and waterfalls (for gas transfer modeling) New model segmentation protocol Genetic algorithm for auto-calibration Monte Carlo simulation Transient storage zones Computation of evaporation |

| Model | Water Quality State Variables | Sediment Simulation | Other Changes |
|-------|--|---|---|
| HSPF | <ul style="list-style-type: none"> • Simulation of up to 4 algal types • Nitrification and denitrification as water column processes • New state variables for phosphate and ammonium in suspended and bed sediment | Sediment–nutrient interaction simulation (adsorption and desorption of P and N) | <ul style="list-style-type: none"> • Wetlands and shallow water-table hydrology • Irrigation capabilities • Alternative simplified snow algorithms • BMP and REPORT modules |

For all models, many of the model applications were conducted by state and federal agencies such as USGS, USACE, and state environmental agencies. In addition, the models have also been used by academic researchers nationally and internationally. It is very important for model practitioners to use defensible parameter values for TMDLs and other regulatory and planning purposes. There is a potential for misuse if model practitioners utilize abbreviated and incomplete model parameter tables without a complete understanding of antecedent environmental conditions for the model application, geographic scale and applicability, and other relevant study-specific information, as well as specific limitations acknowledged by the model practitioner. Although the quality criteria review for this study disqualified papers with no discussion of model setup and input data, some literature did report abbreviated lists of parameter values. It is the responsibility of the modeler to assess the relevance of specific values before use and to document all values.

There are some differences in the availability of model parameter values in the literature depending on the model. Many of the WASP, CE-QUAL-W2, Q2K, and Q2Kw studies were conducted by federal and state agencies with complete, publicly available reports, making the identification and extraction of RCK parameter values relatively easy for these models. It is also standard reporting practice for some federal and state agencies to include tables of calibrated model parameters for these models. In many cases, these reports contained complete parameter tables as well as abundant supporting hydrologic, environmental, climatic, and sampling information. Access to the full input sequences and metadata allows a motivated modeler to discern the importance of hydroclimatic, hydrographic, physical, chemical, and biotic model parameter values in relation to each other. The approach of presenting full and complete metadata and parameter value tables may allow a modeler to develop more defensible parameter values compared to using abbreviated tables from peer-reviewed journal papers.

Although HSPF is used extensively for TMDL modeling, fewer publicly available reports that contain parameter tables were identified using the search strategy used for this report. The available HSPF literature describes study setup and results; however, some literature sources, especially peer-reviewed journal articles, often include abbreviated parameter tables and minimal amounts of supporting information on environmental setting and model setup. By contrast, the EPA-funded database HSPFParm contains full input sequences and metadata for model applications in more than 70 watersheds in 14 states, which can help prevent model misuse. Many of these applications are runoff and land-surface simulations, but some studies used the receiving waters HSPF module RCHRES, which is the relevant module for this task. Additional full parameter lists for calibrated HSPF models are included in gray literature model calibration reports (e.g., for TMDL studies) that were not identified or selected by the search strategy.

All four models have been used in studies in the United States and internationally, in climates ranging from semi-arid to tropical and in both warm and cool environments. Hydrologic regimes in the areas studied included snowmelt dominated, storm dominated, and monsoonal, although there are few cold-climate applications. It is unlikely that the settings represented in the literature investigated for this task are exhaustive, and therefore do not reflect the full application capabilities of the models.

For QUAL2Kw, WASP, and certain modeling options for HSPF, the use of the model for benthic algae simulation is focused on relatively shallow and clear Western streams. In the case of HSPF, this is a function of the formulations used in the post-1985 benthic algae enhancements, which are optimized for those conditions; the pre-1985 benthic algae formulations for HSPF, which are retained as a modeling option, are more generalized in nature and therefore applicable to a wider range of settings.

It is clear that all of these models are applicable in a variety of climatic conditions and waterbody types. Because the criteria used to select studies disqualified those papers and reports without reported RCK parameter values and without clear documentation of model setup and calibration, the RCK data included in the data tables were extracted from only a small subset of the universe of studies that use these models. Nevertheless, it is possible to identify water quality processes with notable variability in rate values. In general, the largest variation in model coefficients between studies exists in phytoplankton and benthic algae rates, nutrient recycling rates, and nutrient partitioning coefficients.

Monitoring and sampling programs are often inconsistent with phytoplankton growth and death dynamics, likely resulting in difficulties with model calibration. As would be expected, these difficulties result in significant variation from site to site and application to application. Similarly, there is significant site-specific variation in nutrient recycle rates. A problem encountered during the literature review and population of the RCK data tables is that there are very few studies that present empirical information to constrain rates; the majority of RCK parameters included in the studies and the data tables developed for this effort are calibration parameters derived from the model. Future study could focus on constraining rates with empirical data (e.g., laboratory algal growth rates for a variety of species; nitrification rates, etc.). Given the lack of empirical parameter data, the model practitioner must rely on the body of parameters estimated through calibration; these data are presented in the RCK data tables created for this effort.

The largest data gap for all the models involves the data used for calibration. All the models can be calibrated using a limited amount of data (e.g., a single sampling season), but use of limited data can produce a model that is less able to simulate years with different hydrologic and biogeochemical conditions accurately. Due to limited time, funding, and resources, many studies are not able to collect multiple years of data, and studies with relatively short calibration periods were included in the data compiled for this task if the studies presented sufficient documentation, and rates were within reasonable ranges as determined by expert judgment. Although fewer studies calibrate using multiple years of data, it has become increasingly common for model practitioners to revisit existing calibrated models (i.e., calibrated for a specific river) and add additional calibration years as data become available or it becomes clear that the calibrated model cannot accurately simulate water quality for different hydrologic conditions.

Updates and enhancements to these models since 1985 have resulted in new RCK parameters, examples of which should be available to model practitioners. Although the acceptable ranges for many model parameters are still informed by the 1985 Rates Manual, changes to the models since 1985, particularly

for algal simulation and sediment diagenesis/flux, have resulted in additional parameters that are necessary for successful model application. The data tables in this report can serve as a reference for model users and that can be expanded in the future to incorporate additional studies.

7. Future Research Opportunities

In addition to the literature review and parameter value compilation discussed above, the project team considered other aspects of model parameter value compilation during the project including:

- The availability and applicability of empirically derived parameter values;
- Cross-model applicability of parameter values; and,
- Comparison and mapping of similarities and differences between the governing equations for each model.

Information on these topics could augment the parameter value tables that accompany this report. Preliminary considerations related to empirically derived parameter values, cross-model applicability of values, and comparison of similarities and differences of governing equations are briefly noted below as background for potential future research of these topics related to the update of the 1985 Rates Manual.

Empirical Data

We conducted an initial assessment of the feasibility of compiling empirically derived rates in addition to model application parameters, looking first at citations in the original 1985 Rates, Constants, and Kinetics manual. Of the 116 citations in the 1985 manual, a large majority were modeling studies. Many of these modeling studies contained references to rates and other parameters based on laboratory data, but most of the initial rates manual was based on modeling studies, similar to this project.

Following an assessment of the 1985 Rates Manual, the research team investigated the availability of empirical studies related to the Group 1 water quality parameters. In conducting this search, several issues were identified that inhibited a comprehensive assessment of empirical studies and the inclusion of empirical data in the parameter data tables. These issues included:

1. **Presentation of environmental conditions** – The applicability of empirically derived values was a concern given the tight coupling of environmental conditions to algal behavior, nutrient cycling, and sediment diagenesis. Many of the studies evaluated during the preliminary assessment of empirical data presented multiple parameter values across a range of conditions, making it difficult to extract a single parameter value from a report.

The parameter value tables for this project were not designed to include details on the project-specific applicability for a given parameter. For instance, various studies focused on representation of a single algal species and the resulting rates are applicable to the species in question (e.g., some harmful algal bloom (HAB) species, such as *Microcystis* or *Anabaena*), but may not be informative to a modeler who wishes to model an algal functional group such as diatoms, greens, or dinoflagellates. This level of detail is not available in the tables presented herein. Furthermore, studies report diverse types and levels of information, making it difficult to extract the same information on methods and environmental conditions from all sources.

Accurately representing the environmental or laboratory conditions for specific parameter values is necessary, and should be a significant component of potential future projects to identify and compile empirical values.

2. **Identification and Accessibility of Literature** – The preliminary assessment of the availability of empirical parameter values indicated that it would be particularly difficult to assess the applicability of studies based on the results of keyword searches; a comprehensive assessment of empirical studies since 1985 would be a very large undertaking. The limited amount of empirical parameter values proved difficult to find because they represent foundational data that are often not published in peer-reviewed reports. Future research could focus on the identification of the most applicable laboratory and field studies that provide empirically derived parameters.
3. **Selection of appropriate parameters** – It is not possible to determine a value empirically for every parameter listed in the parameter value tables that accompany this document; some parameters are difficult to determine through field or laboratory experiments. Selecting the parameters to investigate in a literature review of empirical studies was difficult given the range of parameters in the models. For example, although there are many studies that provide empirical values for algal parameters (e.g., growth, death, N/P requirements, etc.), it is challenging to determine sediment flux rates in the field due to the sensitivity of sediment diagenesis to environmental conditions such as DO, pH, and temperature, which can vary significantly over a short distance. A comprehensive literature review of empirical studies could potentially identify studies that did investigate the more complex or variable parameters.
4. **Differences between empirical and calibration methods** – The preliminary assessment of empirical data sources indicated significant differences across empirical studies and between empirical studies and model applications. Consistency in methods used to calculate parameters is a factor. For example, a kinetics model for a constituent in an empirical study may not match the method employed by one of the water quality models (e.g., zero order vs. first order kinetics; variable models for algal growth). Similarly, many empirical studies do not report values in the same units as the model applications, requiring careful and complete conversion and standardization of units. Reconciling these differences and presenting metadata to explain the differences will likely take effort and time.

For this report, an empirical data assessment and collection was deferred due to the challenges summarized above. Future identification, assessment, and compilation of empirical parameter values could be conducted and provided as a supplemental table to, and additional context for, those tables of calibrated parameter values produced for this project.

Comparison of Model Kinetic Formulations

During the development of the model-specific parameter value tables that accompany this report, the project team investigated the possibility that the values for certain parameters might be applicable across models. For example, kinetic formulations for processes such as nitrification may be similar and the parameters relevant to more than one model (if units are consistent). To determine the level of consistency in the kinetic formulations across models, a selected subset of governing equations was evaluated to identify parameters that are model-agnostic and those that are model-specific. However,

full cross-model parameter value comparisons are difficult because each model handles kinetic formulations in slightly different ways, including how those formulations are incorporated into the model. It is, therefore, difficult to identify if a parameter is truly held in common between multiple models. In some cases, the governing equations presented in model documentation are not identical to the model code, making it difficult to compare models based on their documentation. The project team determined that, due to the uncertainty in how similar or identical parameters are treated in each model, parameter values should be considered model-specific for the purposes of this project and the associated data tables.

The project team conducted a preliminary comparison of the governing equations for each model and concluded that through this process it might be possible to identify a subset of the parameter values that could be used in multiple models. Subsequent research could initially assess the similarities and differences of governing equations between the different models, with a focus on identification of parameters that can confidently be applied to any of the water quality models. Such an effort would require both an investigation of the governing equations in the model documentation and a detailed assessment of the model code. Important next steps would include extracting as many governing equations as possible and linking them to the parameter data that are presented in the parameter value tables that accompany this report. This could identify parameter values that could be removed from the model-specific tables and used to create a model-agnostic parameter value table to facilitate cross-model applications.

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