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Using Qual2K Modeling to Support Nutrient Criteria Development and Wasteload Analyses in Utah

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A cooperative data collection and modeling effort between the Utah Department of Environmental Quality (Utah DEQ), Division of Water Quality and Utah State University (USU) began in 2010. The primary objectives of this study were to 1) design a data collection approach appropriate to support the population and calibration of QUAL2Kw models for use in a variety of applications; and 2) develop a methodology for populating and calibrating QUAL2Kw given these data. The intended use of the resulting models was to assist in developing numeric nutrient criteria for the state of Utah and provide a starting point for the development of new waste load allocations (WLAs) for 9 water reclamation facilities (WRFs). The objectives were completed by assisting DEQ in collecting the appropriate data in the reaches below WRFs around the state and using these data to populate and calibrate QUAL2Kw models for each of these study sites.

Background

Over the last few years the state of Utah has been working towards understanding the implications of instituting numeric nutrient criteria. To do this they have initiated a publicly owned treatment works (POTW) nutrient removal cost study [*UDEQ*, 2009], an economic evaluation study [*UDEQ*, 2011], and a nutrient criteria ecological study [*UDEQ*, 2010]. The Nutrient Removal Cost Impact Study, completed in 2009, evaluated the economic impacts of potential new nutrient removal requirements for Utah's POTWs. The study estimated economic, financial, and environmental impacts interrelated with a range of potential nutrient discharge standards for every discharging mechanical POTW in the State and one lagoon system [*UDEQ*, 2009]. The economic evaluation study, which is still in progress, is intended to quantify the economic benefits and costs of implementing nutrient criteria for surface waters in Utah [*UDEQ*, 2011].

When investigating nutrient criteria based on the ecological implications, EPA recommends three types of scientifically defensible empirical approaches for establishing numeric thresholds intended to limit nitrogen/phosphorus pollution: reference condition approaches, mechanistic modeling, and stressor-response analysis [*US EPA*, 2010]. The DEQ is currently investigating all three recommended approaches to establish numeric nutrient criteria. In order to complete two of the recommended approaches the DEQ, along with USU, are investigating the ecological impacts of nutrients on Utah waterbodies using both a stressor response approach combined with the predictive capabilities of the mechanistic modeling approach. To do this a data collection strategy was developed to meet the needs of both recommended approaches. By combining the results of the economic study with the predictive capabilities of the modeling efforts and ecological response information, the proposed instream nutrient criteria can be linked to the expected economic costs of the treatment upgrades as well as forecasting the potential impact of nutrient loading on the ecological health of the downstream waterbodies.

This report covers the general approaches taken in the mechanistic modeling portion of the Nutrient Criteria study for data collection, model population, and calibration/validation. However, it is important to note that the data collection approaches and models are intended to have multiple applications and therefore, have been made very generic in order to support: 1) development of statewide numeric nutrient criteria; 2) development of site-specific criteria for rivers and streams where the statewide nutrient criteria do not appear valid; 3) wasteload analyses to determine water quality based effluent limits (WQBEL), and 4) determination of TMDL endpoints. Details regarding the associated ecological measures and reference condition information can be found at http://www.nutrients.utah.gov/nutrient/index.htm.

QUAL2Kw Model

Utah DEQ uses low flow conditions to determine WQBELs for point sources under the Utah Pollution Discharge Elimination System (UPDES) program (*UDEQ*, 2012) due in part to these corresponding with limiting conditions. This led to selecting a model that would be appropriate for these conditions. QUAL2K [*Chapra et al.*, 2004] is a USEPA approved model that has been commonly used in WLAs and total maximum daily loads (TMDLs) (e.g., [*Bischoff et al.*, 2010; *Kardouni and Cristea*, 2006]), and even development of nutrient criteria [*Flynn and Suplee*, 2011]. This quasi-dynamic, one dimensional instream water quality model includes the dominant processes of concern within Utah waters, predicts the required water quality variables, and is feasible to populate and calibrate given the limited data available in most waterbodies of the state. In order to understand the associated daily minimum and maximum instream concentrations, the model provides a 24 hour diel response in water quality given an appropriate or representative 24 hour weather pattern. QUAL2Kw [*Pelletier and Chapra*, 2008], a sister model to QUAL2K developed within the state of Washington, built in additional functionality (e.g., automatic calibration algorithms) into QUAL2K based on their identified needs. With the anticipation of having some similar needs as Washington and the possibility of identifying additional needs, Utah DEQ elected to use QUAL2Kw in their instream modeling applications.

Details regarding the version of QUAL2Kw used in this application (version 5.1) are provided within the user's manual [*Pelletier and Chapra*, 2008] and a number of publications [*Cho and Ha*, 2010; *Kannel et al.*, 2007; *Pelletier et al.*, 2006]. In short, the state variables (Table 1) include the macro nutrients (C, N, and P) of interest and the critical nutrient species (e.g., inorganic P, nitrate, and ammonia) in surface waters.

Using the same notation as that of Table 1, the QUAL2Kw composite or calculated variables are (Pelletier and Chapra, 2008):

Total Organic Carbon (mgC/L):

$$TOC = \frac{c_s + c_f}{r_{oc}} + r_{ca} a_p + r_{cd} m_o \quad \textbf{(1)}$$

Table 1. QUAL2Kw State Variables (taken directly from [*Pelletier and Chapra*, 2008]).

Variable	Symbol	Units*
Conductivity	s_1, s_2	μmhos
Inorganic suspended solids	$m_{i,1}$, $m_{i,2}$	mgD/L
Dissolved oxygen	o_1, o_2	mgO_2/L
Slow-reacting CBOD	$c_{s,1}$, $c_{s,2}$	mg O_2/L
Fast-reacting CBOD	$c_{f,1}$, $c_{f,2}$	mg O_2/L
Organic nitrogen	$n_{o,1}$, $n_{o,2}$	μgN/L
Ammonia nitrogen	$n_{a,1}$, $n_{a,2}$	μgN/L
Nitrate nitrogen	$n_{n,1}$, $n_{n,2}$	μgN/L
Organic phosphorus	$p_{o,1}$, $p_{o,2}$	μgP/L
Inorganic phosphorus	$p_{i,1}$, $p_{i,2}$	μgP/L
Phytoplankton	$a_{p,1}$, $a_{p,2}$	μgA/L
Detritus	$m_{o,1}$, $m_{o,2}$	mgD/L
Pathogen	x_1, x_2	cfu/100 mL
Generic constituent	gen_1, gen_2	user defined
Alkalinity	Alk_1, Alk_2	$mgCaCO_3/L$
Total inorganic carbon	$c_{T,1}$, $c_{T,2}$	mole/L
Bottom algae (a_b in the surface water layer), biofilm of attached heterotrophic bacteria (a_h in the hyporheic sediment zone for the Level 2 option)	a_b,a_h	gD/m^2
Bottom algae nitrogen	IN_b	mgN/m^2
Bottom algae phosphorus	IP_b	mgP/m^2

* mg/L ≡ g/m^3

Total Nitrogen (μgN/L):

$$TN = n_o + n_a + n_n + r_{na} a_p \tag{2}$$

Total Phosphorus (μgP/L):

$$TP = p_o + p_i + r_{pa} a_p \tag{3}$$

Total Kjeldahl Nitrogen (μgN/L):

$$TKN = n_o + n_a + r_{na} a_p \tag{4}$$

Total Suspended Solids (mgD/L):

$$TSS = r_{da} a_p + m_o + m_i \tag{5}$$

Ultimate Carbonaceous BOD (mgO_2/L):

$$CBOD_u = c_s + c_f + r_{oc} r_{ca} a_p + r_{oc} r_{cd} m_o \tag{6}$$

Additionally, the model provides the ability to predict the associated biological effects of various nutrient concentrations since photosynthesis, respiration, and death of phytoplankton and bottom algae are included within the model. As the version of QUAL2Kw applied within this study is quasi-dynamic, it provides the ability to deal with steady flow, but does allow for non-uniform flow. This means that while the flow conditions cannot change over time, they can vary longitudinally downstream due to point or distributed inflows or abstractions.

Given the capabilities of this version of QUAL2Kw, there are environmental conditions that are suited for this type of modeling approach. The time period over which this model should be applied require that 1) stream conditions are completely mixed since the model assumes all model elements are completely mixed, 2) boundary condition concentrations can be approximated by consistent 24 hourly values; 3) distributed flows are constant, 4) point inflows follow a consistent diel pattern or are constant, and 5) weather conditions over the simulation period have a consistent diel pattern.

Study Site Locations

Nine sites were selected for the nutrient criteria ecological study and represent the different types of receiving waterbodies around the state of Utah (Figure 1). Using these sites as a representative sample of the state's waterbodies, the QUAL2Kw, ecological stressor-response, and reference condition findings will be used to extrapolate information regarding possible ranges of nutrient criteria for the remaining state waters [*UDEQ*, 2010]. The selected sites (Table 2) are located within different order streams with varied background water quality, surrounding land uses, and amounts of wastewater effluent that have been treated to different levels. The sections studied were those influenced by WRF effluents since these areas generally have enhanced nutrient loads. More detail regarding each site (e.g., location, study reach length, etc.) are provided in a separate report in preparation by the Division of Water Quality that evaluates structural and functional responses to nutrients. Detailed information about unique sampling requirements associated with each site and the specific information regarding model population, calibration, and validation are provided within the QUAL2K modeling files and site specific model documentation provided to Utah DEQ as project deliverables (see Appendix B for an example).

Figure 1. Study site locations within the state of Utah.

Table 2. Study site locations, water reclamation facilities, and dates sampled within the state of Utah.

Waterbody	Facility	Dates Sampled
Box Elder Creek	Brigham City WRF	Aug. 9 - 11, 2010
San Pitch River	Fairview City WRF	Aug. 2 - 5, 2010 Oct. 11 - 13, 2010
San Pitch River	Moroni City WRF	July 28-30, 2010
Weber River	Oakley City WRF	Aug 23-26, 2010
Price River	Price River Water Improvement District	Aug. 30 - Sep 1, 2010
Dry Creek	Spanish Fork City WRF	July 23 - 26, 2010
Silver Creek	Snyderville Basin-Silver Creek Water Reclamation Facility	July 20 - 22, 2010 Sep. 30 - Oct 4, 2010 Aug 22-30, 2011
Malad River	Tremonton City WRF	Aug. 13 - 16, 2010
Little Bear River	Wellsville Lagoons	Sept 10-13, 2010

Project Results

Since the key objectives in this project were to develop the appropriate data collection methodologies to support QUAL2Kw model population and calibration, this report provides general information regarding the field data requirements, approaches to model population using these data, strategies used in model calibration, and the steps required for model validation (if these data sets exist).

Supporting field data

Data must be collected at 3 general locations for instream modeling. The beginning of the study reach (also called the headwater or upstream boundary condition), inflows/outflows (point sources or tributary inflows and diversions/abstractions), and at least one location downstream for model calibration. The data types required at these locations will vary and are discussed below. For the 2010 data collection efforts, data collection at each location spanned a 2 day period during low flow conditions.

Figure 2 shows a generalized schematic used within the 2010 data collection efforts. Data for the modeling efforts were gathered at Station B (headwater/upstream boundary condition), Station C (wastewater treatment plant effluent before it enters the stream), Station D (at a location where the stream and point source effluent was completely mixed), and Station E (the calibration location downstream at the end of the study reach). Information gathered at Station A was only used in the ecological portion of the study. If a tributary entered the modeling reach, data were also collected at T1. Similarly, if a diversion was present, the quantity of water leaving the system was determined.

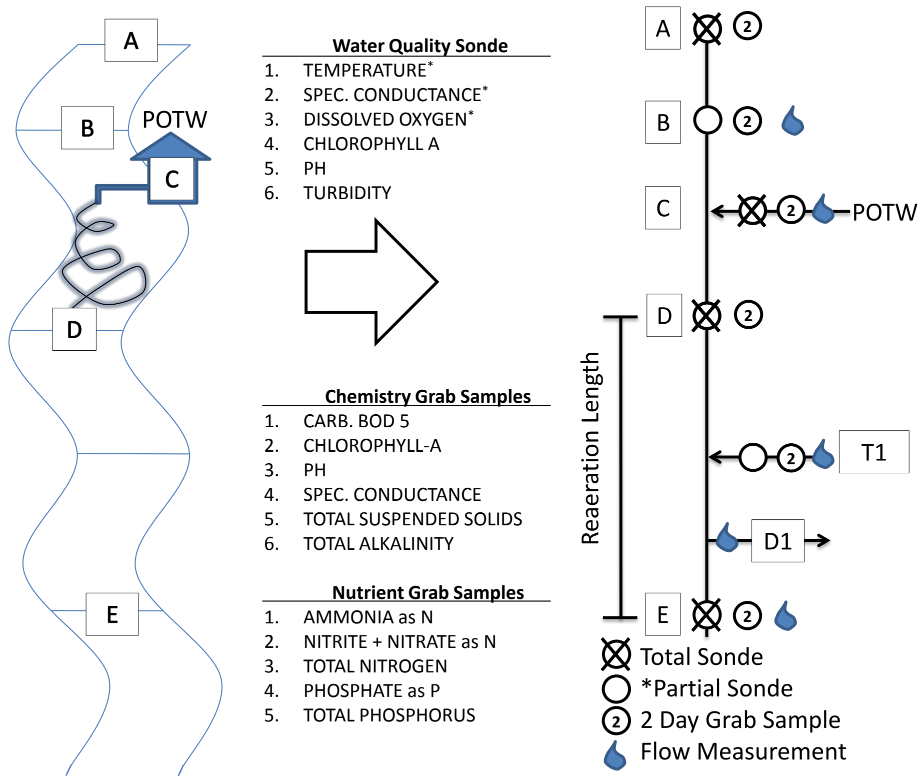

Figure 2. Generalized data collection locations within the 2010 sampling efforts. Required locations of flow measurements and the multi-parameter water quality sondes are also shown. Since 2010 modeling efforts used Station B as the headwater location, the information for chlorophyll-a and pH is taken from Station A.

For the 2010 data collection, the location of the completely mixed conditions downstream of the WRF was determined by measuring specific conductance or temperature across the channel to determine where uniform conditions existed. In some cases where the differences in temperature and/or specific conductance were too small, rhodamine WT was used as a visual indicator. To support and integrate these efforts with the ecological study needs the distance between Station D and E was estimated using methods described in Grace and Imberger [2006] which designate the optimum distance between stations for calculating open water metabolism using the single station method (Eqn. 7).

$$X = 0.693 \cdot \frac{v}{k_a} = \frac{v^{0.33}}{0.0137 \cdot \left(D^{-0.85}\right)} \qquad \textbf{(7)}$$

Where X = optimum station distance (km), v = velocity (cm s^{-1}), D = depth (cm), and k_a = reaeration coefficient for oxygen (d^{-1}). As discussed later, we found this method to result in distances that were in general too short to meet the diverse needs of this study and often times did not include the compliance point for WLAs.

The information necessary at each of these stations is dependent on whether it is the headwater location, a load, or a diversion. Water quality models require an understanding of both the water balance and the mass balances for each constituent modeled. Flow measurements may be required at all stations in order to establish a water balance. Water quality information is not, however, required for diversions or abstractions since the mass loss will be a function of the instream concentrations predicted by the model and the volume of water taken out that is specified by the user.

The specific water quality constituents measured at each station and the frequency they were collected are detailed within Table 3. There are a number of constituents that were measured using multi-parameter sondes (e.g., temperature, dissolved oxygen, conductivity) at five minute increments over each of the two day sampling period. Grab samples of most constituents requiring laboratory analyses were gathered each day and usually in the mid-morning. Benthic algae sampling was only conducted once at some point in time close to the study periods. A number of constituents within this list, indicated by a * in the table, were not sampled directly and had to be estimated. The appropriate values for modeling were estimated using the relationships between measured constituents and model variables as described below. Additional data types that could be collected that would be useful in the modeling include a measure of sediment oxygen demand, total organic carbon, and volatile suspended solids. None of these measures were completed in the 2010 data sets.

Data to characterize each site is additionally necessary to support model population or calibration. Table 4 provides a list of the data types requiring collection, some procedural information, locations where these data are required within or near the site, and the utility of the data in the context of the modeling effort. A number of these data types are collected within routine Utah's Comprehensive Assessment of Stream Ecosystems (UCASE) surveys based on protocols adapted from the USEPA [2007]. It is important to note that all locations where data are collected must have GPS coordinates established for documentation purposes.

Model Population

Once the data have been collected, they must be translated from observations to model inputs. The model state variables (Table 1) can be related to measurements as follows [taken directly from Pelletier and Chapra, 2008]:

$$\text{Conductivity} = s = \text{COND} \tag{8}$$

$$\text{ISS} = m_i = \text{TSS} - \text{VSS or TSS} - r_{dc}\,(\text{TOC} - \text{DOC}) \tag{9}$$

$$\text{Dissolved Oxygen} = o = \text{DO} \tag{10}$$

$$\text{Organic Nitrogen} = n_o = \text{TKN} - \text{NH4} - r_{na}\,\text{CHLA} \quad \text{or} \tag{11}$$

$$n_o = \text{TN} - \text{NO2} - \text{NO3} - \text{NH4} - r_{na}\,\text{CHLA}$$

$$\text{Ammonia Nitrogen} = n_a = \text{NH4} \tag{12}$$

$$\text{Nitrate Nitrogen} = n_n = \text{NO2} + \text{NO3} \tag{13}$$

$$\text{Organic Phosphorus} = p_o = \text{TP} - \text{SRP} - r_{pa}\,\text{CHLA} \tag{14}$$

$$\text{Inorganic Phosphorus} = p_i = \text{SRP} \tag{15}$$

$$\text{Phytoplankton} = a_p = \text{CHLA} \tag{16}$$

Table 3. Water quality constituents sampled and the frequency of sampling for QUAL2Kw modeling.

Multi-Parameter Sonde Data	**Abbreviation/QUAL2Kw Units**	**Frequency**
Water Temperature	Temp (C)	5 min samples
Specific Conductance	COND (mhos)	5 min samples
Dissolved Oxygen	DO (mgO_2/L)	5 min samples
pH	pH	5 min samples
Chlorophyll a	CHLA (gA/L)	5 min samples
Turbidity		5 min samples
Laboratory Analysis		
5-Day Soluble Carbonaceous BOD, sCBOD5		1 each day
Total Nitrogen	TN (gN/L)	1 each day
Ammonia Nitrogen	NH_4 (gN/L)	1 each day
Nitrate+Nitrite Nitrogen	NO_3 (gN/L)	1 each day
Total Phosphorus	TP (gP/L)	1 each day
Soluble Reactive Phosphorus	SRP (gP/L)	1 each day
Volatile Suspended Solids*	VSS (mgD/L)	1 each day
Total Suspended Solids	TSS (mgD/L)	1 each day
Alkalinity	ALK ($mgCaCO_3$/L)	1 each day
Chlorophyll a	CHLA (gA/L)	1 each day
Dissolved Organic Carbon, DOC	DOC (mgC/L)	1 each day
Dissolved Organic Phosphorus, DOP*		1 each day
Dissolved Organic Nitrogen, DON*		1 each day
Benthic Chl-a		1 per sampling time period
Benthic AFDM		1 per sampling time period
Benthic TP		1 per sampling time period
Benthic TN		1 per sampling time period
Benthic TOC		1 per sampling time period
SOD#		1 per sampling time period
TOC#	TOC (mgC/L)	1 each day

* = not gathered or required estimation for QUAL2Kw
# = data that would be useful in model population/calibration but were not directly measured in these efforts

Table 4. Site characterization data types.

Data Type	Procedure	Locations	Reasoning
Average Cross Sectional Velocity*	See methods provided within Data Collection and/or UCASE SOP. Information from HEC-RAS modeling applications can also be extracted to supplement data collected.	Station D, E, and above and below any inflow or outflow. Additional locations along study reach would be beneficial.	Provides observations of velocity in different reaches to compare with the predicted velocities. This can be used with the depth and tracer information to ensure appropriate representation of the hydraulics and reasonable travel times.
Average Cross Sectional Depth*	See methods provided within Data Collection and/or UCASE SOP.	Station D, E, and above and below any inflow or outflow. Additional locations along study reach would be beneficial.	Provides observations of depths in different reaches to compare with the predicted depths. This can be used with the velocity and tracer information to ensure appropriate representation of the hydraulics and reasonable travel times.
Average Channel Bottom Width	Bottom width estimates were calculated using side slope, average depth, and top width values in the formula: Top Width – Depth x 1/tan(radians(°SSLEW)) – Depth x 1/tan(radians (°SSREW)), where width and depth are in meters and side slope is in radians in the form of Run/Rise.	Station D, E, and above and below any inflow or outflow. Additional locations along study reach would be beneficial.	Model input.
Channel Bottom Slope	See methods provided within UCASE SOP.	Should estimate bottom slope from beginning to end of study reach at 10% increments of total reach length and/or when changes in bottom slope are observed.	Model input.
Channel Side Slope	See methods provided within UCASE SOP.	Station D, E, and above and below any inflow or outflow. Additional locations along study reach would be beneficial.	Model input and can be used to calculate bottom width from measured top widths.
Weather data	Onsite weather station or nearest Mesowest Station.	Near study site would be most appropriate and 15-30 minute data are preferred.	Wind speed, air temperature, shortwave solar radiation, humidity/dewpoint temperature are all used within the model as forcing information. Precipitation data shows whether there was significant rainfall in the area that would influence instream flows.
Tracer Study	Inject tracer at Station B or C and measure response at Station E. Can also use HEC-RAS model if available.	Measure tracer response at Station E, but additional locations along the study reach would be beneficial to capture heterogeneity.	Provides information regarding average travel time through system and can be used in calibration of hydraulic parameters (e.g., Manning's roughness coefficient).
Substrate type*	See methods provided within Data Collection and/or UCASE SOP.	Information should be gathered at cross sections in subreaches that represent the variability in substrate types.	Provides a method to approximate the Mannings roughness coefficient and determine fraction of bottom substrate appropriate for bottom algae.
Shading*	See methods provided within Data Collection and/or UCASE SOP.	Information should be gathered at locations that represent the variability in shading.	Model input. If riparian or topographic shading drastically influences instream temperatures, estimates of the shading % for each hour of a day will be necessary to scale the incoming shortwave solar radiation.

Detritus = m_o = VSS – r_{da} CHLA or r_{dc} (TOC – DOC) – r_{da} CHLA **(17)**

pH = PH **(18)**

Alkalinity = Alk = ALK **(19)**

While a number of these relationships are straightforward, it is important to realize that the typical Organic N and Organic P measurement cannot be directly compared to the Organic N and Organic P QUAL2Kw predictions. As shown in equations 11 and 14 above, the QUAL2Kw versions of organic N and P only represent the dissolved and detritus portion of each organic nutrient pool since the portion associated with the live algae are subtracted out. It is also important to note that detritus (Eqn 17) only contributes to the carbon budget and does not influence other nutrient pools.

Given the data available from the 2010 sampling, we needed additional methods based on some assumptions or established equations to calculate the variables necessary for model population and calibration. These included the need to convert $sCBOD_5$ measurements to the sCBOD ultimate values required within QUAL2Kw (Eqn 20).

sCBOD ultimate = c_f or c_s = $sCBOD_5/(1\text{-}exp(\text{-}k_d\ (5days))$ **(20)**

Further, since we did not have direct measures of VSS or ISS in the 2010 data sets, we had to come up with methods and a logic tree to estimate these values for model population (Figure 3).

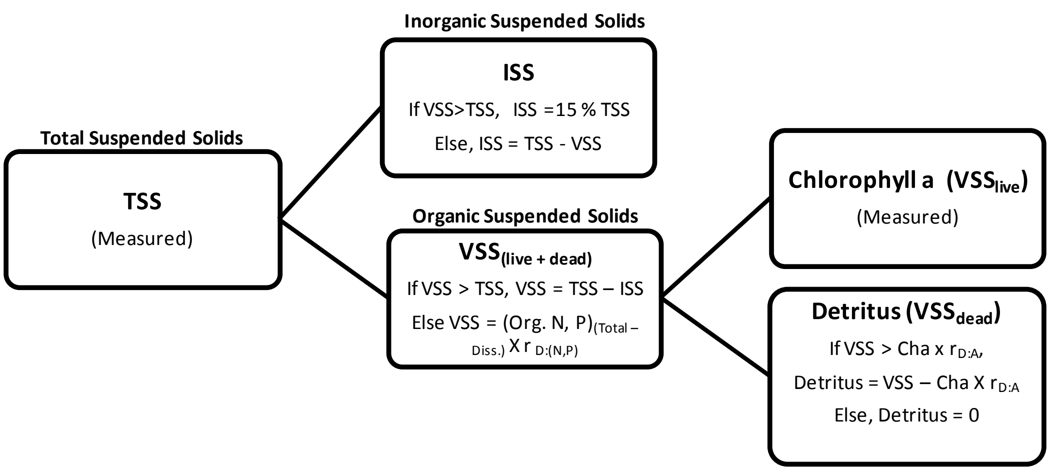

Figure 3. Logic used in estimating VSS and ISS from TSS, followed by logic for estimating detritus from VSS.

To populate the model, information regarding the reach, initial conditions, headwater conditions, weather data, point sources and distributed sources must be provided (Table 5). More specifically, observations from the headwater location and any point flow (inflow or abstraction) or distributed flows must be entered into the model framework. Any flow information provided for these locations must be a representative value for the entire modeling period. The necessary sampling frequency of specific water quality data is dependent upon whether it is a point source or headwater (Table 6). The other forcing data

Table 5. General information required for QUAL2Kw model population.

QUAL2Kw Sheet	Information Required
Reach	
	Reach segmentation
	Hydraulic characteristics
	% suitable substrate
	Bottom algae % cover
	SOD
	Thermal properties
Initial Conditions	
	Constituent concentrations (See Table 6)
Headwater Data	
	Average flow
	Constituent concentrations (See Table 6)
Weather Data (hourly average values)	
	Air temperature
	Dewpoint temperature
	Solar radiation
	Shading
	Cloud cover
	Wind speed
Point Sources	
	Average flow
	Constituent concentrations (See Table 6)
Distributed Sources	
	Average flow
	Constituent concentrations (See Table 6)
Rates	
	Primarily set in calibration. See Model Calibration section below.

Table 6. Model input constituent concentrations requirements and the associated observed data used in population of QUAL2Kw.

		Point Source	**Headwater**	**Distributed Inflow**
Model Parameter	**Data Collected**	Mean + Range/2 or 2 Day Mean	Hourly Average or 2 Day Mean	Average
Alkalinity	Total Alkalinity	X	X	X
$sCBOD_{ultimate}$	$sCBOD_5$	X	X	X
Specific Conductivity	Specific Conductivity	X	X	X
Detritus (POM)	(Org - Diss. N, P) X r(POM/N, P)	X	X	X
Dissolved Oxygen	Dissolved Oxygen	X	X	X
Inorganic Phosphorus (SRP)	Inorganic Phosphorus (SRP)	X	X	X
Inorganic Solids	TSS - VSS	X	X	X
NH_4-Nitrogen	NH_4-Nitrogen	X	X	X
NO_3-Nitrogen	NO_3-Nitrogen	X	X	X
Organic Nitrogen	TN - (NH_4) - (NO_3 + NO_2)	X	X	X
Organic Phosphorus	TP - Inorg P	X	X	X
pH	pH	X	X	X
Phytoplankton	Chlorophyll a	X	X	X
Water Temperature	Water Temperature	X	X	X

required by the model is meteorological information which includes hourly average air temperatures, wind speeds, and dewpoint temperatures from a nearby, representative weather station. Shortwave solar radiation can be estimated automatically within the modeling framework, however, if using these estimates, hourly cloud cover values would be required. In the 2010 modeling efforts, we instead used actual shortwave radiation observations from a local source.

When populating the models, censored data, or concentrations that are below the analytical detection limits (i.e., non-detects) commonly occur. Within the 2010 modeling, non-detects were assigned a concentration of half of the detection limit. More accurate statistical analysis of limited amounts of censored data should be investigated. The detection limits associated with key parameters are detailed within Table 7.

Table 7. Detection limits for constituents based on the procedures applied within specific laboratories.

Constituent	Laboratory	Analytical Detection Limit (mg/L)
TN, TP	Baker Lab – USU	0.0057
TDN, TDP	Baker Lab – USU	0.0025
NO_3+NO_2 -N	Baker Lab – USU	0.0006
NH_4 -N	Baker Lab – USU	0.00395
PO_4 -P	Baker Lab – USU	0.0008
$sCBOD_5$	Utah DEQ Laboratory/AWAL	3/5
Chlorophyll a	Utah DEQ Laboratory	0.0007
Specific Conductance	Utah DEQ Laboratory	2 (uS/cm)
Total Suspended Solids	Utah DEQ Laboratory	4
Total Dissolved Solids (180 °C)	Utah DEQ Laboratory	10
Turbidity	Utah DEQ Laboratory	0.1 (NTU)

To assist in ensuring model population consistency given the relatively consistent data collection strategies implemented in 2010, we developed two supporting sheets within the QUAL2Kw files delivered to DEQ. A "Data Input" and "Addt Info" sheet provides a number of tables that can be populated with observations, and this information automatically populates the QUAL2Kw sheets. Further, these sheets facilitate some of the additional calculations that were completed and suggested in future applications (described further below). Information regarding these features is included within Appendix A.

Most information within the Rates Sheet was not changed at all or was adjusted in model calibration (described further below). However, specific values of some parameters were established within the 2010 modeling efforts that may be appropriate for other Utah model applications. First, we measured CBOD decomposition rates (k_d) by taking 6 samples from the Silver Creek WRF effluent. These samples were analyzed in triplicate resulting in 18 total measurements of 30 day CBOD using methods detailed in Environmental Protection Division [1989]. The resulting data were analyzed using a Nonlinear Least Squares Method and the Thomas Method (Table 8). Given that Chapra [1997] reports values ranging 0.05-0.1 d^{-1} at 20°C for waste streams treated using activated sludge, we assumed the average value of 0.103 d^{-1} was an appropriate value for all the 2010 study sites and this value was not varied in calibration. Further, this value was used to convert any measured concentrations of $sCBOD_5$ to the sCBOD ultimate values required by the model (Table 6). We do, however, suggest that a Utah specific number be established for the dominant wastewater treatment types of activated sludge and membrane mechanical treatment as well as for lagoon systems.

Table 8. CBOD decomposition rate statistics based on samples from Silver Creek WRF effluent.

	NLS Method	**Thomas Method**
	k_d, 1/d	**k_d, 1/d**
Min	0.095	0.076
Max	0.125	0.124
Mean	0.103	0.096
StDev	0.011	0.012
95% CI	0.013	0.013

The thermal properties of the Silver Creek substrate were also measured since these dictate the rate of heat exchange between the water column and the sediments. While there are a number of values reported within the QUAL2K and QUAL2Kw manual, it can be important to have site specific thermal properties. The thermal property values based on measurements from Silver Creek with a sandy-gravel substrate were a thermal diffusivity of 0.72 $mm^2 s^{-1}$ and a thermal conductivity of 2.25 $W m^{-1} k^{-1}$.

Model Calibration

Calibration within this effort consisted of a number of manual calibration steps followed by autocalibration using the genetic algorithm within QUAL2Kw. The data used in calibration included hydraulics data (longitudinal depths, velocities, and travel time) and water quality data (Table 3) including the mean, minimum, and maximum values at each calibration location (only station E for the 2010 effort). For those data types where only 2 samples were taken, the minimum and maximum values were not always representative of the daily variability and only provided an understanding of the range at these sampling times.

Manual Calibration Steps

A number of manual calibration steps and or checks were identified to ensure that the model was representing the system well based on site specific data. These steps are key since they ensure that the foundational model components (e.g., flow balance, volumes, and instream temperatures) are correct before moving onto the more interconnected mechanisms associated with nutrient cycling.

Flow Balance/Hydraulics - To ensure that the representation of the hydraulics was appropriate, a number of steps were taken and many data types must be considered. Initially, to make sure discharge matched empirical observations, predicted values were compared to measured values. If the values differed, it could have been due to inflows or outflows from unknown sources or from groundwater exchanges. Although the reaches in these studies did not have significantly large differences, in some cases it may be necessary to incorporate a distributed inflow or abstraction to represent groundwater influences.

Specific conductance values were used in a number of different ways. Predicted values were compared to observed specific conductance values including the diel fluctuations. Since specific conductance is a measure of relatively conservative dissolved species, if predictions did not match the observations, this could indicate the presence of unknown inflows and may suggest the need for additional time in the field determining the source of the inflow.

Travel times within the study reach are dependent on having the channel geometry, water depth, and velocities correct. After data collection efforts were completed, we conducted a tracer study using either salt or rhodamine WT to provide data regarding travel times within the study reaches. Because Manning's equation is used to route the water through the study reach, additional information must be provided at a subreach scale about bottom widths, side slope, channel bottom slope, and Manning's roughness coefficient. Top widths, side slopes, and bottom slopes are measured at consistent increments along the channel. From these data, as described in Table 4, bottom width estimates were calculated using side slope, average depth, and top width values. Once the bottom width, side slope, and bottom slope values were entered into the model and the model was run, the predicted top widths were compared to field-derived data. If necessary, the bottom widths or side slopes were adjusted within reason. While good estimates of water depth and velocity were available at a number of discharge measurement locations, these values were not always recorded. After model setup, where available, predicted water depths and velocities were compared to measurements from locations downstream. At the same time**,** predicted travel times were compared to those estimated from tracer injection responses at various locations downstream. If necessary Manning's n and possibly bottom slope were adjusted to ensure water depths, velocities, and travel time predictions were similar to observations. Once the hydraulic representation was appropriate, it was necessary to determine if the temperature and ISS predictions were acceptable.

<u>Temperature</u> - First, predicted and observed temperatures at different locations downstream were compared. If predictions were inaccurate, shading data and trial and error approaches were used to adjust the hourly percent shading values. Another consideration was the accuracy of the predicted top widths. This was key because the predicted surface heat flux values are dependent upon the surface area of the air water interface. At times, it may be necessary to revisit the top width predictions to ensure the accuracy of temperature predictions. Additionally, if there were inflows, the temperature of these inflows may have required adjustment if they were not measured in the field.

<u>Inorganic Suspended Solids (ISS)</u> - Second, predicted and estimated ISS concentrations were compared at various locations longitudinally. The settling velocity was adjusted to vary the predicted concentrations. Ensuring these values were correct was important for photosynthesis due to its influence on light penetration. However, the ISS observations were calculated and it was unclear if they were accurate.

<u>Reaeration Rates</u> - Finally, to minimize the number of parameters that are varied in the autocalibration we developed an approach to determine the appropriate reaeration formula to apply within the model and a method of approximating SOD using the dissolved oxygen timeseries collected at each site. To determine a representative reaeration formula, whole stream metabolism methods were applied to estimate gross primary production (GPP) and ecosystem respiration (ER) using the concentrations at most stations where DO was measured within the study reach. As part of this, it is necessary to estimate a reaeration rate (k_a). Various "open-water" methods of determining GPP, ER and k_a have been established including the Delta Method [*McBride and Chapra*, 2005], Night Time Regression [Young et al 2004], and Inverse Method [Holtgrieve et al 2010]. It is possible to select the appropriate method for sites based on recommendations of Aristegi et al. [2009] where the Delta method was found to be best in open canopy

and clear conditions (using the point method if data are smooth and the centroid method if data are noisy) and the Night Time method was inappropriate in turbulent reaches and where WRF effluent is dominant and there are highly variable flows. For various sites in Utah, the Inverse Method was found to produce the most consistent results based on estimates for many systems and sites across the state.

To support the QUAL2Kw modeling, the Night Time Regression and Inverse Methods were applied to estimate the GPP, ER, and/or k_a at locations along the study reach. Given the variability of predicted reaeration rates from the formulas included within QUAL2Kw and the associated uncertainty, a number of steps were taken to determine the most appropriate formula. First, we would run QUAL2Kw model using each reaeration formula. These predicted reaeration rates in each reach segment were compared to the k_a values estimated from the metabolism methods and an RMSE was calculated. Next, we determined the most appropriate formula based on the lowest RMSE value and set this within the model. If multiple equations were appropriate, we selected one where all assumptions (e.g., depth and velocity ranges) were met.

As described within Appendix A and B, these steps have been automated within the "Data Input" sheet that USU added for the 2010 modeling. It is important to note that it would be possible to set the reaeration rates based on the values obtained from the metabolism measurements directly, however, this would limit the applicability of the model to predict reaeration under other flow conditions (i.e., due to different velocities and depths) and within reach segments where k_a values were not measured.

<u>Sediment Oxygen Demand</u> - Another significant source of uncertainty in QUAL2Kw modeling, particularly in shallow streams, is the amount of SOD present within each system. While QUAL2Kw has the functionality to estimate SOD based on a sediment diagenesis algorithm, there is often more SOD present than is predicted. The need to prescribe SOD has been associated with the deposition of organic matter outside of the time period of the model simulation (i.e. during snowmelt runoff) and the deposition of coarse particulate organic matter (CPOM) that typically is not captured by standard sampling techniques. This extra SOD became an issue within the Jordan River TMDL [*Stantec Consulting*, 2010] and was addressed through direct measurements of SOD to determine reasonable ranges that would be acceptable within QUAL2Kw modeling. In many cases, however, these types of measurements will not be available due to cost and the personnel requirements to collect them and there is significant variability in the results. We know that the change in oxygen over time is a result of oxygen sources (primary production and reaeration) and oxygen sinks (autotrophic and heterotrophic respiration, BOD, and other oxygen consuming reactions within the water column and sediments). However, when using metabolism methods, the equation describing the change in oxygen is reduced to:

$$dO/dt = GPP + reaeration - ER \qquad \textbf{(21)}$$

where *GPP* = gross primary production and *ER* = ecosystem respiration.

In this context, *ER* is now a net sink term. If we assume autotrophic respiration approximately equals *GPP* (it may need to be some fraction of *GPP [Jones et al., 1997]*), then any extra oxygen consumption is due to heterotrophic respiration and other oxygen consuming reactions within the sediments and water column. If this value is positive (meaning *ER* is higher than primary production), this provides an estimate of a total SOD (heterotrophic respiration + oxygen demanding reactions within the sediments) and some oxygen demanding reactions within the water column (e.g., BOD decomposition and nitrification). Within QUAL2Kw, it can be assumed that this total SOD value would provide a maximum SOD that could be prescribed within the model. In most cases, the maximum SOD should include the prescribed SOD plus the SOD estimated within the sediment diagenesis algorithm within QUAL2Kw (described within [*Pelletier and Chapra*, 2008]). In these efforts, we assumed that the *ER* minus *GPP* approximation for SOD is appropriate since the streams included in this study are relatively shallow and sediment processes will significantly influence the water column DO response. In larger rivers, it is possible that other processes more significantly influence the water column oxygen responses (e.g. chemical reactions within the water column, phytoplankton, etc.) and these approaches may not be applicable or include more error due to the aforementioned assumptions.

Since SOD measurements were not gathered during the 2010 data collection efforts, we used *ER* values minus the *GPP* estimates at Station E (and at times Station D) to determine a reasonable average and range of SOD values for the portion of the study reach below the WRF. Where appropriate, an average value of SOD was established and set within the model before autocalibration.

Autocalibration

With a number of parameters set based on the prior manual calibration steps, the remaining parameters that were appropriate to include in model calibration were autocalibrated. The parameters that should be included in calibration as well as the appropriate parameter ranges were set based on recommendations from Dr. Steven Chapra [*Stantec Consulting*, 2010] and from Bowie et al. [1985] (Table 9). Within the autocalibration, a fitness statistic is evaluated for each state variable as the reciprocal of a weighted average of the normalized RMSE and estimated as follows:

$$f(x) = \left[\sum_{i=1}^{q} w_i\right] \left[\sum_{i=1}^{q} \frac{1}{w_i} \left[\frac{\frac{1}{m}\sum_{j=1}^{m} O_{i,j}}{\left[\frac{1}{m}\sum_{j=1}^{m}\left(P_{i,j} - O_{i,j}\right)^2\right]^{1/2}}\right]\right] \quad \textbf{(21)}$$

where $O_{i,j}$ = observed value, $P_{i,j}$ = predicted value, m = number of pairs of predicted and observed values, w_i = weighting factor, and q = number of different state variables (e.g., dissolved oxygen, pH) in a bounded n-dimensional space for $x \equiv (x_1, x_2, ..., x_n) \quad x_k \in [0.0, 1.0]$ (Pelletier et al. 2006). This tool, allows the coefficient of variation of the RMSE (model results versus observed data) between each constituent along with appropriate, individual weighting factors (Table 10), to be summarized in a single value that the genetic algorithm seeks to maximize by adjusting all desired parameters.

The constituents included in the fitness statistic for the 2010 modeling efforts heavily weighted DO average, minimum, and maximum values at Station E as indicted by a weighting factor of 5 and were established via discussions with Greg Pelletier and Nick von Stackelberg. The preliminary calibration parameters for each study site were established by the autocalibration algorithm and are outlined within each model and the associated documentation delivered to UDEQ.

Table 9. Appropriate ranges (Min Value and Max Value) of parameters for QUAL2Kw modeling with the "Value" column showing the default value used. The "Auto-Cal" column indicates if a parameter was autocalibrated in the 2010 modeling efforts.

				Autocalibration inputs		
Parameter	***Value***	***Units***	***Symbol***	***Auto-cal***	***Min value***	***Max value***
Stoichiometry:						
Carbon	40	gC	gC	No	30	60
Nitrogen	7.2	gN	gN	No	5	9
Phosphorus	1	gP	gP	No	0.5	2
Dry weight	100	gD	gD	No	100	100
Chlorophyll	1	gA	gA	No	0.5	2
Inorganic suspended solids:						
Settling velocity	Manual	m/d	v_i	No	0.2	2
Oxygen:						
Reaeration model	Manual Determination of Appropriate Formula			No		
Temp correction	1.024		q_a			
Reaeration wind effect	None					
O2 for carbon oxidation	2.69	gO_2/gC	r_{oc}			
O2 for NH4 nitrification	4.57	gO_2/gN	r_{on}			
Oxygen inhib model CBOD oxidation	Exponential					
Oxygen inhib parameter CBOD oxidation	0.60	L/mgO2	K_{socf}	No	0.60	0.60
Oxygen inhib model nitrification	Exponential					
Oxygen inhib parameter nitrification	0.60	L/mgO2	K_{sona}	No	0.60	0.60
Oxygen enhance model denitrification	Exponential					
Oxygen enhance parameter denitrification	0.60	L/mgO2	K_{sodn}	No	0.60	0.60
Oxygen inhib model phyto resp	Exponential					
Oxygen inhib parameter phyto resp	0.60	L/mgO2	K_{sop}	No	0.60	0.60
Oxygen enhance model bot alg resp	Exponential					
Oxygen enhance parameter bot alg resp	0.60	L/mgO2	K_{sob}	No	0.60	0.60
Slow CBOD:						
Hydrolysis rate	0	/d	k_{hc}	No	0.05	0.25
Temp correction	1.047		q_{hc}	No	1	1.07
Oxidation rate	0.103	/d	k_{dcs}	No	0.05	0.25
Temp correction	1.047		q_{dcs}	No	1	1.07
Fast CBOD:						
Oxidation rate	10	/d	k_{dc}	No	0	10
Temp correction	1.047		q_{dc}	No	1	1.07
Organic N:						
Hydrolysis		/d	k_{hn}	Yes	0.05	0.3
Temp correction	1.07		q_{hn}	No	1	1.07
Settling velocity		m/d	v_{on}	Yes	0.05	0.25
Ammonium:						
Nitrification		/d	k_{na}	Yes	0.05	4
Temp correction	1.07		q_{na}	No	1	1.07
Nitrate:						
Denitrification		/d	k_{dn}	Yes	0.05	2
Temp correction	1.07		q_{dn}	No	1	1.07
Sed denitrification transfer coeff		m/d	v_{di}	Yes	0	1
Temp correction	1.07		q_{di}	No	1	1.07
Organic P:						
Hydrolysis		/d	k_{hp}	Yes	0.05	0.3
Temp correction	1.07		q_{hp}	No	1	1.07
Settling velocity		m/d	v_{op}	Yes	0.05	0.25
Inorganic P:						
Settling velocity		m/d	v_{ip}	Yes	0	2
Sed P oxygen attenuation half sat constant		mgO_2/L	k_{spi}	Yes	0	2
Phytoplankton:						
Max Growth rate		/d	k_{gp}	Yes	1.5	3
Temp correction	1.07		q_{gp}	No	1	1.07
Respiration rate		/d	k_{rp}	Yes	0.05	0.5
Temp correction	1.07		q_{rp}	No	1	1.07
Death rate		/d	k_{dp}	Yes	0	1
Temp correction	1		q_{dp}	No	1	1.07
Nitrogen half sat constant	15	ugN/L	k_{sPp}	No	10	25

				Autocalibration inputs		
Parameter	***Value***	***Units***	***Symbol***	***Auto-cal***	***Min value***	***Max value***
Phosphorus half sat constant	2	ugP/L	k_{sNp}	No	1	5
Inorganic carbon half sat constant	1.30E-05	moles/L	k_{sCp}	No	1.30E-06	1.30E-04
Phytoplankton use HCO3- as substrate	Yes					
Light model	Smith					
Light constant	57.6	langleys/d	K_{Lp}	No	40	110
Ammonia preference	15	ugN/L	k_{hnxp}	No	15	30
Settling velocity		m/d	v_a	Yes	0.05	0.5
Bottom Plants:						
Growth model	Zero-order					
Max Growth rate		gD/m^2/d or /d	C_{gb}	Yes	1.5	200
Temp correction	1.07		q_{gb}	No	1	1.07
First-order model carrying capacity	100	gD/m^2	$a_{b,max}$	No	50	200
Basal respiration rate		/d	k_{r1b}	Yes	0.02	0.2
Photo-respiration rate parameter	0.39	unitless	k_{r2b}	No	0	0.6
Temp correction	1.07		q_{rb}	No	1	1.07
Excretion rate		/d	k_{eb}	Yes	0	0.5
Temp correction	1.07		q_{db}	No	1	1.07
Death rate		/d	k_{db}	Yes	0	5
Temp correction	1.07		q_{db}	No	1	1.07
External nitrogen half sat constant		ugN/L	k_{sPb}	Yes	100	500
External phosphorus half sat constant		ugP/L	k_{sNb}	Yes	25	100
Inorganic carbon half sat constant		moles/L	k_{sCb}	Yes	1.30E-06	1.30E-04
Bottom algae use HCO3- as substrate	Yes					
Light model	Half saturation					
Light constant		langleys/d	K_{Lb}	Yes	40	100
Ammonia preference		ugN/L	k_{hnxb}	Yes	15	30
Subsistence quota for nitrogen		mgN/gD	q_{0N}	Yes	0.36	1.44
Subsistence quota for phosphorus		mgP/gD	q_{0P}	Yes	0.05	0.2
Maximum uptake rate for nitrogen		mgN/gD/d	r_{mN}	Yes	350	1500
Maximum uptake rate for phosphorus		mgP/gD/d	r_{mP}	Yes	50	200
Internal nitrogen half sat ratio			$K_{qN,ratio}$	Yes	1.05	5
Internal phosphorus half sat ratio			$K_{qP,ratio}$	Yes	1.05	5
Nitrogen uptake water column fraction	1		$N_{UpWCfrac}$	No	0	1
Phosphorus uptake water column fraction	1		$P_{UpWCfrac}$	No	0	1
Detritus (POM):						
Dissolution rate		/d	k_{dt}	Yes	0.05	5
Temp correction	1.07		q_{dt}	No	1.07	1.07
Settling velocity	0.4033805	m/d	v_{dt}	Yes	0.05	0.5

Table 10. Weighting factors for each constituent used to calculate the fitness in model calibration.

Parameter	Weighting Factor
DO (mgO_2/L)	5
CBODs (mgO_2/L)	1
Norg (ugN/L)	2
NH4 (ugN/L)	3
NO3 (ugN/L)	3
Porg (ugN/L)	2
Inorg P (ugP/L)	4
Phyto (ugA/L)	1
Alk (mg$CaCO_3$/L)	4
pH	4
TN (ugN/L)	3
TP (ugP/L)	3
TSS (mgD/L)	1
CBODu (mgO_2/L)	1
DO (mgO_2/L) - Min	5
DO (mgO_2/L) - Max	5
CH-A - Min	1
CH-A - Max	1

Model Validation/Corroboration

At two locations (Silver Creek and Fairview) validation or corroboration data sets (identical to the calibration data sets) were collected during a different time period. The objectives of these data sets were to determine if the model calibrations held during a different time period under somewhat different conditions. For model corroboration we updated the boundary condition, point inflow, and weather data to coincide with the conditions during the validation time period. All other site specific information (e.g., channel characteristics) and parameters set during calibration were held constant. The exception was SOD which can change during the year due to the transfer of oxygen demanding material into the study reach. The SOD value for the validation period was again estimated based on ER- GPP at station E.

Findings/Recommendations/Suggested Future Work

In general, we have found that the models resulting from this study have been able to meet the diverse intended uses. For example, a number of the models have already been foundational in developing WLAs and they are currently in the process of being used to assist in statewide nutrient criteria development. However, given the generic nature of the data collection and automatic calibration methods necessary to meet these varied needs and applications, there is at times significant uncertainty in important mechanisms and therefore in predictions. In some circumstances, additional data collection efforts, sensitivity and uncertainty analyses will be necessary to ensure the appropriate confidence in model predictions. Recommendations and suggested future efforts have also been identified.

Data Collection

In general, one of the most important lessons learned from this effort was the need for a larger number of samples due to the short timescale of the data collection campaigns (2-3 days). These data collection efforts focused on collecting data during presumed steady state conditions which further led to the assumption that many of the data types we gathered would not vary significantly throughout each day (including flow and water quality). The exceptions from this assumption were temperature, DO, pH, specific conductance, and chlorophyll a which were measured at small time increments over 3-4 days in an effort to get a good understanding of this daily variability. While the streams themselves and the conditions at station A and B were relatively stable during these late summer time periods, the conditions downstream of many of the WRFs were not. Based on these studies, stable conditions do not exist for many of these plants and the loads are highly variable throughout the day. This becomes critical to consider when sampling and modeling effluent dominated systems (e.g., Silver Creek, Moroni). This variability caused significant problems during model population and calibration due to samples often not representing the average conditions and resulting in very different values between days where grab samples were collected. The Washington Department of Ecology generally samples twice a day for two days in a row in the stream. They also use a 24-hour composite for two days from the WRF effluent. Further, they average three benthic algae samples at randomly selected sites where periphyton are present. A similar approach may be warranted within the state of Utah, however, the representativeness of this sampling regime should be investigated.

We also found that samples taken at different locations often did not coincide with the samples taken at a calibration location. To illustrate some of the disconnects we encountered, assume a sample is taken at station E (calibration location) at 10:00 am and this corresponded to the WRF release at 8 am (i.e., there is a 2 hour travel time between the WRF and Station E). The sample then taken at the WRF for the modeling occurs at 10:30 am. This and the measured flow value from the WRF is then used to calculate the load within the model that gets decayed and transported downstream to station E (the calibration location). In this example, if the WRF effluent varies significantly over short time periods you can see how the samples used in model forcing and calibration can easily be disconnected and influences model calibration and ultimately interpretation. These sorts of issues could be dealt with by taking more samples throughout the study period (e.g., 3 per day) which would provide a much better understanding of the mean and variance throughout the entire study period. However, the constituents requiring higher frequency sampling will likely be site specific and depend on the loads impacting the system (e.g., highly variable WRF versus a lagoon system). Due to the WRF variability, the 2 data points gathered often times provided a large range of possible concentrations and made it difficult to decide on an appropriate representative average to be used in the load estimates or in calibration. Another concern was that there were many times that data points were either missing, resulted in non-detects, etc. These missing data left us with even less information for model population and/or calibration. In the future when dealing with effluent dominated streams with highly variable loads, it would be more appropriate to gather time-variable data and use the newly developed version of QUAL2Kw that allows for non-steady flow with a continuous simulation option over a 365 day simulation period.

When it came to understanding loads, we also identified the need to collect enough flow information to ensure an appropriate water balance throughout the study reach. Since the ability to predict accurate concentrations hinges on correct volumes, in cases where the inflows were variable or discharge measurements showed variability, more measurements were necessary. This includes ensuring accurate flow estimates at each of the study sites throughout the study period and may require the use of various flow measurement methods (e.g., slug injections rather than velocity area methods). Good flow data provides information regarding the appropriateness of the steady flow assumption and also provides a more solid estimate of average flow conditions if there is variability present. This again highlights the need to understand the variability in WRF effluent. To assist in these efforts and all load allocation decision making (e.g., TMDLs or NPDES permits), we recommend that the state requires WRFs to track subhourly effluent rates and provide these to the state quarterly. It may be worthwhile to also have them install a water quality sonde and track the effluent DO, temperature, specific conductance, and pH since these data provide information regarding the plant effluent concentration variability and potential plant upsets.

The other key concern identified within these data had to do with analytical methods and the associated errors. For example, the sCBOD method detection limits are 3 or 5 mg/L depending on the lab. With low sCBOD both in WRF effluent and many of the streams not being highly influenced by high BOD loads, we were forced to calculate the actual BOD loads (from the WRF or at the upstream boundary condition) based on concentrations assumed to be half the method detection limit. While other, less biased techniques exist to handle these censored values (i.e., trimmed mean, Winsorized mean, Cohen's maximum likelihood method), they are incapable of handling cases where more than 25% of the data is censored. These types of assumptions lead to significant errors in loads and the resulting sCBOD predictions. This may become a significant enough issue that new analytical methods need to be developed. Similarly, we ran into issues with analytical error when it came to estimating some constituent concentrations based on differences (e.g., Organic N, Organic P, and detritus). The various sources of sampling and analytical error can produce significant errors in model loads and model calibration. This was particularly important given the limited number of samples and again illustrates the need for additional sampling throughout the study period. Further, we identified that a measure of VSS should be included in the sampling protocol to better estimate detritus concentrations. Detritus could then become part of the fitness statistic and used in calibration.

Model Population/Calibration

Many of the issues associated with data collection have an obvious link to the success of model calibration, the ability to minimize model uncertainty, and the utility in decision making. Other concerns were identified that were more specifically related to model population or calibration.

A key concern was the very short spatial scale over which data were collected. In an effort to minimize the influence of tributaries, withdrawals, etc. and to meet the needs associated with quantifying open water metabolism, data were collected over short reaches based on Eqn. 7. This equation provides an estimated reach length where half of the oxygen has exchanged with the atmosphere via reaeration [*Grace and Imberger*, 2006]. While these distances were appropriate for the metabolism estimates, the associated short travel times resulted in many of the chemical reactions having minimal influence within the study reach. In other words, over these travel time scales many reactions had minimal impact on instream concentrations resulting in relatively insensitive parameters. To address this concern, additional data sets were gathered in summer 2011 and the reach lengths were extended as much as possible given the tributary inflows, diversions, etc. that would require even more extensive data collection. For most future modeling applications (with the exception of WLA analyses) it would be best to make reach lengths as long as possible for the modeling study and deploy dissolved oxygen sensors within the reach at the optimal lengths based on Eqn. 7. If the approach provided by Grace and Imberger [2006] is still used, we suggest maximizing the multiplier (use 3 instead of 0.693, increasing importance of instream processes from 50% to 95%, -ln(.05) ≈ 3) to ensure longer study reaches for the modeling and maintain the ability to still use the one or two station metabolism methods.

Another key issue identified in QUAL2Kw modeling is the need to decrease the number of parameters that are autocalibrated. As discussed previously, when possible, parameters should be measured or estimated for the study site of interest. Some key rates that can be estimated include:

1. BOD decomposition rates (k_d) could be estimated for each of the WRF types (lagoons, oxidation ditch, membrane) in Utah.
2. Nitrification rates could be estimated for each study site.
3. Photosynthetic Active Radiation (PAR) attenuation within the water column given the importance of bottom algae in many of these systems.

The other key parameter, at least in some systems, is SOD. While we established a method of estimating SOD using dissolved oxygen measurements and metabolism methods, further investigation into the assumptions made regarding the minimal influence of other oxygen demanding reactions that are reflected by the in-situ dissolved oxygen measurements and the amount of autotrophic respiration should be considered. Further, the application of these methods to all systems needs to be investigated.

When it comes to autocalibration, there is an obvious need to decrease the number of parameters and potentially come up with narrower ranges to confine autocalibration estimates. In these model applications, over 30 parameters are being optimized. This number is extremely high, but without more information regarding which parameters are unimportant, it is not clear which should be dropped from the autocalibration. We have seen that the phytoplankton parameters seem to be insensitive. However, the bottom plants predictions are very important in many Utah streams and it is unknown which bottom algae parameters are sensitive and should be included in autocalibration. Approximately 15 of the parameters being optimized are associated with bottom plant growth and there is minimal information regarding the spatial and temporal concentrations to be used in calibration. Benthic algae carbon, nitrogen, and phosphorus ratios were established within some streams to provide an understanding of autotrophic nutrient limitation and provide insight into the heterotrophic resource quality. These data could be useful in bottom algae parameter estimation, however, they show there is significant spatial and temporal variability in stoichiometry along study reaches. This presents additional challenges in developing the appropriate sampling approaches to collect representative data at the reach or sub reach scales. The utility of these data types and sampling techniques need to be further investigated. Additionally, the number of simulation days influence the bottom plant concentrations and guidance regarding how best to set the simulation time period should be developed.

We recommend a sensitivity analysis be completed for all these case studies to determine if there can be global reduction (meaning for all study sites) in the number of parameters autocalibrated and then which parameters are insensitive in different systems. This will result in a reduction of parameter sets that produce similar output responses. Within this effort, it would be important to identify which output parameters are important and influence the fitness statistic since the objective function (i.e., fitness) guides the calibration. If output values are not sensitive, they can influence the calibration algorithm performance.

In these applications, given the number of calibration parameters, short travel times, and limited amount of data, the resulting calibrations may or may not be appropriate for different circumstances. We say this because there were some consistent findings that suggest that we are missing key processes, some parameters included in calibration were insensitive, or our approach to autocalibration may need some refinement. For example, the autocalibration algorithm consistently set sediment denitrification rates and inorganic phosphorus settling rates to relatively high values (Table 11). Both of these parameters basically provide a way to remove N and P from the water column, but in general this is done in way that does not provide any insight into underlying mechanisms. In other words, these model terms are merely a N and P sink. It is recommended that the influence of these parameters in autocalibration be investigated. If these additional N and P sinks truly exist, there is a need to investigate which mechanisms are not present within the model but are being consistently observed in these systems. Another interesting result of these calibrations are predicted pH values that are consistently too high. This can be important in the ability to predict other constituent concentrations and the mechanisms leading to this should be revisited.