Notes on QUAL2E and QUAL2K

QUAL2E/QUAL2K are a computer codes long supported and distributed by the US E.P.A. (Environmental Research Laboratory, Athens, GA) for the purpose of modeling conventional pollutants and nutrients in rivers. Their mechanistic forumlations are echoed in other widely used models (e.g., WASP). Version 3.3 represents the most recent Fortran code in a long line of programs dating back to the late 1960's. This latest version is equipped to simulate up to 15 constituents:

Conventional Pollutants:
1. Dissolved Oxygen (DO)
2. Biochemical Oxygen Demand (BOD)
3. Coliforms

Nutrients & Algae:
4. Chlorophyll a

Nitrogen Species
5. Organic Nitrogen
6. Ammonia
7. Nitrite
8. Nitrate

Phosphorus Species
9. Organic Phosphorus
10. Dissolved Phosphorus

Others:
11. Temperature
12. One Arbitrary Non-conservative constituent
13. Three Arbitrary Conservative constituents

This model can be used with branched rivers. It is a one-dimensional model (river is segmented along the longitudinal axis), and therefore presumes complete mixing in cross-section. QUAL2E can accommodate a very large number of point and non-point sources and withdrawals. These sources or withdrawals must be treated as constant in time, however.

QUAL2E may be used as either a steady-state or a limited dynamic model. Most applications to conventional pollutant modeling will use the steady-state mode of operation. Dynamic modeling is primarily used when information on diurnal variations in algal metabolism is desired. Impacts from single events (e.g., pollutant spill) cannot be simulated with QUAL2E, because the only time-varying inputs allowed are the meterological ones (i.e., temperature, sunlight).

The basic kinetic formulations are centered around dissolved oxygen. Figure 1 shows how the DO, BOD, nutrients, and algae interact in this modeling framework. The symbols shown in Figure 1 are further defined in Table 1 which follows. They all describe, in some way, the rate of transformation of the various constituents. Temperature may be provided by the user, or it may be modeled from meterological data. It is then used to adapt the various rate constants. Coliforms and the arbitrary conservative and non-conservative substances are treated separately, and do not interact with each other or with any other constituents.

QUAL2K is an updated version of QUAL2E, programmed in the Windows macro-language; Visual Basic for Applications (VBA). Microsoft Excel is the graphical user interface

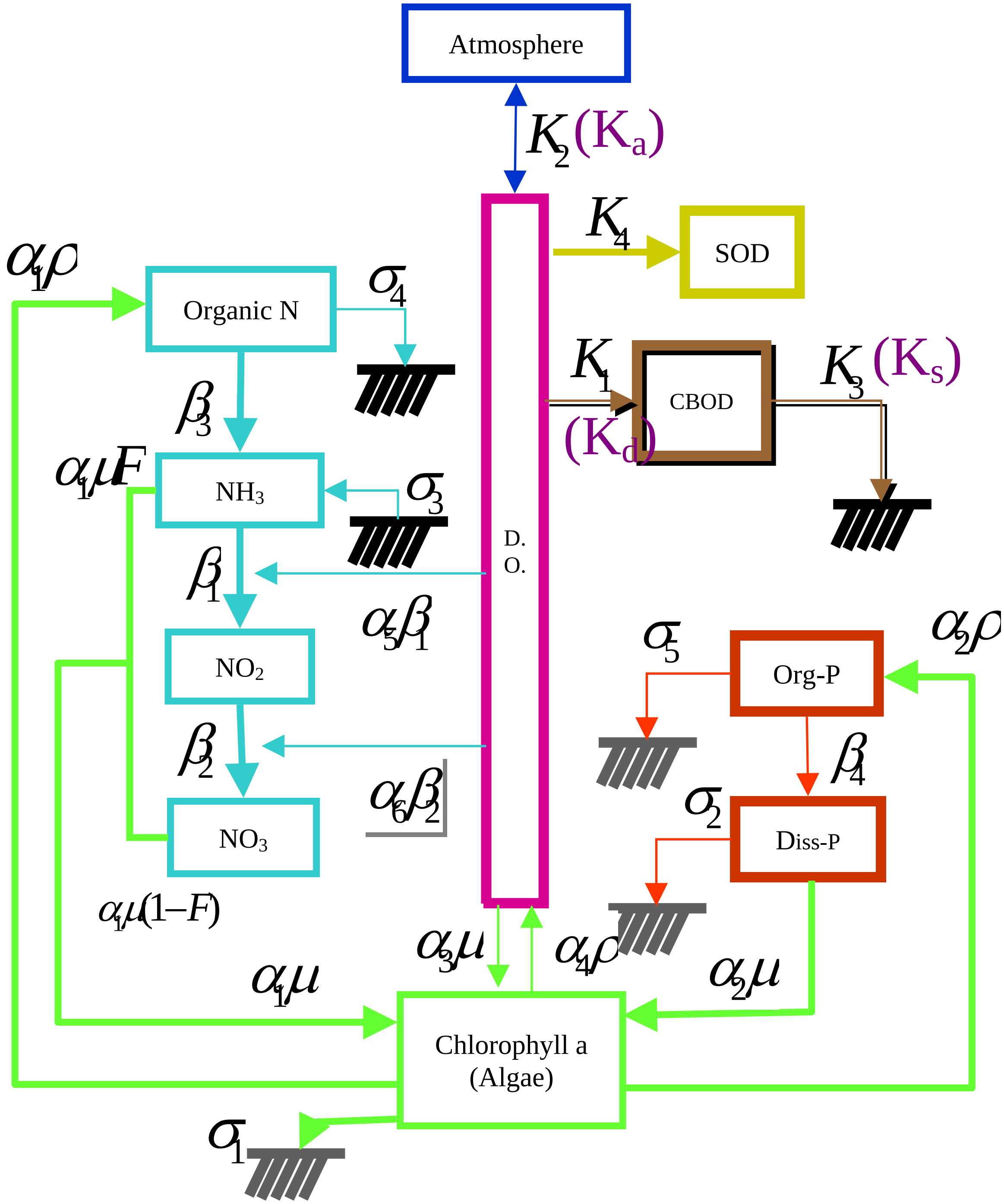

Figure 1

Major Constituent Interactions in QUAL2E
(After Brown & Barnwell, 1987[1])

1. Brown & Barnwell, "The Enhanced Stream Water Quality Models: QUAL2E and QUAL2E-UNCAS: Documentation and User Model", EPA/600/3-87/007, 1987.)

TABLE I
DO/BOD REACTION COEFFICIENTS

Variable[a] QUAL2E(T&M)	Description	Units	Range of Values	Variable by Reach.	Typical Value .
AE	Evaporation coefficient	ft/hr-in-Hg	No	0.00068	
AFACT	Light averging factor	none		No	0.92
BE	Evaporation coefficient	ft/hr-in-Hg	No	0.00027	
K	Dispersion constant		5.9-6000	Yes	5.9
K_1 (K_d)	Carbonaceous deoxygeneration rate constant (in-stream)	day^{-1}	0.02-3.4	Yes	
K_2 (K_a)	Reaeration rate constant	day^{-1}	0.0-100	Yes	
K_3(K_s)	Rate of loss of BOD due to settling	day^{-1}	-0.36-0.36	Yes	0
K_4(S_B)	Benthic O_2 uptake (SOD)	mg-O_2/ft^3-day	0-100	Yes	
K_5	Coliform die-off rate	day^{-1}	0.05-4.0	Yes	
K_6	Arbitrary non-conservative decay coefficient	day^{-1}	Variable	Yes	
K_b (K_1)	Bottle constant for rate of CBOD deoxygenation	day^{-1}	0.05-0.4		0.2
K_L	Michaelis-Menton half-saturation constant for light (Option 1)	Btu/ft^2-min	0.02-0.10	No	
K_L	Light saturation Coefficient (Option 3)	Btu/ft^2-min	0.25-0.90		0.75
(K_N)	NBOD deoxygenation rate	day^{-1}			
K_N	Michaelis-Menton half-saturation constant for nitrogen	mg-N/L	0.01-0.40	No	0.20
K_p	Michaelis-Menton half-saturation constant for phosphorus	mg-P/L	0.01-0.05	No	0.04
KNITRF	Nitrification inhibition coefficient	L/mg	0.3-5	No	0.65
P_N	Algal preference factor for ammonia	-	0.0-1.0	No	
TFACT	Fraction of photo-synthetically active radiation	none		No	0.45
α_0	Ratio of chlorophyll-a to algal biomass	ug Chl a/mg A	10-100	No	20

TABLE I (cont.)
DO/BOD REACTION COEFFICIENTS

Variable[a] QUAL2E(T&M)	Description	Units	Range of Values	Variable by Reach.	Typical Value
α_1	Fraction of algal biomass that is Nitrogen	mg-N/mg A	0.07-0.09	No	0.085
α_2	Fraction of algal biomass that is Phosphorus	mg-P/mg A	0.01-0.02	No	0.014
α_3	O_2 production per unit of algal growth	mg-O/mg A	1.4-1.8	No	1.6
α_4	O_2 uptake per unit of algae respired	mg-O/mg A	1.6-2.3	No	2.0
α_5	O_2 uptake per unit of NH_3 oxidation	mg-O/mg N	3.0-4.0	No	3.43
α_6	O_2 uptake per unit of NO_2 oxidation	mg-O/mg N	1.0-1.14	No	1.14
β_1	Rate constant for the biological oxidation of NH_3 to NO_2	day^{-1}	0.10-1.00	Yes	0.30
β_2	Rate constant for the biological oxidation of NO_2 to NO_3	day^{-1}	0.20-2.0	Yes	0.60
$\beta_3(K_{12})$	Rate constant for the hydrolysis of organic-N to ammonia	day^{-1}	0.01-0.4	Yes	0.03
β_4	Rate constant for the decay of organic-P to dissolved P	day^{-1}	0.01-0.70	Yes	0.05
λ_0	Non-algal light extinction coefficient	ft^{-1}	Variable	No	
λ_1	Linear algal self-shading coefficient	1/ft/ug Chl-a/L	0.002-0.02	No	0.00268
λ_2	Nonlinear algal self-shading coefficient	$1/ft/(ug\ Chl\text{-}a/L)^{2/3}$	0.0165 (Riley)	No	0.0165
μ_{max}	Maximum algal growth rate	day^{-1}	1.0-3.0	No	2.5
ρ	Algal respiration rate	day^{-1}	0.05-0.5	No	0.10
σ_1	Algal settling rate	ft/day	0.5-6.0	Yes	1.0
σ_2	Benthos source rate for dissolved phosphorus	mg-P/ft^2-day	0.001-0.01	Yes	0.0015
σ_3	Benthos source rate for ammonia nitrogen	mg-O_2/ft^2-day	0.004-0.02	Yes	0.002

TABLE I (cont.)
DO/BOD REACTION COEFFICIENTS

Variable[a] QUAL2E(T&M)	Description	Units	Range of Values	Variable by Reach.	Typical Value
σ_4	Organic nitrogen settling rate	day^{-1}	0.001-0.10	Yes	0.01
σ_5	Organic phosphorus settling rate	day^{-1}	0.001-0.10	Yes	0.010
σ_6	Arbitrary non-conservative settling rate	day^{-1}	Variable	Yes	
σ_7	Benthal source rate for arbitrary non-conservative settling rate	mg-ANC/ft^2-day	Variable	Yes	

[a]First symbol is that used in QUAL2E documentation (Brown & Barnwell, "The Enhanced Stream Water Quality Models: QUAL2E and QUAL2E-UNCAS: Documentation and User Model", EPA/600/3-87/007, 1987.); the second, when present, is that used by Thomann and Mueller, Principles of Surface Water Quality Modeling and Control

New Features in QUAL2K

QUAL2K (Q2K) incorporates the framework estabilished by QUAL2E with the following changes and enhancements:

1. Model segmentation. Q2E segments the system into river reaches comprised of equally spaced elements. In contrast, Q2K uses unequally-spaced reaches. In addition, multiple loadings and abstractions can be input to any reach.
2. Carbonaceous BOD speciation. Q2K uses two forms of carbonaceous BOD to represent organic carbon. These forms are a slowly oxidizing form (slow CBOD) and a rapidly oxidizing form (fast CBOD). In addition, non-living particulate organic matter (detritus) is simulated. This detrital material is composed of particulate carbon, nitrogen and phosphorus in a fixed stoichiometry.
3. 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.
4. Sediment-water interactions. Sediment-water fluxes of dissolved oxygen and nutrients are 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.
5. Bottom algae. The model explicitly simulates attached bottom algae.
6. Light extinction. Light extinction is calculated as a function of algae, detritus and inorganic solids.
7. pH. Both alkalinity and total inorganic carbon are simulated. The river's pH is then simulated based on these two quantities.
8. Pathogens. A generic pathogen is simulated. Pathogen removal is determined as a function of temperature, light, and settling.

Portions of ths are from EPA’s modeling web page. You should consult:

http://www.epa.gov/Athens/wwqtsc/html/qual2k.html

For more on QUAL2K and to download the program