International Journal of Advance Research and Innovation
Vol. 4(2), Apr-Jun 2016, pp. 66-70
Doi: 10.51976/ijari.541710
www.gla.ac.in/journals/ijari

Article Info
Received: 25 Jan 2016 | Revised Submission: 20 Feb 2016 | Accepted: 28 Feb 2016 | Available Online: 15 Jun 2016

Application of Qual2e Model for River Water Quality Modelling

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ABSTRACT

QUAL2E is modeling software which simulates up to 15 water quality parameters in branching stream system. The model uses mathematical equations like finite-difference solution of the adjective- dispersive mass transport and reaction equations. The program computes a series of steady- state water surface profiles and simulates changes in flow conditions along the stream. The model is applicable only to dendritic streams that are well mixed and it assumes that the major transport mechanism, advection and dispersion are significant only along the main direction of flow of the stream. QUAL2E can operate as either a steady state or a dynamic model and it simulates dynamic dial heat budget and water quality kinetics for a one dimensional and steady flow system. QUAL2E program performs dissolved oxygen balance by including source and sink terms in mass balance equation and is used to quantify the non point sources loading rate, determine the pollutants, calculate the phosphorus and estimate the natural conditions. It accommodates four types of hydraulic and mass load functions in addition to local climate factors: headwater-inputs, point sources, inflow/outflow and downstream boundary conditions.

Keywords: *Qual2e Model; Water Quality; Heat Balance; Kinetic Processes and Mass Transfer Processes Kinetic Processes; Mass Transfer Processes.*

1.0 Introduction

QUAL2K is a modernized version of the QUAL2E which was developed by Brown and Barnwell (1987) and it employs Microsoft Excel as the graphical user interface. At present there are total two versions of QUAL2K available: version 2.11b8 of QUAL2K an updated version based on QUAL2K 2.04 which was first developed by Chapra et al. (2006) and the QUAL2Kw model supported by the Washington State Department of Ecology (Washington State Department of Ecology 2007). QUAL2Kw contains a genetic algorithm for the automatic calibration of kinetic rate parameters and generic algorithm used in this is the PIKAIA algorithm while QUAL2K does not (Pelletier et al. 2006). QUAL2K has the ability to model a main channel with several tributaries whereas QUAL2K only be used to model a main channel without a branching network of the stream. Both versions of the QUAL2K model have been used in order to assess the fate and transport of conventional pollutants to estimate river pollution loading for input into a river model (Capodaglio et al. 2005). QUAL2K is a time-variable, steady flow model with constant coefficients in each designated reach of the stream and it simulates various constituents such as temperature, carbonaceous BOD, DO, phytoplankton, phosphorus and nitrogen. It also simulates pH, alkalinity, inorganic suspended solids, pathogenic bacteria and bottom algae of river stream. The advantage of the QUAL2K model is its ability to incorporate hourly data. It has the ability to simulate a system stream which is comprised of a main branch and several tributaries. This model is one-dimensional with the assumption that the channel is well mixed in the vertical and lateral directions and simulates the impacts of point and non point pollutant loading. All hydraulic characteristics are simulated as one dimensional, steady state with non-uniform flow i.e. water depth and velocity may vary depending on location in the channel. The model captures dial variations as water quality kinetics and the heat budget are determined on a dial time scale as the

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calculations are dynamic for dial heat budget. QUAL2K divides a study river stream into segments which are called reaches, that are further divided into elements and these elements are the basic computational unit (spatial step, P*x*).

Reaches are assigned based on the hydraulic characteristics present in the study river having the sections of river with similar slope, Manning roughness coefficient, bottom width, and side slope will be defined as a reach. Some other factors which also define reaches are constant longitudinal dispersion, bottom algae coverage, bottom sediment oxygen demand (SOD) coverage, and the rate constants for mass transfer (to the air and sediment) of oxygen, methane, ammonium, and inorganic phosphorus. Representation of QUAL2K model for the study of river is created by sequentially numbering the reaches starting from the headwaters of the main channel.

2.0 Material and Method

QUAL2Kw can simulate number of constituents that includes temperature, pH, carbonaceous biochemical demand, sediment oxygen demand, dissolved oxygen, organic nitrogen, ammonia nitrogen, nitrite and nitrate nitrogen, organic phosphorus, inorganic phosphorus, total nitrogen, total phosphorus, Phytoplankton and bottom algae.

Water quality parameters measured from QUAL2K model are: flow, water temperature, pH, electrical conductivity (EC), dissolved oxygen (DO), total suspended solids (TSS), total alkalinity as $CaCO_3$ (alkalinity), orthophosphates as phosphorus (PO_4P), total phosphorus (TP), ammonium as nitrogen (NH_4N), nitrate as nitrogen (sum of NO_3N and NO_2N), 5 days biochemical oxygen demand as O_2 (CBOD or BOD) and chemical oxygen demand as O_2 (COD).

2.1 Hydraulic modeling:

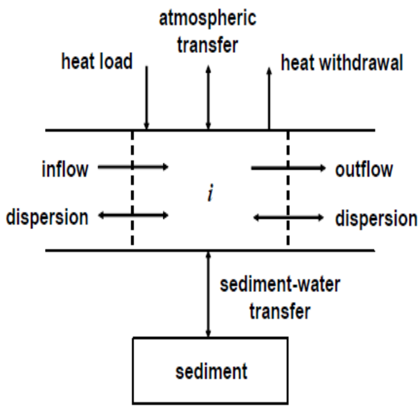
Once the boundaries of each reach are defined, QUAL2K will determine the water depth and velocity using Manning's equation

$$Q = \frac{S_0^{1/2} A_c^{5/3}}{n P^{2/3}} \quad (1)$$

Where, Q is the discharge in $m^3 s^{-1}$, S_0 is the bottom slope, A_c is the cross-sectional area in m^2, n is Manning's roughness coefficient, and P is the wetted perimeter in meters. QUAL2K can also determine water depth and velocity based on weir heights and rating curves.

2.2 Heat balance: By performing a heat balance on each element in the study area, temperature is modelled in QUAL2K. Transfer of heat in the model includes the inflow and outflow of heat from water flowing into and out of the particular element. The model also takes into account the water flowing into and out of each element from point and non-point inputs and withdrawals. Dispersion of heat, heat transfer to and from the atmosphere, and heat transfer to and from sediments are also included in the heat balance for each element.

Fig 1: Heat Balance for an Element



3.0 Modelling Tool

QUAL2Kw has a general mass balance equation for a constituent concentration in the water column of reach(Pelletier et al.,2006) which is given by:

$$\frac{dC_i}{dt} = \frac{Q_{i-1}}{V_i} C_{i-1} - \frac{Q_i}{V_i} C_i - \frac{Q_{ab,i}}{V_i} C_i + \frac{E'_{i-1}}{V_i}(C_{i-1} - C_i) + \frac{E'_i}{V_i}(C_{i+1} - C_i) + \frac{W_i}{V_i} + S_i$$

The general mass balance for the model constituents in element *i* (except bottom algae and sediments) is written as follows: where Q_{i-1} is flowrate from the i - 1th element, $L^3 T^{-1}$, Q_i is flowrate from the *i*th element, $L^3 T^{-1}$, $Q_{out,i}$ is total out flow from the *i*th element due to point and non-point withdrawals, $L^3 T^{-1}$, V_i is the volume of the *i*th element, L^3, E'_{i-1} is the bulk dispersion coefficient between elements i - 1 and i, $L^3 T^{-1}$, E'_i is the bulk dispersion coefficient between elements i and i + 1, L3 T-1, C*i*-1 is the constituent concentration in the *i* – 1th element, M T-1, *ci* is the constituent concentration in the *i*th element, M T-1, *ci+1* is the constituent concentration in the *i* + 1th element, M T-1, *Wi* is the external point and non- point source loading of the constituent to the *i*th element, M T-1, and *Si* is sources and sinks of the constituent due to reactions and mass transfer mechanisms in the *i*th element, M L-3 T-1. The *Si* term in the mass balance is the generic term for a variety of different biological, chemical, and physical reactions which may occur in each model element.

Fig 2: Transformation of a Hypothetical River (a) Into the QUAL2K Representation of That River (b) (Adapted From Chapra Et Al. 2006).

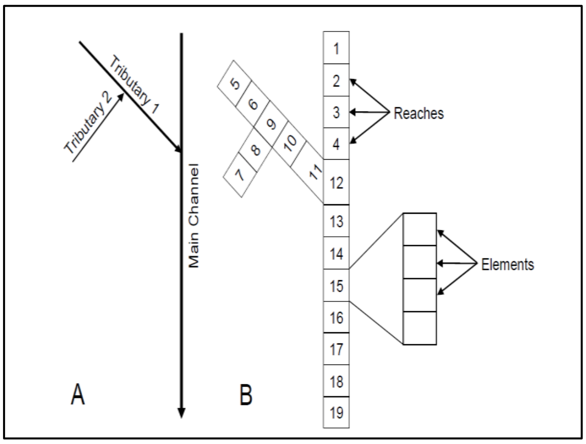


Fig 3: QUAL2K Segmentation Scheme for a River with No Tributaries

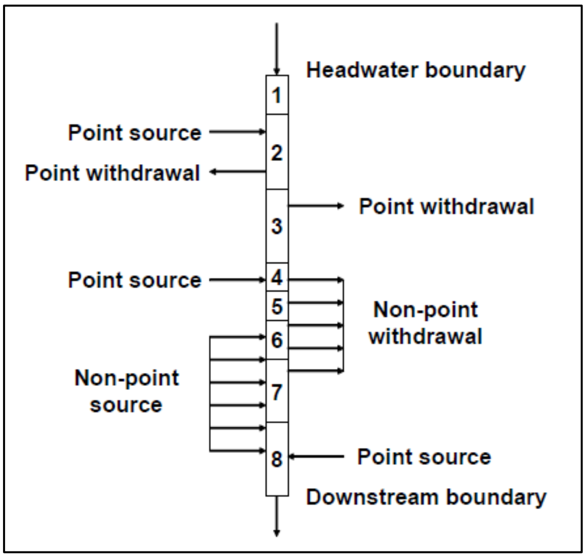


Fig 4: Processes Included in the General Mass Balance in the Modelling of QUAL2K Water Quality Parameters for a Segment Without a Tributary (Adapted From Chapra Et Al. 2006).

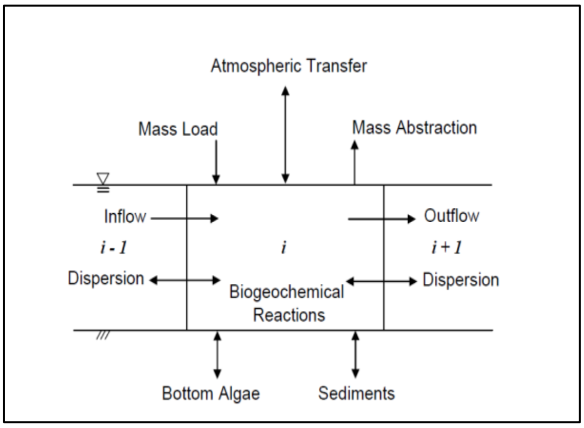


Table 1: Water Quality Parameters Simulated in the QUAL2K Model

Variable	Symbol	Units
Specific conductivity	s	µmhos/cm
Inorganic suspended solids	m_i	mgD L^{-1}
Dissolved oxygen	o	mgO_2 L^{-1}
Slowly reacting CBOD	c_s	mgO_2 L^{-1}
Fast reacting CBOD	c_f	mgO_2 L^{-1}
Organic nitrogen	n_o	µgN L^{-1}
Ammonia nitrogen	n_a	µgN L^{-1}
Nitrate nitrogen	n_n	µgN L^{-1}
Organic phosphorus	p_o	µgP L^{-1}
Inorganic phosphorus (orthophosphate or soluble reactive phosphorus)	p_i	µgP L^{-1}
Phytoplankton biomass	a_p	µgA L^{-1}
Detritus	m_o	mgD L^{-1}
Pathogen	X	cfu 100 mL^{-1}
Alkalinity	Alk	mgCaCO_3 L^{-1}
Total inorganic carbon	c_T	mole L^{-1}
Bottom algae biomass	a_b	mgA m^{-2}
Bottom algae nitrogen	IN_b	mgN m^{-2}
Bottom algae phosphorus	IP_b	mgP m^{-2}

Source: Chapra et al. 2006

3.1 Model calibration and confirmation

3.1.1 Input data:

The river geometries, its depth and water velocities were used to determine the hydraulic characteristics at each sampling locations of the streams. The model inputs the hydraulic characteristics of the river for each reach (i.e. coefficients and exponents of velocity and depth) as empirical equations to estimate average water velocity (*V*) and depth (*D*) of the river:

V = aQb and D = cQd - (2)

The coefficients a,c and exponents b,d were computed using flows, mean depth and velocities measured in the winter and post-monsoon seasons.

The water quality input parameters included in the model were flow, temperature, pH, DO, BOD, organic nitrogen, ammonium nitrogen, nitrate (nitrite + nitrate) nitrogen, organic phosphorus and inorganic phosphorus.

Table 2: Kinetic Processes and Mass Transfer Processes Incorporated in the QUAL2K Model.

Kinetic Processes	Mass Transfer Processes
Dissolution	Reaeration
Hydrolysis	Settling
Oxidation	Sediment Oxygen Demand
Nitrification	Sediment Exchange
Denitrification	Sediment Inorganic Flux
Photosynthesis	
Death	
Respiration/Excretion	

3.2 Prototype representation:

QUAL2E permits simulation of any branching, one-dimensional stream system.

The first step of modelling is to subdivide the system into the reaches having the uniform hydraulic characteristics. Each reach is then divided into computation element which has equal length. So, all the reaches have the computation elements.

There are total seven computation elements:

1. Headwater element
2. Standard element
3. Element just upstream from the junction
4. Junction element
5. Last element in the system
6. Input element
7. Withdrawal element

3.3 Model limitations:

- Reaches : maximum of 25
- Computation elements: no more than 20 per reach or total of 250
- Headwater elements : maximum of 7
- Junction elements : maximum of 6
- Input and withdrawal elements : maximum of 25

4.0 Systematic Parameters

Mathematical model: Used to simulate the prototype behaviour by applying a mathematical model on a digital computer proceeds through three phases:

1. **Conceptual representation**: It involves a graphic idealization of the prototype by description of geometric properties and by the identification of boundary conditions.
2. **Functional representation**: Formulation of physical features, processes and boundary conditions into set of algebraic equations.
3. **Computational representation** : Functional model is transformed into mathematical forms

4.1 Program language and operating requirements:

QUAL2K and QUAL2Kw are open sources, which are very cost-effective and the main advantage of these modelling software are that they are packaged as an Excel Workbook. It is implemented within the Microsoft Excel. Excel is used as an interface for the input, output and running of the model. And because of this major quality, sharing of the model become very simple and quick because no special software needs to be purchased and no installation is necessary.

The programming of the model is written entirely in Visual Basic for Applications (VBA) programming language, which is Excel's Macro coding language and numerical integration during modelling is performed by a compiled FORTRAN 95 program which is run by Excel VBA program. FORTRAN execution has proven to be very time efficient during multiple model runs as it is much faster than the VBA execution (seconds vs. minutes). The genetic algorithm used in QUAL2KW is called PIKAIA which essentially models natural selection to derive the optimal rate parameters and fitness of the model (Charbonneau & Knapp, 1995; Pelletier et al., 2006; Pelletier & Chapra 2008). PIKAIA is incorporated into QUAL2Kw as an Excel VBA Macro.

Some of the major limitations include:

1. Non-uniform mixing (2D or 3D);
2. Unsteady flow;

3. Watershed processes;
4. Reservoirs;
5. Sediment adsorption/desorption.

5.0 Conclusions

QUAL2K and QUAL2Kw output data can be viewed in tabular or graphical format within Excel. The model produces diurnal data for each reach, and also tabulates the average, maximum, and minimum value of each parameter or constituent for each reach of the stream system. The average, minimum, and maximum values of each modelled parameter are automatically organized into three separate tabs within the QUAL2K model and it gives a 24-hr diurnal plot of specified parameters for each reach of the system or a plot of the average, maximum, and minimum values for each parameter as a function of distance downstream. Using a Macro in Excel is an ideal approach for a number of reasons. The entire QUAL2Kw model can be run using Macros by clicking the "Run VBA" macro button, so adding one more macro to export the desired output data.

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