Re-oxygenation Coefficient in QUAL2E: a Prediction Methodology

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The water quality model QUAL2E has been applied worldwide to modeling dissolved oxygen (DO) and biochemical oxygen demand (BOD) in rivers. The model is an important management tool for environmental impact studies, however a difficulty relating to its application for DO and BOD computations is the quantification of the re-aeration or re-oxygenation coefficient K_2 . The procedure used to establish K_2 is extremely important if the model is to represent real water stream conditions. A simple methodology for estimating QUAL2E input parameters related to re-aeration coefficient calculations based on open channel hydraulic characteristics is described in this chapter. It aims to give guidelines to professionals and researchers who plan to use QUAL2E. A brief review of the re-aeration process in water streams is briefly reviewed.

10.1 Modeling and the QUAL2E Model

Modeling consists of simplifications based on hypotheses about the structure and behaviour of a physical system. Using a model one tries to explain the properties of the system and estimate its response to different stimuli. Through a model it is possible to quantify a river's self-purification capacity and then to foresee the impacts resulting from a waste discharge. This way, the model can indicate the reason why some management alternatives are better than others, thus presenting an important tool for environmental impact studies. According

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to Thomann and Mueller (1987), surface water quality modeling brings a better knowledge of the mechanisms and interactions that justify various water quality behaviours, and comprises a rational base for decision making on stream water management.

QUAL2E has been developed by researchers world-wide in the last 30 years and has a long history of usage (Bittencourt et al., 1995; Cubillo et al., 1992); Demetracopoulos and Stefan, 1983a; Gastaldini, 1982; Lo and Chen, 1991; Siqueira, 1996; Walton and Webb, 1994). QUAL2E computes the changes of several water components such as DO, coliforms, temperature, nitrogen, phosphorus, conservative and non-conservative components. Barnwell et al., (1989) mention that this model has been mainly applied to dissolved oxygen. QUAL2E has proven to be effective for dissolved oxygen modeling analysis in rivers and contains one of the more sophisticated kinetics of current water quality models (Walton and Webb, 1994). One difficulty related to its application for DO and BOD is the quantification of the re-aeration or re-oxygenation coefficient, K_2 .

10.2 Re-oxygenation and its Quantification

The process of oxygen exchange between atmosphere and the water stream is called re-aeration or re-oxygenation. Oxygenation is the physical absorption of oxygen from the atmosphere into flowing water. In running waters, re-aeration has an extremely important role in maintaining aerobic and facultative aquatic life because it brings in oxygen from the atmosphere in a natural way to the aquatic medium. Currently re-aeration in streams is still being extensively investigated (Qaisi and Thibodeaux, 1997; Thibodeaux et al., 1994; Koh et al., 1995; Moog and Jirka, 1999a; Moog and Jirka, 1999b; Weiss, 1998).

Several models for the quantification of the coefficient K_2 exist. Rathbun (1977), in a review about re-aeration coefficient in flowing waters, emphasised three measuring techniques: the oxygen balance technique, the disturbed balance technique and the tracer technique. Besides these three methods, Bicudo and James (1989) and Giorgetti (1991) described an indirect method for quantifying the re-aeration coefficient using a soluble probe. Bennett and Rathbun (1972, p.58) concluded that the technique using tracers is better than other techniques used for quantifying the re-aeration coefficient in open channels because it has the advantage of measuring re-aeration independently of other DO sources and sinks in water. Barbosa and Giorgetti (1995) reaffirmed that the most acceptable method is the gaseous tracer technique. However this method requires considerable field and laboratory work, specialised equipment and skilled technicians.

Although the gaseous tracer technique is the most recommended, from the technical point of view, Rathbun, 1977) indicates that in some studies of water quality modeling no technical or financial conditions are available to perform such field measurements. In this case, the use of predictive equations for K_2 based on literature is most appropriate.

These equations should be used with caution, realising the experimental conditions in which they were generated. Preferentially, they should be applied in similar hydraulic conditions, being aware of their accuracy and limitations. It is common that these different methods will present quite different results for the same hydraulic conditions.

Moog and Jirka (1999a) mentioned that errors remain large in these equations, pointing to a need for additional investigation. In an evaluation of ten commonly used equations Moog and Jirka (1998) found values of K_2 in error by a factor of two or greater from measured values in more than half of the cases; many produced five-fold errors in more than 10% of cases. Moog and Jirka (1999b) also presented a model then still under development which could provide proper scaling for oxygen transfer in small-roughness flows by accounting for the increase in near-surface turbulent energy dissipation rates.

QUAL2E offers eight K_2 calculation options; six predictive equations from literature and two options for measured values. The six predictive equations for K_2 incorporated in the QUAL2E model were analysed by several authors (Bowie et al., 1985; Bennett and Rathbun, 1972; Schultz, 1989) and are listed in Table 10.1. QUAL2E model equations are mostly empirical and semi-empirical equations are proposed for relating K_2 to measurable flow parameters like velocity and depth. These equations were obtained from regression analysis of field data.

Barbosa (1989) mentions that the semi-empirical formulations have been obtained from a theoretical model for the mass transfer process and that their coefficients were determined by regression analysis of experimental data. Empirical formulae were obtained from dimensional analysis, involving flow and gas-liquid system mean parameters and from regression analysis that determined the equation that best fitted the experimental data. Some equations include factors like Froude Number, friction velocity and others. Formulations include Froude Number ($Fr = U / \sqrt{gH}$) in an attempt to consider the wave action effects and other surface disturbances affecting re-aeration. Once the turbulence generated at the bottom of the channel can be seen at the surface level, the friction velocity ($u^* = \sqrt{gHS}$), in terms of the slope of the energy grade line or channel slope, S , is also included in some equations.

Table 10.1 Predictive equations in small roughness for the re-aeration coefficient, K_2 (day⁻¹), in logarithmic base 10 at 20 °C, incorporated in QUAL2E (Siquera, 1996).

Authors	Equations (SI Units)	Equations (English System)
CHURCHILL et al., (1962)	$5.03 \frac{U^{0,969}}{H^{1,673}}$	$11.6 \frac{U^{0,969}}{H^{1,673}}$
LANGBEIN and DURUM (1967)	$5.14 \frac{U}{H^{1,33}}$	$7.6 \frac{U}{H^{1,33}}$
O’CONNOR and DOBBINS (1958)	$3.93 \frac{U^{0,5}}{H^{1,5}}$	$12.9 \frac{U^{0,5}}{H^{1,5}}$
OWENS et al., (1964)	$5.34 \frac{U^{0,67}}{H^{1,85}}$	$21.7 \frac{U^{0,67}}{H^{1,85}}$
TRACKSTON and KRENKEL (1969)	$\frac{24.9(1 + F^{0,5})u^*}{H}$	$\frac{24.9(1 + F^{0,5})u^*}{H}$
TSIVOGLOU and WALLANCE (1972)	$86400cSU$	$86400cSU$

g = gravity acceleration, (m/s²)
V = mean velocity in the river stretch,
(ft/s) or (m/s)
H = mean depth in the river stretch ,
(ft) or (m)
S = slope in the river stretch,
(ft/ft) or (m/m)
U* = shear velocity, (ft/s) or (m/s)
F = Froude Number, (dimensionless)
($Fr = V / \sqrt{gH}$)
Q = flow rate, (ft³/s) or (m³/s)

Units in English System:
c = 0.054 ft⁻¹ for 15 ft³/s ≤ Q ≤ 3000 ft³/s
Units in International System (SI):
c = 0.177 m⁻¹ for 0.42 m³/s ≤ Q ≤ 84.96m³/s

10.3 Re-oxygenation Coefficient Quantification for the QUAL2E Model, Methodology

Table 10.1 shows that K_2 calculation for the QUAL2E model is made from water stream flow characteristics (mean depth, slope and mean velocity). These hydraulic characteristics, however, are indirectly calculated in QUAL2E as a function of flow rate, through two methods: discharge coefficients or Manning coefficient for trapezoidal cross section.

The user selects the method for computer simulation. According to Barnwell et al. (1989), preference should be given to the discharge coefficient method, since error occurs in the K_2 calculation resulting from estimating Manning coefficient for a trapezoidal cross section.

For the discharge coefficient method, mean velocities and depths are calculated as a function of the flow rate (Q), using the following equations:

$$V = aQ^b \quad (10.1)$$

$$H = cQ^d \quad (10.2)$$

where:

- H = depth (L);
- a, b, c, d = discharge coefficients;
- V = stream mean velocity (LT^{-1}).

Obtaining the necessary data for re-aeration coefficient calculation requires fieldwork followed by computer work. Initially, discharge coefficients (a, b, c, d) for a water stream should be determined using field observations from a river stretch selected for estimating the discharge coefficients. A location with a representative cross section should be determined. At this location flow rates, depth and mean velocity are measured. These measurements should be taken at at least three different times of the year in order to include a considerable variation in the flow rates. This variation should include the flow rates range at the location where the model will be used for computer simulations. The choice of the flow rate measurement method should be made according to local conditions, availability of measuring equipment, human resources and site characteristics.

Data are plotted twice, the first graph showing mean depth versus flow rate and the second, mean velocity versus flow rate, as shown in Figure 10.1. From the graphs, with the support of a regression program, a non-linear adjustment is made in order to determine coefficients a, b, c , and d in Equations 10.1 and 10.2. These coefficients are incorporated into the model. The model also requires other data for the re-aeration coefficient calculation, however these are not discussed in this chapter.

When a simulation for a given flow rate condition is desired, flowrate-related velocities and depths are calculated and QUAL2E then calculates the re-aeration coefficient, K_2 .

Figure 10.1 Method stages - schematic flowchart(Siqueira and Cunha, 1997)

10.4 Conclusion

Three field quantification methodologies for K_2 are discussed, the tracer technique being currently the most widely accepted. When the financial, technical and human resources conditions are insufficient for tracer testing, the re-aeration coefficient has to be obtained by predictive equations from literature.

A simple methodology for quantifying re-aeration, K_2 has been described for application to QUAL2E. For proper re-aeration coefficient determination in a given river stretch using the QUAL 2E model empirical and semi-empirical equations, at least three field measurements are required at different conditions of flow rate, followed by statistical data analysis.

Finally, until more detailed studies are conducted determining self purification in streams subject to waste water dumping, the proposed methodology appears to be a viable alternative for determining environmental impacts in flowing waters.

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