# Steady and non-steady flow models for simulation of water quality in rivers

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Models for unsteady conditions were developed ABSTRACT by improving the solution of St Venant equations due to the need to solve an estuary type of problem. An unsteady water quality model which solves flow equations through a forward implicit finite difference scheme and the transport equation by a backward implicit finite difference scheme is compared to the Qual-I model which is a steady flow model. The comparison is done on the Sinos River (Brazil), a highly polluted river, based on the BOD and DO water quality parameters. Sources of pollution were evaluated and the level, flow and water quality parameters were recorded at time intervals. Results showed the influence of flow behaviour on the transport processes and the need for an unsteady flow model for that type of river.

## INTRODUCTION

Low flow during the dry season is the water quality critical condition for most of the rivers. Usually a steady uniform or nonuniform flow condition is assumed in order to simulate the transport equation.

Streeter and Phelps (1925) published the first theoretical model of stream waste assimilative capacity using a uniform flow assumption. The Qual-I model by the Texas Water Development Board (1971) is based on a non-uniform steady flow equation. These models are very useful when the flow does not change much during the critical period.

During the low flow season in rivers near an estuary, the upstream condition is almost a constant discharge but in some reaches downstream, the flow changes due to tidal effect. Water quality simulation in such cases is often done by a steady model, assuming the upstream discharge as constant and disregarding the downstream daily flow fluctuation. This simplification could be serious when flow amplitude is high, which creates a need for unsteady flow models. This paper explores the use of both types of models in such a situation showing the flow effect on the substance concentration distribution. 236 C.E.M. Tucci & L. Moretti

MODELS

Governing Equations

The gradually varied unsteady flow in a river can be described by two partial differential equations: the continuity equation which takes into account the continuity of the mass flow and the momentum equation which represents the dynamics effects of the flow.

The two basic St Venant equations are:

$$\frac{\partial Q}{\partial x} + T \frac{\partial Y}{\partial t} = q_e$$
(1)  
$$\frac{\partial Q}{\partial t} + \frac{\partial (QV)}{\partial x} + gA \frac{\partial Y}{\partial x} = \rho gA(S_o - S_f)$$
(2)

in which x = the horizontal distance along the channel; t = time; A = the cross-sectional area; Q = the flow discharge; T = top width; q = the lateral inflow; v = the mean flow velocity; y = the flow depth; g = the gravity acceleration; S = the mean bed slope; S = the friction slope.

<sup>I</sup> The transport of mass in an environment is due to the advection, diffusion and dispersion processes. The one-dimensional transport equation is:

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(QC)}{\partial x} = \frac{\partial}{\partial x} (EA \frac{\partial C}{\partial x}) + S_{i}$$
(3)

where E is the longitudinal dispersion coefficient, S, accounts for the losses and gains of the system, C is the substance concentration.

The source and sink term used for biochemical oxygen demand is

$$S_{i} = (K_{1} + K_{3})AC + AL_{a} + q_{e}C_{e(bod)}$$
 (4)

where  $K_1$  is the BOD carbonaceous reaction rate  $(day^{-1})$ ,  $K_3$  is the rate coefficient for the removal of BOD by sedimentation and adsorption  $(day^{-1})$ ,  $L_1$  is the rate of addition of BOD along the reach  $(ppm \ day^{-1})$  and  $C_{e(bod)}$  is the concentration of BOD in the lateral flow (ppm).

The source and sink term for dissolved oxygen used is:

$$S_{i} = K_{1}AC_{bod} + K_{2}A(C_{s}-D) - D_{b}A + q_{e}C_{e(do)}$$
(5)

where C<sub>bod</sub> is the BOD concentration (ppm), K<sub>2</sub> is the reaeration coefficient (day-<sup>1</sup>), C is the saturation dissolved oxygen concentration (ppm), D<sub>b</sub> is the removal of oxygen by benthal deposits and plant respiration and the increase in oxygen through photosynthesis (pp day-<sup>1</sup>), and C<sub>e(do)</sub> is the concentration of DO in the lateral flow (ppm).

## Water Quality Steady Model

The Qual-I model developed by the Texas Water Development Board (1971) is based on a steady continuity equation, in which the flow

coming out of a reach is the algebraic sum of the upstream reach flow and the tributary or lateral flow. The uniform flow relationship given by the rating curve and the velocity-discharge function are the relations used in each reach by the hydraulic part of the model. The flow is constant but the velocity and depth may vary from reach to reach.

The transport equation used is equation 3. Since Q is constant it comes from the second derivative term. This is a parabolic partial differential equation. Numerical solution of this equation is performed by an implicit backward scheme.

$$\frac{\partial f}{\partial x} \cong \theta \left( \frac{f_{i} - f_{i-1}}{\Delta x} \right)^{t+1} + (1-\theta) \left( \frac{f_{i} - f_{i-1}}{\Delta x} \right)^{t}$$

$$\frac{\partial^{2} f}{\partial x^{2}} = \frac{1}{\Delta x^{2}} \left[ \theta \left( f_{i+1} - 2f_{i} + f_{i-1} \right)^{t+1} + (1-\theta) \left( f_{i+1} - 2f_{i} + f_{i-1} \right)^{t} \right]$$

$$\frac{\partial f}{\partial t} \cong \frac{1}{\Delta t} \left( f_{i}^{t+1} - f_{i}^{t} \right)$$
(6)

where  $0 \le \theta \le 1$  . Applying the scheme to equation 3 for a general section, i yields:

$$L_{i} c_{i-1}^{t+1} + M_{i} c_{i}^{t+1} + N_{i} c_{i+1}^{t+1}$$
(7)

where  $L_{i}$ ,  $M_{i}$ ,  $N_{i}$  and  $C_{i}$  are functions of A, E, Q, x,  $\theta$ . This model uses  $\theta = 1$ . Equation 7 is applied to the river reaches resulting in a system of equations which is solved for each time step. This type of equation requires the specification of the initial and boundary conditions. In steady flow models the initial concentrations are not so important because one is often concerned with steady-state concentration profiles and the simulation converges to it after several time steps. The boundary conditions should be specified in order to solve this system of equations. Assuming that the river has two boundaries they can be specified by the following procedures; (a) when the concentration function of time at the boundaries is known, (b) assuming the concentration does not change with x at the downstream boundary; (c) assuming the second partial derivative of the concentration is equal to zero, which means the concentration has a linear relationship with x at the boundary. If conditions b and c can be used, then the point source is far from the boundary.

#### Water Quality Unsteady Flow Model

Tucci (1978) presented a finite difference water quality model for a river network. This model uses an implicit scheme to solve equations 1 and 2.

$$\frac{\partial f}{\partial x} \cong \left(\frac{f_{i+1} - f_i}{\Delta x}\right)^{t+1}$$

$$\frac{\partial f}{\partial t} \cong \frac{1}{2\Delta t} \left[ \left(f_i + f_{i+1}\right)^{t+1} - \left(f_i + f_{i+1}\right)^{t} \right]$$
(8)

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in which f is a variable representing Q, y, A, etc., substituting the numerical scheme in equation 8 into equations 1 and 2 for reaches, results in a set of linear equations. A detailed formulation on the system of linear equations is given by Tucci (1978). Adding the boundary equations to this set of linear equations results in the total number of equations being equal to the number of unknowns. This permits solution of the equations. In order to proceed with the calculations it is necessary to specify the stages and discharges at all computation sections at the initial time step. Usually these values are not known and should be estimated. In a river reach with two boundary sections, there is an option to specify stages, discharges or stage discharge relations as the boundary conditions. When the flow is subcritical, it is necessary to specify one condition at the upstream boundary and the other at the downstream boundary.



FIG. 1 Sinos River.

The transport equation is solved by the numerical scheme of equation 6. In this model  $\theta$  is not permanent, it can be chosen by the user.

Simulation is done by first solving equation 1 and 2 and then in the same time step, equation 3. It is called an uncoupled solution. The transport equation is solved for each parameter, first for BOD and later for DO.

#### THE DATA

The River Sinos flows into the Jacui Delta, a small delta located in the south of Brazil in the State of Rio Grande do Sul. The Jacui Delta is a complex system of branches, confluences and storage basins. Below the downstream section of the Delta, there are a series of large lakes that are linked together until they reach the Atlantic Ocean.

The River Sinos has a basin area of about 3700 km<sup>2</sup> and 190 km channel length. The water level in this delta shows a cyclic variation with an amplitude of about 30 cm within a 24 hour time period. This cyclic variation is sometimes altered by wind effects or floods. In the dry season when the flow is low a flow inversion can occur due to the backwater effects from the lakes. The downstream effects on the river are felt up to 44 km upstream. Domestic and industrial waste are dumped directly into this river reach without treatment (figure 1). The BOD and the discharge of large amounts of waste effluent were recorded and are presented in Table 1.

Number on Figure 1	Identification	Discharge	BOD <sub>5</sub>
		(l s- <sup>1</sup> )	(ppm)
1	Paper factory (I)	51	395
2	J. Correia Creek (urban waste)	95	170
3	Portao Creek (urban waste)	161	291
4	J. Joaquim Creek (urban waste)	15	55
5	Riogradense Steel Mill	275	18
6	Pirelli factory	22	4
7	Vacchi tannery	29	421
8	Lansul factory	14	160
9	Paper factory	22	81
10	SAMRIG factory	141	408
11	Petrobras refinery	156	14

TABLE 1 BOD concentration from the waste disposals

There are municipal and State companies recording BOD and DO in this river. Also, in a research programme, the Institute of Hydraulic Research (IPH) has 15 sections where these parameters are recorded. The sampling is often done weekly. The IPH made a continuous recording (four hour intervals) of BOD and DO at these 15 sections during 24 hours (1200 hours 24 April, 1978 to 1200 hours 25 April, 1978). During this field compaign the flows were recorded (t = 4 h) at section 14 and levels (t = 0.5 h) at 5 sections. During those 24 hours the flow at section 14 ranged from 16 to 18 m<sup>3</sup>s<sup>-1</sup>.



FIG. 2 DO Concentration profiles - steady flow water quality simulation.

The geometrical characteristics of 14 sections in 44.1 km reach length were obtained together with their reference levels. Upstream on the River Sinos there is a stage station with a long record and rating curve. This section does not suffer backwater effects. RESULTS

The water quality data was classified according to upstream discharge. These data which were collected under similar conditions of flow and temperature were put together. The Qual I model was applied using 15 sections and 67 km of river. The numerical discretization was  $\Delta x = 1610$  m and  $\Delta t = 3$  h. The hydraulic data was obtained through the geometrical characteristics of the sections.

The flow is the upstream boundary condition. The lateral inflows of waste effluent were taken into account.

The water quality parameters  $K_2$  reaeration coefficient and  $K_1$  BOD carbonaceous reaction rate were adjusted based on the  $q = 16 \text{ m}^3 \text{s}^{-1}$  profile (figure 2d). The best adjusted  $K_2$  was obtained through the O'Connor & Dobbins (1956) equation. The adjusted value of  $K_1$  was 0.15 day<sup>-1</sup>. The  $K_3$  parameter was not taken into account. The dispersion coefficient was calculated internally in the programme by the modified Taylor's equation (Harleman, 1971). The steady profile of the model was well fitted to the banded samples concentrations along the river. The Qual I fitted parameters were verified for three other profiles (figure 2a, b and c) with upstream discharge ranging from 20 to  $32 \text{ m}^3 \text{s}^{-1}$ . The results presented in figure 2 for all profiles show that the model fitted the recorded concentration of DO very well. The results on BOD are similar.

When the upstream flow was  $4 \text{ m}^3 \text{s}^{-1}$ , the Qual I simulation with the parameters determined gave poor results (figure 4a and b) due to flow variation in the reach from section 5 to 14 (figure 1). It can be seen in figure 4 that the DO profile starts to be unreliable downstream from section 5.

The unsteady water quality model described was applied to this set of data. The 14 sections of figure 1 were used, the  $\Delta x$  of the sections ranged from 2.2 km to 3.8 km. First the roughness coefficient from Manning's equation was fitted using the hydraulic data. The boundary conditions were the levels at section 1 and 14 during 24 hours. The initial conditions were the recorded and interpolated values at 1200 h on 24 April 1978. The time step chosen for calculations was 30 min. The adjusted roughness was 0.03 and results are presented in figure 3. It can be seen that the calculated levels and the hydrograph are very well fitted to the recorded values.

The K<sub>1</sub> parameter adopted was the same one adjusted in the steady simulation (K<sub>1</sub> = 0.15). The reaeration coefficient predicted by the equations developed for unidirectional rivers estimated small values due to low velocities. The Kanishwer (1963) equation applicable to estuaries were used based on depth and wind velocity. The longitudinal dispersion coefficient was calculated by the modified Taylor's equation. The concentration boundary conditions were those recorded at sections 1 and 14. The initial conditions were the recorded and interpolated values.

In order to allow for direct comparison, the results were grouped in two sets, the first are corresponding to positive flow in the downstream reach  $(Q_{14})$  and the second one to negative flow. The unsteady model simulations presented in figure 4 are the profiles of 16 h (4/24) and 8 h (4/25). Those profiles shows that this model follows the river concentration distribution and those concentration peaks are mainly due to the flow inversion. Downstream from section



FIG. 3 Level and flow on 24 and 25 April 1978 in River Sinos.

14 is the delta, in which water is not polluted and with greater discharge than in the River Sinos, which improves the DO when the discharge is negative. It can also be seen that for  $Q_{14}(+)$  the profile is low since the dilution discharge comes only from upstream. The small concentration peak is due to the non-uniform flow distribution in the transient behaviour.



FIG. 4 DO and BOD profiles for steady and unsteady flow water quality simulation at River Sinos.

The lower limit for application of the steady model was around 15  $m^3s^{-1}$  for upstream flow with a 25% probability of occurrence. Below this value the downstream effects are important. The upstream discharge of 4  $m^3s^{-1}$  has about 5% of probability.

## CONCLUSION

The water quality in water courses where the flow changes continuously due to downstream tidal effects cannot be accurately simulated by steady flow transport models. The critical condition, which is a low flow upstream, increases the tidal influence upstream of the river mouth.

For the River Sinos, this upstream flow direction increases the river oxygen capacity during the inversion flow period because the delta downstream has a high oxygen concentration, but it could be worse if the situation were inverted.

The steady flow solution which under-estimated the DO concentration was unreliable. If it were used in order to design treatment plants, cost would be higher.

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