NUMERICAL ANALYSIS TO RESOLVE POLLUTED RIVER FLOW

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Channel characteristic in middle part of the lower Tapti River (Loaction: Mandavi Gujrat).

Abstract

A simple mathematical model for river pollution is presented and investigates the effect of aeration on the degradation of pollutant. The model consists of a pair of coupled reaction–diffusion–advection equations for the pollutant and dissolved oxygen concentrations, respectively. The coupling of these equations occurs because of reactions between oxygen and pollutant to produce harmless compounds. Here we consider the steady-state case in one spatial dimension. For simplified cases the model is solved analytically. We also present a numerical approach to the solution in the general case. The extension to the transient spatial model is relatively straightforward. The study is motivated by the crucial problem of water pollution in many countries and specifically within the Tapti River in India. For such real situations, simple models can provide decision support for planning restrictions to be imposed on farming and urban practices.

Keywords: Pollution; Dispersion; Aeration; Michaelis–Menten model; Decision support

1. Introduction

Industrial or domestic Water pollution from human originated activities is a burning problem in so many countries [Tchobanoglous, G. Burton F.L. 1991]. As a result of water pollution, approximately 25 million persons die every year. Developing models to enable to understand how to control and predict water quality is of crucial interest. When assessing the quality of water in a river, there are many factors to be considered: the level of dissolved oxygen; the presence of nitrates, chlorides, phosphates; the level of suspended solids; environmental hormones; chemical oxygen demand, such as heavy metals, and the presence of bacteria. Pollutants from agricultural operations can be a significant contributor to the impairment of surface and groundwater quality [Knight, R.L. . Payne Jr., V.W.E Borer, R.E. Clarke Jr., R.A. Pries J.H. 2000].

Models of Mathematical water quality date back to the 1920s: in 1925, the well-known model of Streeter and Phelps [Streeter, H.W. Phelps E.B. 1925] described the balance of dissolved oxygen in rivers. Following this model has been amended in various ways (cf. [James, A. Beck (Ed.), M.B. 1987]).

The primary purpose of the present study was to investigate the alleviation of pollution by aeration within a flowing river contaminated by distributed sources and the associated depletion of dissolved oxygen. [Gupta, S.K., 2011] The particular river whose water quality was the motivation for the study is the Tapti River in India. It is assumed that the pollutants are largely biological wastes which undergo various biochemical and biodegradation processes using dissolved oxygen. For fish to survive we require dissolved oxygen concentrations everywhere to remain at least at 30% of the saturated value [Murphy, S., 2007] and so this helps to set limits on how much pollution can be tolerated. Simplified models for this real situation will aid decisions concerning future restrictions to be imposed on farming and urban practices.

2. Description of the mathematical model

The flow in the river as being one-dimensional is modelled, using a single spatial parameter $x\,(m)$ to describe the distance down the river from its source. Quantities, such as pollutant or oxygen concentrations, are only allowed to vary along the length of the river and they are treated as homogeneous across the river cross-section. This assumption is justified by fulfilling Dobbins' criterion [Dobbins BOD W.E. and Oxygen 1964]. For the present we allow for variation with time t (days); however, in the latter part of the work we focus on seeking steady-state solutions and so we will drop the time dependence. A single quantity to measure water pollution is used the concentration.$P(x,t)(\text{kg m}^{-3})$ Dissolved oxygen within the river has concentration.$X(x,t)(\text{kg m}^{-3})$ This latter quantity is crucial both for the survival of aerobic communities living in aquatic systems and also for the potential remediation of some of the unwanted pollutants by oxidation.

Table 1.
Variables and parameter values

Parameters	SI units
L is the polluted length of river (m)	325,000[a]
D_p is the dispersion coefficient of pollutant in the x direction ($\text{m}^2\ \text{day}^{-1}$)	3,456,000[a]
D_x is the dispersion coefficient of dissolved oxygen in the x direction ($\text{m}^2\ \text{day}^{-1}$), taken to be the same as D_p	3,456,000
v is the water velocity in the x direction (m day^{-1})	43,200[a]
A is the cross-section area of the river (m^2)	2100[a]
q is the rate of pollutant addition along the river ($\text{kg m}^{-1}\ \text{day}^{-1}$)	0.06[a]
K_1 is the degradation rate coefficient at 20 °C for pollutant (day^{-1})	8.27[c]
K_2 is the de-aeration rate coefficient at 20 °C for dissolved oxygen (day^{-1})	44.10[b]
k is the half-saturated oxygen demand concentration for pollutant decay (kg m^{-3})	0.007[d]
α is the mass transfer of oxygen from air to water ($\text{m}^2\ \text{day}^{-1}$);	16.50[b]
This is calculated as a product: re-aeration rate $\times A'$; the re-aeration rate is 0.055 day^{-1}[b] and A' (the top surface area per unit length) is the product of the river width of 300 m with the unit length (1 m).	
S is the saturated oxygen concentration (kg m^{-3})	0.01[b]

a [8]
b [7]
c Based on the molecular weights in the chemical reaction $K_1 = (3/16)\,K_2$
d Estimated

The model consists of two joined advection–dispersion equations. These equations account for the evolution of the pollutant and the dissolved oxygen concentrations, respectively. The rates of change of the concentration with position x and time t are expressed as

$$\frac{\partial(AP)}{\partial t} = D_P \frac{\partial^2(AP)}{\partial x^2} - \frac{\partial(vAP)}{\partial x} - K_1 \frac{X}{X-k} AP + qH(x), (x < L \leqslant \infty, t > 0) \tag{2.1}$$

$$\frac{\partial(AX)}{\partial t} = D_X \frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(vAX)}{\partial x} - K_2 \frac{X}{X-k} AP + \alpha(S - X), (x < L \leqslant \infty, t > 0) \tag{2.2}$$

Tapti River

where $H(x)$ is the Heaviside function $H(x) = \begin{cases} 1, & 0<x \\ 0, & \text{otherwise} \end{cases}$

The limits concerning with these equations and appropriate modelling values are presented in Table 1. These standard equations are developed by Chapra [Chapra, S.C. 1997]. The first equation consists both addition of pollutant at a rate $qH(x)$, and its removal by oxidation. The river has been divided into two sections: upstream $x<0$ near the source, where it is assumed that there is no added pollution, and downstream $0<x<L$ where pollution is added at a rate q. For simplicity, the addition of pollutant, which is strictly a function of time and position, will be taken to be constant along the downstream portion of the river. The second equation is a mass balance for dissolved oxygen, with addition through the surface at a rate proportional to the degree of saturation of dissolved oxygen $(S-X)$, and consumption during the oxidation of the pollutant. The rate of depletion of pollutant concentration P, due to the biochemical reaction with dissolved oxygen, has been described using a "Michaelis–Menten" term .$-K_1 \frac{X}{X+K} AP$ This term enables pollution to be removed at a rate proportional solely to the pollution concentration when oxygen levels are high. However, at low levels of oxygen the reaction must also be proportional to the oxygen concentration, as also allowed for by this term. [Chin Devid, A.2012] In the second equation, the coefficients of the corresponding dissolved oxygen concentration depletion term differ because of the different weights of oxygen and pollutant involved in the reaction

To simplify the equations, the values of the cross-sectional area of the river A, it is set the downstream velocity of the river v, the rate of addition of pollutant q, the rate of transfer of oxygen through the surface of the river α, the saturated oxygen concentration, and the dispersion rates of pollutant and dissolved oxygen, D_P and D_x, respectively, to be constant.

It is considered the steady-state solutions, for which the left-hand sides of Eqs. and vanish. The only variation applicable is with the distance downstream on the river and so it is written

$P(x,t)=P_s(x)$ and $X(x,t)=Xs(x)$. It is first considered that various special cases for which the equations simplify and can be solved analytically and then describe a preliminary numerical approach to solving the more general problem. For the present we will ignore the restriction $x<L$, due to the finite length of the river.

3. Analytic steady-state solutions for special cases

3.1. Zero dispersion

It begins by considering the case when the dispersion can be taken to be negligible, $D_P = 0, D_x = 0$. For this case the equations reduce to

$$\frac{\mathrm{d}(vAP_s(x))}{\mathrm{d}x} = -K_1 \frac{X_s(x)}{X_s(x)+k} AP_s(x) + q, (x > 0) \tag{3.1}$$

$$\frac{\mathrm{d}(vAX_s(x))}{\mathrm{d}x} = -K_2 \frac{X_s(x)}{X_s(x)+k} AP_s(x) + \alpha\big(S - X_s(x)\big), (x > 0) \tag{3.2}$$

with boundary conditions $P_s(0) = (0)$ and $X_s(0) = S$. For this case there is no pollution upstream because of the absence of dispersion (i.e. $P_s(x) = 0$ and $X_s(x) = S$ for $x < 0$.) In the case where, additionally, the half-saturated oxygen demand concentration for pollutant decay k is negligible ($k \approx 0$), we can calculate the downstream pollutant concentration to be $P_s(x) = (q/K_1A)(1-\exp(-K_1x/v))$, which tends to the limit q/K_1A. The corresponding dissolved oxygen concentration is

$$X_s(X) = S - \frac{K_2 q}{K_1}\left(\frac{1}{\alpha} - \left(\frac{1}{\alpha - K_1 A}\right) e^{\frac{-K_1 x}{v}}\right) - \left(\frac{K_2 qA}{\alpha(\alpha - K_1 A)}\right) e^{-\frac{\alpha x}{vA}} \tag{3.3}$$

Taking the downstream limit we have

$$\lim_{x\to} X_s(x) = S - \frac{K_2 q}{\alpha K_1}$$

In this simplified model at downstream, the dissolved oxygen requirement for fish survival, which is that X is greater than 30% of the saturated value S [5], is achieved for levels q which satisfy $q<0.7\,\alpha K_1 S/K_2$. In this case, with our parameter values, the fish survival constraint is . $q < 0.015 \text{ kg m}^{-1} \text{ day}^{-1}$(The actual rate of pollutant insertion in the Tapti River corresponds to $q = 0.06 \text{ kg m}^{-1} \text{ day}^{-1}$.)
The dispersion-free equations can also be solved for small values of k. In this case

$$\big(P_s(x), X_s(x)\big)|\text{large } x = \left(\frac{q}{K_1 A} + \frac{\alpha k q}{\alpha k_1 S - qK_2}, S - \frac{qK_2}{\alpha K_1}\right). \tag{3.4}$$

This solution is not valid if $q \geqslant \alpha K_1 S/K_2$ and, in that case, the value of the dissolved oxygen concentration reaches zero at a point $x = \bar{x}$, and, thereafter, for $x > \bar{x}$, $X_s\ (x)=0$. Later work will provide ways of estimating $\bar{x}$.

3.2. *Models including dispersion with linear kinetics*

It is now considered that the case where dispersion terms are included, causing the second-order derivative terms to survive, but for which k is assumed to be negligible ($k \approx 0$). Then the equations become

$$D_p \frac{d^2(Ap_s(x))}{dx^2} - \frac{\mathrm{d}(vAP_s(x))}{\mathrm{d}x} - K_1 AP_s(x) + qH(x) = 0, \tag{3.5}$$

$$D_x \frac{d^2(AP_s(x))}{dx^2} - \frac{\mathrm{d}(vAX_s(x))}{dx} - K_2 AP_s(x) + \alpha\big(S - X_s(x)\big) = 0. \tag{3.6}$$

We find the pollution concentration

$$P_s(x) = \begin{cases} \frac{q}{K_1 A}\left(1 - \left(\frac{\delta+\beta}{2\beta}\right) e^{(\delta-\beta)x}\right), & x \geqslant 0 \\ \frac{q}{K_1 A}\left(\frac{\beta-\delta}{2\beta}\right) e^{(\delta+\beta)x}, & x < 0. \end{cases} \tag{3.7}$$

where $\delta = v/2D_p$ and $\beta = \left(\sqrt{v^2 + 4D_pK_1}\right)/2D_p$ and the dissolved oxygen concentration is

$$X_s(x) = \begin{cases} S - \frac{K_2 q}{K_1 \alpha} + \frac{K_2 q}{K_1}\left[\left(\frac{\gamma+\eta}{2\eta\alpha} - \frac{\delta+\beta}{4\beta\eta A^*} + \frac{\delta-\beta}{4\beta\eta B^*}\right)e^{(\gamma-\eta)x} - \frac{\delta-\beta}{2\beta A^*}xe^{(\delta-\beta)x}\right], x \geqslant 0 \\ S + \frac{K_2 q}{K_1}\left[\left(\frac{\gamma-\eta}{2\eta\alpha} - \frac{\delta+\beta}{4\beta\eta A^*} + \frac{\delta-\beta}{4\beta\eta B^*}\right)e^{(\gamma+\eta)x} - \frac{\delta-\beta}{2\beta B^*}xe^{(\delta+\beta)x}\right], x < 0 \end{cases} \tag{3.8}$$

Where

$$\gamma = \frac{v}{2D_X}, \qquad \eta = \frac{\sqrt{v^2 + \frac{4\alpha D_x}{A}}}{2D_X}, A^* = 2AD_X(\delta - \beta) - vA, B^* = 2AD_X(\delta + \beta) - vA.$$

It is required that $P_S(\infty) < \infty$ and $P_S(-\infty) < \infty$. There are no point sources of pollutant (only distributed sources), and so $P_S(x)$ is assumed to be continuous at $x = 0$. Since the dispersive flux $DP'_S(x) - vP_s(x)$ is also continuous this further implies that $P'_s(x)$ is continuous. We use the boundary conditions $X_s(\infty) < \infty$ and $X_s(-\infty) = S$. Also it is required $X'_s(x)$ and $X'_s(x)$ to be continuous where the input of pollutant starts at $x = 0$. The resulting pollutant concentration $P_S(x)$ is relatively smooth with a discontinuity of q/D_PA in the second derivative at $x = 0$. The dissolved oxygen concentration $X_s(x)$ has a discontinuity in the fourth derivative at $x = 0$.

4. Numerical approach for finding the steady-state solution when k is non-zero

In the general case, the boundary concentrations for pollutant and dissolved oxygen are still $P_S(-\infty) = 0$ and $X_s(-\infty) = S$ far upstream and far downstream, respectively.

$$P_s(\infty) = \frac{q}{K_1 A}\left(1 + \frac{k}{X_s(\infty)}\right) \text{ and } X_s(\infty) = S - \frac{K_2 q}{K_1 \alpha}.$$

Furthermore, it can be obtained flux conditions directly by mathematical analysis: $P'_0(0) \leqslant P'_K(0) \leqslant q/Av$ and $X'_0(0) \leqslant X'_K(0) \leqslant 0$, where $P_0(x)$ and $X_0(x)$ are the steady-state solutions for $k = 0$ and $P_k(x)$ and $X_k(x)$ are the corresponding cases for non-zero k.

To search for the result, a primary numerical routine has been developed. It is integrated from a grid of initial values at $x = 0$ and progressively refine this grid to find the solution to the boundary conditions. The Euclidean norm is used for measuring the agreement of trial initial conditions with pollutant and dissolved oxygen concentration far upstream and downstream. The numerical routine has been used in an exploratory investigation with the calibrated parameters given in Table 1 for the Tapti River. For initial testing of the algorithm the case where k is negligible is used. The results agree with the analytical solution under the conditions of no pollution and saturated dissolved oxygen far upstream, tending to a steady state far downstream for a long (considered infinite) river.

5. Concluding remarks

A mathematical model is presented for river pollution comprising a coupled pair of nonlinear equations and has investigated the effect of aeration on the degradation of pollutant. In some simplified cases, analytic steady-state solutions were obtained. The preliminary numerical approach agrees with these analytical solutions under relevant conditions. This model and its solutions could aid in decision support on restrictions to be imposed on farming and urban practices, e.g. it can enable scenarios to be tested for fish survival. Further features can be readily included in this simplified model such as variable pollutant input, tidal flow and the like. The model can also be used to illustrate the effect of aeration processes to increase dissolved oxygen to the water. The extension to the transient spatial model is relatively straightforward.

For the model presented here, it is observed that a pollution insertion rate of $q = 0.06$ kg m^{-1}(as for the Tapti River) would result in an ecologically dead river at far downstream distances when dissolved oxygen falls below the ideal level required for fish to survive [5]. The pollutant being inserted into the river is about 4 times too high and this implies that the total biological oxygen demand (BOD) rate for the river should have a maximum insertion of 5000 kg BOD day^{-1}. However, fortunately, further investigation shows that for a river of the length in this study (the lower 325 km of the Tapti River), the dissolved oxygen level remains above the critical value of 30% of the saturated value in agreement with previous conclusions [Bhatt, Himanshu. 2013]. The critical value is not reached in the Tapti River because of the finite length over which pollution is actually discharged so that the river reaches the sea before this environmental catastrophe can occur. [Goel, P.K 2011] Further details of the model are given elsewhere.

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