MATHEMATICAL MODELLING OF WATER QUALITY IN RIVER CHANNELS AND ITS SYSTEMS

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PREFACE

This paper is a brief review of the theoretical concepts underlying the contemporary approach to the modelling of water quality in rivers and its systems. Special attention is given to some specific mathematical questions when one is considering, numerically, a network of channels. The subject of the paper is of professional interest to the author and at the same time, has direct relation to Task 2 on Models for Environmental Quality Control and Management, of the Resources and Environment Area, in the current Research Plan of IIASA.

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SUMMARY

This paper describes the principles of the contemporary approach to mathematical modelling of water quality in river channels and their networks, including the formulation of basic equations for the hydrophysical and chemical-biological processes involved, the role of longitudinal dispersion, and the initial and boundary conditions. Special emphasis is given to some specific questions related to the numerical computation of channel networks.

Mathematical Modelling of Water Quality in River Channels and its Systems

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In assessing the effects of pollution sources on water bodies, related hydrophysical and chemical-biological processes need to be taken into account. For the description of these processes in river systems, mathematical models have been developed which are based on the use of hydraulic one-dimensional equations for open-channel flows and of balance equations for various substances as well as for heat and oxygen. Such models make possible the prediction of the content of oxygen, substances, and also of water temperature along the channels of a river system, dependent on its hydrological behavior and on the intensities of pollution sources (the rates of effluent disposals). From the physical point of view, the principle point in formulation of convective-diffusion equations describing the processes of substances and heat transfer, is the question of exchange coefficients. In the case of one-dimensional models, the question is reduced to that of the coefficient of longitudinal dispersion of substances (or heat).

Here we will not consider the local phenomena taking place in the zones of mixing and will address the problem of mathematical description of the processes of transfer and transformation of substances and heat in the zones of complete vertical mixing. For simplification, the problem of the distribution of water quality characteristics along a water course can be reduced to a one-dimensional model with the use of averaging variables over flow cross-sections.

1. Basic Equations

A one-dimensional model of water quality for rivers can be based on the equations of unsteady open-channel flow to describe the hydraulic part of the problem under consideration. These include an equation of mass conservation (an equation of continuity)

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q, \quad (Q = UA) \tag{1}$$

and the longitudinal momentum equation (a dynamic equation) [1,2]

$$\frac{\partial}{\partial t}(AU) + \frac{\partial}{\partial x}(QU) = -gA\left(\frac{\partial Z}{\partial x} + \frac{U|U|}{C^2 R} + \frac{h_c}{\rho}\frac{\partial \rho}{\partial x}\right) \quad . \tag{2}$$

Both are written in a one-dimensional approximation.

For the purpose of defining water quality characteristics, the balance equations for transfer of heat, oxygen, and other substances must be formulated. They have a similar structure and may be considered as one-dimensional equations of convective-diffusion. First, let us write equations for heat balance (in a simplified form) and for dissolved conservative matter (or salinity in particular):

$$\frac{\partial}{\partial t}(AT) + \frac{\partial}{\partial x}(QT) = \frac{\partial}{\partial x}\left(AD\frac{\partial T}{\partial x}\right) - k_T A\,(T - T_E) + qT_\ell \tag{3}$$

$$\frac{\partial}{\partial t}(AS) + \frac{\partial}{\partial x}(QS) = \frac{\partial}{\partial x}\left(AD\frac{\partial S}{\partial x}\right) + qS_\ell \quad . \tag{4}$$

These equations must be supplemented with an equation of state connecting the water density (ρ) with temperature and salinity,

$$\rho = f(T,S) \quad . \tag{5}$$

Here t is time; x is the longitudinal coordinate of the cross-section; $A(x,Z)$ is the area of flow cross-section; $Q(x,t)$ is the rate of water discharge; $Z(x,t)$ is the elevation of free-surface level, with respect to horizontal datum; $U = \frac{Q}{A}$ is the mean discharge velocity of flow; $T(x,t)$ is the water temperature; $S(x,t)$ is the salinity (or the concentration of a dissolved matter); $q(x,t)$ is the lateral inflow per unit length of channel (directed normally to the x-axis); R is a hydraulic radius; C is the Chezy coefficient; g is the acceleration of gravity; h_c is the depth of the centroid of the cross-section; D is the coefficient of longitudinal dispersion; T_E is the so-called equilibrium temperature of water (defined as the temperature at which, under given meteorological conditions, the net surface heat flux is equal to zero); k_T is the coefficient of the surface heat exchange; $T_\ell(x,t)$ and $S_\ell(x,t)$ are the temperature and the salinity (or the concentration of a dissolved matter) in the lateral inflow water, respectively.

To describe hydrochemical and hydrobiological processes in a water stream, the above equations must be supplemented with equations for the transfer of dissolved and suspended matter:

$$\frac{\partial}{\partial t}(AS_i) + \frac{\partial}{\partial x}(QS_i) = \frac{\partial}{\partial x}\left(AD\frac{\partial S_i}{\partial x}\right) + qS_{\ell i} + R_i(S_i,S_j,T,I) \quad . \qquad (6)$$

Here $S_i(x,t)$ is the concentration of the i-th component of the passive admixture ($i,j=1,2,3,\ldots,n$). The last term R_i

represents all chemical-biological links and interactions. It characterizes the rate of change of the concentration for the i-th component of the admixture due to chemical and biological transformations (i.e., kinetic interactions between the different components of the admixture). Here the components of the passive (from the hydrodynamical point of view) admixture can include different chemical substances as well as the components of biomass such as phyto- and zooplankton. As can be seen from equation (6), the rate of kinetic interactions R_i generally depends upon the concentrations of the related components of the admixture, S_i and S_j, as well as upon the temperature T and the insulation I. If a certain component of the admixture is conservative, the last term in equation (6) is absent, i.e., $R_i = 0$, and we arrive to the equation (4).

In particular, the latter equation can be applied to consider the balances of carbonaceous organic matter and oxygen in a river flow with the use of the concept of biochemical oxygen demand (BOD) and of the term dissolved oxygen (DO):

$$\frac{\partial}{\partial t}(AL) + \frac{\partial}{\partial x}(QL) = \frac{\partial}{\partial x}\left(AD\frac{\partial L}{\partial x}\right) - k_1AL + qL_\ell \tag{7}$$

$$\frac{\partial}{\partial t}(Ac) + \frac{\partial}{\partial x}(Qc) = \frac{\partial}{\partial x}\left(AD\frac{\partial c}{\partial x}\right) - k_1AL + k_2A(c_s - c) + qc_\ell \quad , \tag{8}$$

where

L(x,t) is the ultimate carbonaceous biochemical oxygen demand (BOD);

$c(x,t)$ is the concentration of dissolved oxygen (DO);

k_1 is the BOD decay coefficient;

k_2 is the surface reaeration coefficient;

c_s is the saturation concentration of dissolved oxygen;

L_ℓ, c_ℓ is the BOD and DO in the lateral inflow water.

Some other possible physical and chemical-biological processes which can occur in a river stretch are not taken into account here. Among them are:

(1) the removal of oxygen by nitrogenous biochemical reactions,

(2) the removal of oxygen by the benthal layer,

(3) the replenishment of oxygen due to the photosynthetic production by phytoplankton (algae) and fixed plants,

(4) the removal of oxygen by the respiration of plankton and fixed plants,

(5) the removal of BOD by adsorption and sedimentation,

(6) the addition of BOD due to the interaction with bottom deposits and the benthal layer (the scour of bottom deposits and the diffusion of organic products from the benthal layer).

In some cases, these processes can make an important contribution to the balance of organic matter and also play a significant role in the oxygen regime of a water course/stream as a whole.

If the heat, the dissolved and suspended substances transported by a flow do not significantly affect the density ρ and consequently the latter term of the dynamic equation (2) is negligible, (the case of passive admixture), the system of hydraulic and transport equations is uncoupled. The hydraulic equations (1), (2) can be solved first, independently of the others and then the results can be used to solve the equations for transfer of substances and heat. In the opposite case, the equations for transfer of matter (and heat), actively influencing the flow dynamics, need to be solved simultaneously with the hydraulic ones (1) and (2). It may take place in case of intrusion of saline water into the lower reaches of rivers near coastal zones (i.e. estuaries) and, at least theoretically, in the case of significant quantities of heated water wastes, discharged into rivers. In accordance with a statement in the introduction of the paper, where the above equations apply, it is assumed that there is a well developed mixing process in a stream (the well mixed state of flow), which prevents density stratification in the vertical direction.

2. Longitudinal Dispersion

The one-dimensional equations given above, of convective-diffusion of heat and dissolved and suspended substances, include the effect of a longitudinal dispersion. G.I. Taylor [3] has demonstrated that the non-uniform distribution of the rate of convective mass transfer (due to the nonuniformity of mean velocity distribution) over the cross-sectional area, and the turbulent lateral mixing (due to lateral velocity fluctuations), together play a major role in the longitudinal spread of the substances. The difference in the longitudinal convective mass transfer which is associated with the actual velocity distribution and that which is accounted for by the average discharge velocity U is taken into account by the term of longitudinal dispersion in the equations of transfer [4,5]. It is necessary to distinguish between turbulent longitudinal diffusivity (caused by turbulent longitudinal fluctuations of velocity) and longitudinal dispersion. The evaluation of the coefficients related to both phenomena shows that, for example, in a uniform turbulent flow in a straight pipe, the latter one is about 200 times larger than the first one: a longitudinal spread of substances due to dispersion is much higher than that due to the diffusivity.

According to Harleman [4], the coefficients of longitudinal dispersion for a flow in a straight open channel can be evaluated by the expression obtained through the reformulation of the G.I. Taylor formula for a pipe flow:

$$D = 20{,}2 \sqrt{g} \frac{UR}{C} \qquad (9).$$

However, Fisher [6] has demonstrated that the longitudinal dispersion coefficient for an arbitrary river channel can be one or two orders of magnitude larger than in a straight channel.

It can be shown that when there is a gradually varied change of temperature or concentration along a channel under steady conditions, the role of dispersion is mostly insignificant. Under steady state conditions, the relative importance of longitudinal advection U, and longitudinal dispersion D for a substance undergoing a first-order decay [rate constant $k_1 (t^{-1})$] is given by the dimensionless ratio

$$4k_1 D/U^2$$

when this ratio is small compared to unity, longitudinal dispersion may be neglected. Accordingly, taking note of longitudinal dispersion may be important in estuaries where the flow is inherently unsteady or in the consideration of rapid unsteady processes such as the emergency release of wastes.

3. Initial and Boundary Conditions

Calculations of unsteady flow and water quality characteristics in systems of open channels come down to finding the solution of the equations (1) - (6) for given initial and boundary conditions.

As initial conditions, the values of state variables Z, Q, T, S_i need to be given along the river channels at an initial moment of time.

The boundary conditions for the hydraulic variables Z and Q are prescribed in the form of functional relations

$$Z = Z(t),\ Q = Q(t) \text{ or } Q = Q(Z) \qquad (10)$$

in the upstream and downstream sections of the channel systems.*

In the inflow and outflow cross-sections of the system it is also necessary to specify one boundary condition for each of the variables characterizing the content of substances transferred by a flow and the water temperature (S_i, T). In the upstream sections where the inflow takes place, it is sufficient to prescribe the value of these variables S_i, T or the integral fluxes of respective substances and heat as the functions of time. For example, in the first case:

$$S_i = S_i(t) \text{ and } T = T(t) \qquad (11)$$

This implies the concentrations of transported substances and the temperature are given in the inflow section.

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*It should be noted , that as usual,when considering subcritical flow regimes, only a single boundary condition needs to be entered for each of these sections.

In the second case, taking into account the role of longitudinal dispersion, the integral flux Φ of a substance characterized by a concentration φ through the cross-section of a channel, should be properly represented by the following expression:

$$\Phi = Q\varphi - AD \frac{\partial \varphi}{\partial x} \qquad (12)$$

The heat flux can be expressed similarly.

Of somewhat greater complexity is the question of imposing physically sound boundary conditions on the downstream cross-sections of the channel system where the outflow of water and consequently of transported substances and heat occurs. The presence of diffusive terms in the equations for transfer of substances and heat needs imposed boundary conditions for S_i and T variables in the downstream sections as well. However, the specification of substances content and temperature (or the fluxes of substances and heat) in the outflow sections would be unnatural from the physical point of view. It appears that more natural conditions can be obtained by suggesting that at an outflow section situated at a distance large enough from the point of the pollutant or heat release, the role of longitudinal dispersion becomes negligibly small and so the substance (or heat) content is mainly determined by the advective transfer. If the equation of transfer of a substance (generally a non-conservative one) or of heat is written as follows:

$$\frac{\partial}{\partial t}(A\varphi) + \frac{\partial}{\partial x}(Q\varphi) = \frac{\partial}{\partial x}\left(AD \frac{\partial \varphi}{\partial x}\right) + F(\varphi, t) \qquad (13)$$

then the boundary condition which follows from the above assumption will have a form [8,9]:

$$\frac{\partial}{\partial t}(A\,\varphi) + \frac{\partial}{\partial x}(Q\,\varphi) = F(\varphi, t). \tag{14}$$

A similar physical consideration of the question was done by D. Harleman et al [1 ,2] in the development of a numerical scheme for the transfer process in an estuary.

The matter is much simpler when the longitudinal dispersion does not play an essential role and the diffusive term is omitted from the transport equations (D = 0). In this case it is mathematically enough to impose the appropriate boundary conditions for S_i and T variables only on the upstream cross-sections.

4. Conjunction Conditions

To complete the mathematical formulation for the problem of a system of channels it is necessary to specify conjunction conditions to be satisfied at the points of abrupt change of cross-section, of channel confluence, of local inflows (and outflows), of local (point) pollutant or heat sources and at hydraulic structures as well.

The conjunction conditions for the hydraulic variables take the form of a balance of discharges Q and of conditions of connection between the levels Z respectively. It seems convenient at each junction to designate the free surface ordinate with Z_* , while the local inflow is denoted by Q_*. For instance, on the boundary of two reaches (Fig. 1) marked by indices 1 and 2 for the upstream and downstream reach respectively, the conjunction conditions may be formulated without taking into account the level difference in the following form:

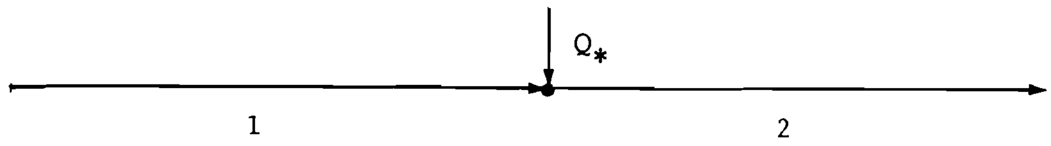

Figure 1. Case of local inflow Q_*

a) equality of levels in adjoining sections of the reaches

$$Z_2 = Z_1 = Z_*, \tag{15}$$

b) balance of discharges

$$Q_2 = Q_1 + Q_* \tag{16}$$

Here it is assumed that the rate of local inflow Q_* may be the specified function of Z_* and t. The conjugation conditions in the case of confluence of two (or more) channels are formulated in an analogous way. These will be discussed below.

The conjunction conditions for water-quality characteristics are also based on the balance considerations. For example, from the formal mathematical standpoint for the diffusion equation of type (13) on the boundary of two reaches with a local (point) pollutant source or a local release of water, we should specify two conditions, such as:

$$\Phi_2 = \Phi_1 + \Phi_*, \qquad Q_2\varphi_2 = Q_1\varphi_1 + \Phi_* \tag{17}$$

(Note: This is so if $D \neq 0$; but if $D = 0$, these conditions are identical). In the case when there is an inflow $Q_* > 0$, the intensity of a pollutant release Φ_* must be given as a function of time t or it can be expressed through the rate of water inflow Q_* and the time-dependent concentration $\varphi_*(t)$ of a matter released (or the temperature of released water)

$$\Phi_* = Q_* \varphi_* \tag{18}$$

In the case of an outflow, $Q_* < 0$, it is expedient to assume that the concentration of a matter (or temperature) in the outflowing water is the same as in the upstream reach:

$$\varphi_* = \varphi_1, \text{ and consequently,} \tag{19}$$

$$\varphi_2 = \varphi_1 = \varphi_*. \tag{20}$$

In a similar way, the conjunction conditions for the case of a bifurcation of upstream channel (Fig. 2) can be obtained:

$$Q_1 = Q_2 + Q_3, \; Z_1 = Z_2 = Z_3 \tag{21}$$

$$\Phi_1 + \Phi_2 = \Phi_3, \quad \varphi_1 = \varphi_2 = \varphi_3 \tag{22}$$

When there is a confluence of two channels (Fig. 3) the conjunction conditions are generally similar to the above ones for the case of a local inflow ($Q_* > 0$):

$$Q_1 + Q_2 = Q_3, \; Z_1 = Z_2 = Z_3 \tag{23}$$

$$\Phi_1 + \Phi_2 = \Phi_3, \; Q_1\varphi_1 + Q_2\varphi_2 = Q_3\varphi_3 \tag{24}$$

The process of solving the longitudinal dispersion equations may be significantly simplified if an approach similar to the one suggested in section 3 is applied; namely, if at the lower end(s) of the upstream reach(es) adjoining a node under consideration, the role of dispersion becomes negligible, as an example, the conditions (24) will take the following form:

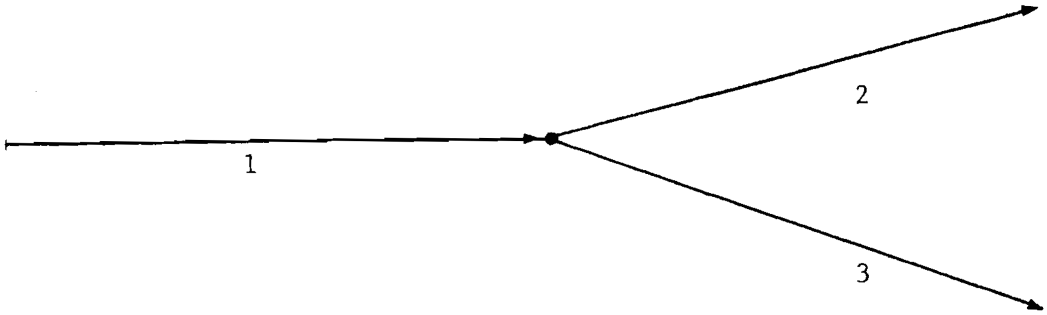

Figure 2. Case of a Channel Bifurcation

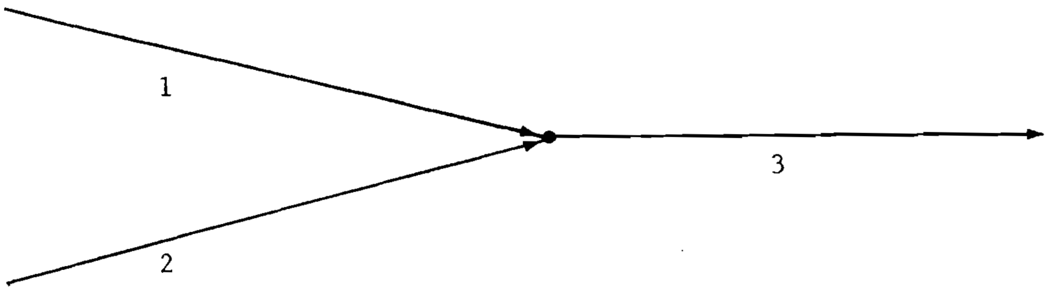

Figure 3. Case of the Channels Confluence

$$\left.\begin{aligned} & Q_1\varphi_1 + Q_2\varphi_2 = \Phi_3, \\ & \frac{\partial}{\partial t}(A\varphi) + \frac{\partial}{\partial x}(Q\varphi) = F(\varphi, t) \text{ at the ends of upstream reaches 1 and 2} \end{aligned}\right\} \quad (24')$$

Similarly, instead of the conditions (17) one can get the following one:

$$\left.\begin{aligned} & \Phi_2 = Q_1\varphi_1 + \Phi_* \\ & \frac{\partial}{\partial t}(A\varphi) + \frac{\partial}{\partial x}(Q\varphi) = F(\varphi,t) \text{ at the end of upstream reach 1} \end{aligned}\right\} \quad (17')$$

Thus, in calculating the transfer of substances and heat, the process of solving convective-diffusion equations for a branching system of channel networks (a tree-type system) is reduced to the consecutive solution for separate elements of the system (from upstream to downstream). These are separated in the corresponding nodes by the second conditions and are conjugated by the first ones in (24') and (17').

Naturally, the consideration of the problem without taking account of longitudinal dispersion (D = 0) greatly simplifies the mathematical description of transport processes in complex channel networks, particularly with regard to conjunction conditions. Under the conditions in (17), (22) and (24), the first expressions (in terms of Φ_i) can be omitted, because they are reduced to the second ones in all these cases.

5. Numerical Computation

The numerical procedures for the computation of hydraulic regimes and related water quality characteristics of unsteady flow in open-channel networks can be found in a number of publications, including the papers [8,10]. Both the branching network system (those of the tree-type) and the general network systems (those with loops) are considered there. The systems differential equations are solved using the implicit finite-difference methods. A number of effective algorithms have been developed, which take into account the three-diagonal structure of difference equations matrix and are variants of the matrix method of factorization. The suggested technique is embodied rather simply in the programming process and can be applied effectively to solve a wide range of problems.

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