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MATHEMATICAL MODEL OF UNSTEADY-STATE POLLUTANTS TRANSPORTED IN NATURAL STREAMS

by

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SOMMAIRE : On a élaboré un modèle mathématique qui permet de prévoir la diffusion transversale et longitudinale de polluants instables libérés dans des cours d'eau naturels. Dans ce document, on discute des arrangements numériques et de la structure du modèle et on explique les essais auxquels on l'a soumis.

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SUMMARY: A mathematical model which predicts the transverse and longitudinal spreading of unsteady-state pollutants released into natural streams has been developed. The numerical scheme, structure and testing of the model have been discussed.

INTRODUCTION

Effective control of pollution in natural streams requires the ability to understand the mixing and transport of pollutants discharged into the stream. To this end, mathematical models based on the mass balance equation have been widely used, with the advantage that the variabilities in channel characteristics and other transport process parameters can be included. A review of the pertinent literature has indicated that most of the existing models [1, 2, 5, 7, 14, 20] deal with the one-dimensional or longitudinal mixing, in which sectional mixing was assumed to be completed. The other models [4, 9, 13, 15, 17, 18, 19, 21], though two-dimensional in nature, have their applications limited mainly to the case where the pollutants are released continuously at a steady rate into the stream.

In this paper, a mathematical model that describes the two-dimensional mixing process of a pollutant released at an unsteady rate has been developed. The model, MABOCOST (Mixing Analysis Based On the Concept Of Stream Tube), is based on the revised mass balance equation originally derived by Yotsukura and Sayre [22]. It is applicable for mixing in natural streams with constant flow rates, for which the cross-sections and the velocity profiles are non-uniform, the channels are sinuous, and localized sources or sinks due to chemical or biological reactions are present. Pollutants which undergo growth or decay can also be modelled within this model.

THEORETICAL FOUNDATIONS

The analysis of two-dimensional mixing in prismatic channels can be based on the depth-averaged mass balance equation derived by Holley et al. [9] as

$$\frac{\partial(hC)}{\partial t} + hu\frac{\partial C}{\partial x} + hw\frac{\partial C}{\partial z} = \frac{\partial}{\partial z}\left(h\,E_z\frac{\partial C}{\partial z}\right), \tag{1}$$

where x,z = longitudinal and transverse coordinates respectively, t = time, h = flow depth, and u,w = longitudinal and transverse depth-averaged velocities respectively, C = depth-averaged volumetric concentration, and E_z = transverse dispersion coefficient.

For the case of natural streams, where the cross-sections are varying, the channels are sinuous, and the velocity and depth quantities vary from point to point, the Cartesian system in which (1) is expressed makes the application of this equation an unduly inconvenient task. To circumvent this difficulty, Yotsukura and Sayre modified this equation according to the concept of stream tubes. The final form of their equation can be given as [22]

$$\frac{\partial C}{\partial t} + \frac{u}{m_x}\frac{\partial C}{\partial x} = \frac{\partial}{\partial n}\left(D\frac{\partial C}{\partial n}\right) + k_1 C + k_2 \quad , \tag{2}$$

where $D = (h^2 u^2 E_z/Q^2)$ is the dispersion factor; x and Q are as defined in Fig. 1, k_1 is the rate of first-order chemical reaction of pollutants, and k_2 is the rate of change in concentration as produced by the presence of a source or sink. In this equation, the independent variable, z, which appears in (1), has been replaced by the fraction of discharge that flows between the right bank and z, that is,

$$n = \frac{q}{Q} = \frac{1}{Q}\int_o^z (m_z\, uh)dz \ . \tag{3}$$

Here, m_x and m_z are metric coefficients to account for the difference in lengths between the respective coordinate surfaces as indicated in Fig. 1.

Mathematical models with different numerical algorithms have been developed for the solution of (2) for the case of steady-state pollutant input (i.e., $\partial C/\partial t = 0$), some examples of which are the RIVMIX [13], the POLDER [11], and the MIXCALBN [8] models.

UNSTEADY-STATE POLLUTANTS

When the pollutants are released at an unsteady rate into the stream, the resulting spatial concentration distribution in the stream will change with time, and the above models are not applicable. Attempts have been made to develop a workable algorithm that represents this case adequately, an example of the more significant contribution is the model of Holly [10], which is based on a finite-difference solution of (2). Through the use of a half-implicit, half-explicit, second-order differencing scheme for the space derivative, Holly has managed to eliminate from the solution numerical instability and damping in the convective stage. However, it was observed that undesirable numerical dispersion, causing additional spreading other than that directly related to the actual physical phenomena, is present in his solution. This problem, which has created fictitious results (e.g., negative concentrations) in some instances, has been described in his paper, and can only be minimized by careful choice of time and distance steps.

Another mixing model for the solution of unsteady pollutant input was developed by Fischer [6]. Fischer, in an attempt to reduce numerical dispersion, proposed an explicit algorithm which involves a step-by-step simulation of the mixing process in a coordinate system moving at the mean flow velocity. Owing to the complexity in the numerical structure, Fisher's model is applicable only to the simplest form of straight and prismatic channels. Natural channels by large do not fit into this category, and hence this limitation restricts very much the application of the model.

NUMERICAL DISPERSION

Although numerical dispersion can occur in both the longitudinal and lateral directions, it is generally believed that its magnitude in the longitudinal direction is much larger than that in the lateral direction. Therefore, more efforts will be geared toward the elimination of the longitudinal numerical dispersion in the present work, while attempts will also be made to reduce the amount of lateral numerical dispersion by reducing the size of Δn through the division of the stream into more tubes.

As described in the works of Beltaos [3], the behaviour of the numerical solution in the longitudinal direction rests heavily on the parameter L, where

$$L = u\Delta t/\Delta x . \tag{4}$$

When $L > 1$, the solution is unstable and will not converge to the real solution,and when $L < 1$, continuous spreading in the longitudinal sense occurs, despite the fact that the nature of the governing equation is purely convective in this direction. In fact, only when $L = 1$ can the problem of longitudinal numerical dispersion be eliminated completely. In a natural stream where the local velocity varies from one point to another, this condition can only be maintained in a space grid constructed in such a way that the length of each element is always the product of the local velocity and the time step, i.e., $\Delta x = u\Delta t$. This results in a grid with variable length elements as shown in Fig. 1.

NUMERICAL SCHEME OF MABOCOST

Based on the above discussions, the mathematical model MABOCOST has been developed. The model uses the time fractional step method as suggested by Verboom [21], which involves a step-by-step simulation of the actual physical processes, with the advantage that stability and consistency of the entire solution can be assured once the numerical scheme chosen for each individual step is stable and consistent.

According to this method, after a stream is divided into stream tubes and subsequently variable length elements, the solution may be obtained by first solving the convective portion of the mass balance equation,

$$\frac{\partial C}{\partial t} + \frac{u}{m_x}\frac{\partial C}{\partial x} = 0 , \tag{5}$$

by approximating it with a first-order, explicit, finite difference expression. Representing the concentration in tube i and element j at time t by $C(i,j,t)$, and applying the condition $L = u\Delta t/\Delta x = 1$, the resulting expression would give the concentration for the next time step as

$$C(i,j,t+\Delta t) = C(i,j-1,t). \tag{6}$$

That is to say, all the materials in an element is advected to the next element along that stream tube with the passage of every time step.

After this, the new advected concentrations are then dispersed laterally to each of the adjacent elements according to

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial n}\left(D\frac{\partial C}{\partial n}\right) = D\frac{\partial^2 C}{\partial n^2} + \frac{\partial D}{\partial n}\frac{\partial C}{\partial n} . \tag{7}$$

Using a simple forward difference expression to represent the left-hand side of (7), and three central difference expressions accurate to the order of $(\Delta n)^2$ to represent the partial derivatives on the right, one obtains

$$C(i,j,t+\Delta t) = C(i,j,t) + \frac{D\Delta t}{(\Delta n)^2}(\Delta C_\ell + \Delta C_r) + \frac{1}{4(\Delta n)^2}(\Delta D_\ell - \Delta D_r)(\Delta C_\ell - \Delta C_r)\ , \qquad (8)$$

where ΔC_ℓ and ΔD_ℓ are the concentration and dispersion factor differences on the left (looking downstream) of the element concerned, and ΔC_r and ΔD_r are the respective differences on the right. When an element has more than one adjacent element on its side, the concentration and dispersion factor differences will be distributed to each of the adjacent elements according to the proportion of their overlapping area.

Finally, the concentration distribution will be changed according to a first-order chemical reaction,

$$C(i,j,t+\Delta t) = C(i,j,t) \cdot e^{k_1 \Delta t}, \qquad (9)$$

and then according to the presence of the source-sink terms for that particular time step

$$C(i,j,t+\Delta t) = C(i,j,t) + k_2 \Delta t\,. \qquad (10)$$

When these processes are repeated for all the time steps, the concentration distribution throughout the entire stream at every time step can be obtained.

The code of MABOCOST was written with an IBM-XT personal computer in Fortran. The data required to be input for MABOCOST includes mainly the geometry and flow characteristics of the stream, as well as the pollutant and source-sink input records. A complete listing of the program, along with all the subroutines, can be found in Ref. [16].

MODEL TESTING

The numerical scheme of MABOCOST has been tested for correctness by comparing the model predictions with the analytical solutions of two cases:

1. A continuous line source stretching from $n = 0$ to $n = 0.2$, with strength $C = 5.0$, is released at $x = 0$. The pollutant is assumed to be a decaying material ($k_1 = -0.01/s$) with a linearly varying dispersion factor, $D = 0.01n + 0.0178$.

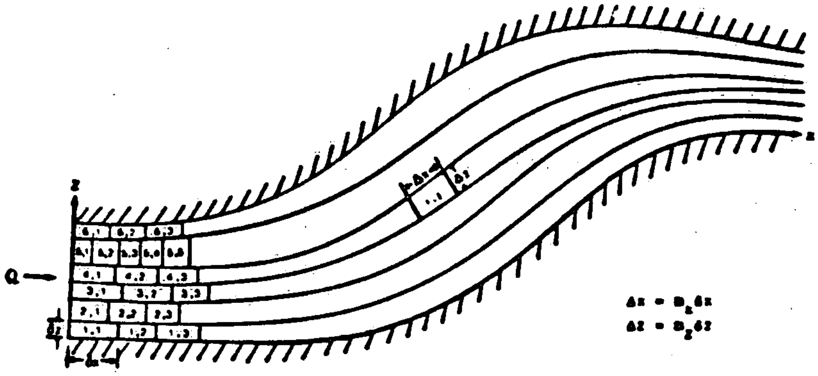
2. An instantaneous vertical unit mass with $E_z = 0.016\ m^2/s$ is released at the centre of the upsteam boundary into a stream with a constant velocity of 1 m/s.

The results of comparisons for the two cases are shown in Figs. 2 and 3 respectively. As can be seen from the figures, MABACOST has produced results that are in excellent agreement with the analytical solution.

The full validity of the model as applied to natural channels still needs to be proven by comparisons with field or laboratory generated data for the case of unsteady state pollutant input. A series of experiments, to be conducted at the Canada Centre for Inland Waters, Burlington, has been planned for this purpose.

CONCLUSIONS

The numerical scheme of MABOCOST has proven to be correct from the favourable comparisons with the analytical solutions of a steady-state line injection and an instantaneous point injection into a prismatic, straight channel. Complete verification of the model can only be possible when field or experimental data for natural or simulated streams become available.



Element (i,j) means the j-th element in tube i

Fig. 1. A Natural Coordinate System with Variable Length Elements

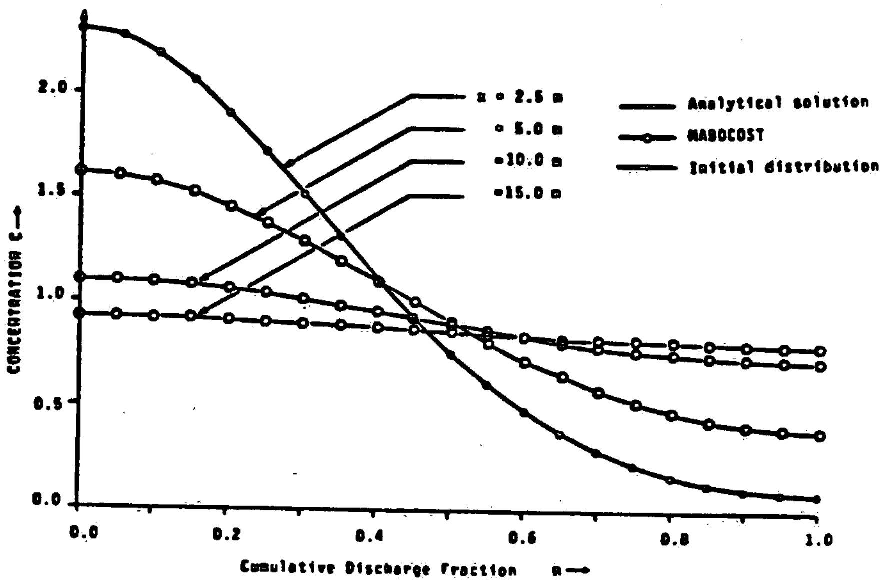


Fig. 2. Comparison Between MABOCOST Prediction and Analytical Solution (Case 1: Continuous Line Source)

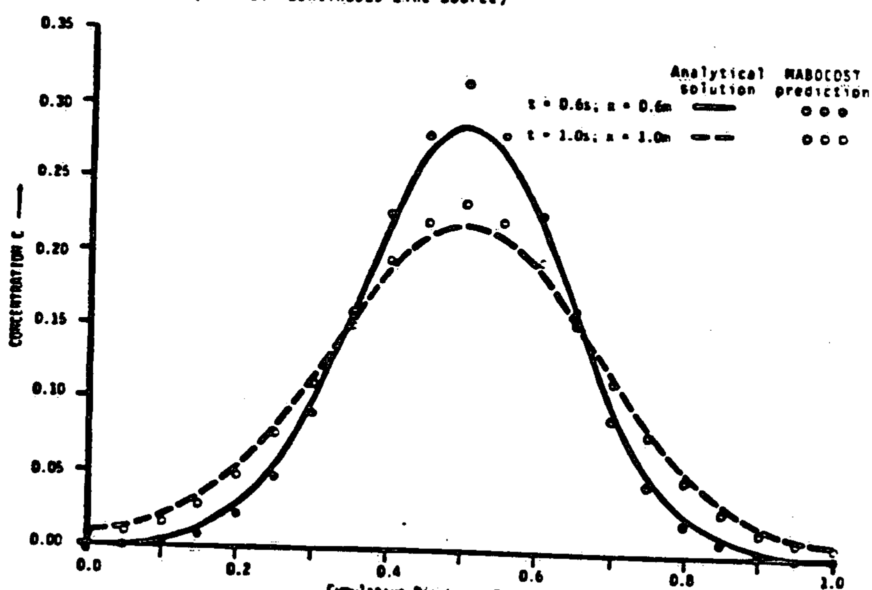


Fig. 3. Comparison Between MABOCOST Prediction and Analytical Solution (Case 2: Instantaneous Vertical Line Source)

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