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Project Summary

Analysis of Mathematical Models for Pollutant Transport and Dissipation

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Four realistic nonlinear models of pollutant transport with turbulent diffusion and reaction in rivers were studied. Exact solutions for all the kinetics models (no transport, no diffusion — the so-called stirred tank reactor) are described. An algorithm for calculating the rate constants from the exact solutions is given.

Exact solutions for all systems are also provided when transport terms are included with the kinetics (plug flow model). The inclusion of turbulent diffusion prevents exact solution, but the methods of perturbation and the maximum (minimum) principle provide approximate solutions and bounds on the traveling wave solution. The steady state is also analyzed by the bounding technique. These bounds, which may be used independently, demonstrate how the various parameters affect the solutions.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Mathematical models of pollutant reaction, diffusion and transport in rivers and streams are nonlinear partial differential equations, primarily because of the nonlinear kinetics of the biochemical reactions. In previous studies, exact solutions have been given for, at most, simplified and/or linearized problems. These solutions, usually, are not good approximations for the true situation. For the nonlinear problems, numerical solutions are usually obtained. Although often useful, numerical solutions are not easily employable in analyzing the adequacy of a model and evaluating parameters. Numerical solutions, without error analysis, must be viewed with caution and even suspicion — doubly so for nonlinear problems that may develop singularities, bifurcations, etc.

In this study, four realistic models of pollutant transport, turbulent diffusion and reaction are employed. In the absence of turbulent diffusion and transport, the kinetic equations are solved exactly in all four cases. When transport is added, the equations are also solved in all four cases. For the full system, exact solutions do not seem possible. For travelling wave problems, however, models I and II can be exactly solved for the active carbon and the bacteria and approximately for the pollutant.

For all travelling wave cases and all steady state cases, upper and lower bounds involving all parameters of the problem are constructed using the maximum (minimum) principle. These bounds are simple negative exponentials and may be used independently — that is, they are not coupled together as are the equations. This is the most useful and interesting result to come out of this work.

Procedure

With $\hat{C}_i$, i = 1,2,3 as the concentrations of pesticide, bacteria and organic carbon; D_i, i = 1,2,3 as the respective diffusion coefficients; k_i, i = 1,2,3 as the appropriate rate constants; v as the mean stream velocity; τ as the time; and x as the distance along the river, the model equations are:

$$\frac{\partial \hat{C}_1}{\partial \tau} + \bar{v}\frac{\partial \hat{C}_1}{\partial \bar{x}} = D_1 \frac{\partial^2 \hat{C}_1}{\partial \bar{x}^2} - k_1 f_1(\hat{C}_1, \hat{C}_2, \hat{C}_3)$$

$$\frac{\partial \hat{C}_2}{\partial \tau} + \bar{v}\frac{\partial \hat{C}_2}{\partial \bar{x}} = D_2 \frac{\partial^2 \hat{C}_2}{\partial \bar{x}^2} + k_2 f_2(\hat{C}_1, \hat{C}_2, \hat{C}_3)$$

$$\frac{\partial \hat{C}_3}{\partial \tau} + \bar{v}\frac{\partial \hat{C}_3}{\partial \bar{x}} = D_3 \frac{\partial^2 \hat{C}_3}{\partial \bar{x}^2} + k_3 f_3(\hat{C}_1, \hat{C}_2, \hat{C}_3)$$

Model I: $f_1 = \hat{C}_1\hat{C}_2$,

$f_2 = f_3 = \hat{C}_2\hat{C}_3$

Model II: $f_1 = \hat{C}_1\hat{C}_2\hat{C}_3$,

$f_2 = f_3 = \hat{C}_2\hat{C}_3$

Model III: $f_1 = \hat{C}_1\hat{C}_2$,

$$f_2 = f_3 = \frac{\hat{C}_2\hat{C}_3}{K + \hat{C}_3} \text{ (Monod)}$$

Model IV: $f_1 = \hat{C}_1\hat{C}_2\hat{C}_3$,

$$f_2 = f_3 = \frac{\hat{C}_2\hat{C}_3}{K + \hat{C}_3} \text{ (Monod)}$$

The analysis had four stages.

1. Stirred tank reactor - Kinetics only. With $D_i \equiv 0$, and $\bar{v} = 0$, the kinetic equations are solved exactly using the methods of ordinary differential equations. An algorithm is described for the evaluation of rate constants, which are employed in subsequent analyses. Solutions are displayed for several models.
2. Plug flow reactor - Kinetics and transport. With $D_i \equiv 0$, the transport equations with kinetics are solved exactly using the method of characteristics of hyperbolic first order equations. The resulting solutions have a number of arbitrary functions that depend upon initial and/or boundary conditions.
3. The Full System. In this case all physical processes, kinetics, transport and turbulent diffusion are included. These parabolic equations admit the important case of travelling wave solutions. In cases I and II, exact solutions are obtainable for the bacteria and active carbon but only a perturbation solution is possible for the pollutant. For all cases uncoupled analytic upper and lower bounds are obtained by means of maximum (minimum) principle. These bounds contain the parameters of the problem and may be used independently.
4. The Steady State. Solutions of the steady state are not obtainable analytically. The maximum (minimum) principle is used to derive upper and lower bounds. These bounds contain the parameters of the problems and are uncoupled.

In this problem the exact values of parameters, such as rate constants, turbulent diffusion constants, etc. are not known exactly but do lie on an interval - i.e., $\underline{\beta} \leq \beta \leq \bar{\beta}$. Interval analysis is employed to obtain information about the solutions in such cases.

Summary and Conclusions

(1) For four stirred-tank-type kinetic models, dimensional analysis has been applied, dimensionless kinetic groups obtained, and analytic solutions developed and analyzed. In the case of Model II (third order kinetics for C_1, second order for C_2 and C_3), the dimensionless equations are also parameter-free. This is an interesting and somewhat unusual situation. From an examination of these exact solutions, the following limiting results (as $t \to \infty$) are obtained.

Model Number	C_1	C_2	C_3
I	0	$\neq 0$	0
II	$\neq 0$	$\neq 0$	0
III	0	$\neq 0$	0
IV	$\neq 0$	$\neq 0$	0

From the exact solutions for the oft-used Model I, it is shown how these equations can be used to obtain rate constant ratios and the individual rate constants.

(2) When transport effects (constant velocity) are included, the resulting first order hyperbolic partial differential equations must be dimensionally analyzed in a manner different from the kinetic models.

(3) When turbulent dispersion effects are included, the equations become coupled reaction-diffusion equations that are parabolic. Dimensional analysis reveals the importance of the reciprocal of a Peclet number (Np_e) for mass transport and reaction rate ratios. None of the model equations possess classical similar solutions, but they all possess travelling wave solutions. For Models I and II, a partial exact solution is constructed that can be used to generate a perturbation solution for the pollutant. Both show the subtle way the problem parameters enter. In particular, the pollutant decays according to the exponential of the negative of the square root of the term $N_{Pe}E$ and by a complicated function of $\lambda = k_3/k_1$ for Model I (E is a constant of integration). On the other hand, the active carbon decays according to the exponential of the negative of the square root of $N_{Pe}Ek_3/k_1$.

(4) The complicated functions experienced in the perturbation analyses suggested that upper and lower bounds be constructed in terms of simple functions (negative exponentials). This has been done for all travelling wave solutions and for the steady state. Those bounds may be used independently. Moreover, the bounds show how the various parameters affect the solutions. This is the most useful and interesting result to come out of this work.

(5) Because none of the parameters are known exactly, interval analysis has been used to give deferred interval bounds in which the upper bound lies.

Some of the results are verified by computer calculations.

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The complete report, entitled "Analysis of Mathematical Models for Pollutant Transport and Dissipation," (Order No. PB 82-256 900; Cost: $10.50, subject to change) will be available only from:
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