Hybrid Solutions for Multidimensional Contaminant Dispersion Models in Rivers and Channels
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Abstract
A hybrid analytical-numerical strategy based on the Generalized Integral Transform Technique (GITT) is used to solve steady-state multidimensional models for contaminants dispersion in rivers, streams and channels. The aim is to analyze and exploit this hybrid approach in the reduction of computational costs associated with convection-diffusion models that contain more than one space variable. The main focus of this work is the proposition of solutions for models that include variable coefficients such as variable velocity fields and turbulent diffusion coefficients along and across the river. The mathematical formulations also allow the use of arbitrarily general inlet conditions such as point, linear and plane sources. A few test cases were simulated and the models were validated both numerically and with experimental data taken from the literature. The models were implemented on the symbolic computation platform of the \textit{Mathematica} system.

Keywords: Hybrid methods, Integral transforms, Symbolic computation, Contaminants dispersion, Turbulence

1. Introduction
In order to make accurate and more realistic predictions of contaminants dispersion in rivers and streams to aid decision makers, mathematical models must account for the variability of flow properties and chemical discharge. Simplified one-dimensional models for contaminants dispersion in rivers have been extensively used and can be found for instance in Zoppou \textit{et al.} (1997) and Runkel (1996). These previous works assume that the contaminant is well mixed both laterally (from one river bank to the other) and vertically (across the depth). Depending on the inlet conditions and the aspect ratio of the width and depth of the river, two-dimensional models can be sufficient for predicting concentration plumes, Fischer \textit{et al.} (1979). The knowledge is fairly well consolidated for models that use constant coefficients such as for the velocity and turbulent diffusion coefficients, including the availability of object oriented computer codes, for instance \textit{User’s Guide for RIVRISK} (2000). Research findings are yet to be pursued in the analytical and robust solution of more generalized models.

The traditional approach has been to assume constant coefficients and use classical mathematical techniques such as the integral transform method. A few works have thus considered constant coefficients in horizontal two-dimensional models (depth averaged), such as \textit{User’s Guide for RIVRISK} (2000), Lew \textit{et al.} (1999) and Codell \textit{et al.} (1982). To account the variability of velocity field, Basha (1997) handles the advection-dispersion equation for a non-uniform velocity, including measured velocity profiles as input data in the proposed model, but still assuming that the turbulent diffusion coefficient is constant all across the river. The same modeling is assumed in Mazumder \textit{et al.} (1994) and Wang \textit{et al.} (1978). It is however common to have non-uniform velocities in rivers, streams and channels mainly because of the uneven geometry of the river bed and these variable velocities depend on the cross sectional topography of the river, Mazumder \textit{et al.} (1994). Yeh \textit{et al.} (1979) analytically solved the transport equation for variable velocity and diffusivity fields with power law profiles in vertical contaminant dispersion. In addition, approximate solutions were obtained for two and three dimensional steady state models with variable diffusivities and velocity by making use of hybrid methodologies, Nokes \textit{et al.} (1984) and Nokes \textit{et al.} (1988). Still, depending on the physical characteristics of the river and the type of inlet condition of the discharge, one and two-dimensional models fail to predict contaminant clouds within the physical domain. For this reason, three dimensional dispersion models are of great importance in predicting the concentration field for near source location, Fischer \textit{et al.} (1979). Zoppou \textit{et al.} (1999) analytically solved the advection-diffusion equation with spatially variable coefficients in three dimensions, but with particular forms for the variable coefficients. Three-dimensional models with variable coefficients have been commonly solved by numerical methods since it is difficult to analytically handle partial differential equations with non-constant coefficients, Nokes \textit{et al.} (1994), Lin \textit{et al.} (1995), Croucher \textit{et al.} (1998) and Mazumder \textit{et al.} (2000). On the other hand, it is also accepted that depending on the complexity of the mathematical formulation, these methods tend to have a considerable computational cost and to be less robust than the so desirable analytical solutions,
when available. Hybrid methods, such as the one used in the present work, maintain the simplicity, accuracy and relative small computational cost of analytical methods, while having the ability to handle more complex physical situations that cannot be treated by pure analytical methods, such as, for example, complex geometries and non-linearities. Therefore, the main objective of this work is to solve two-dimensional and three-dimensional steady state mathematical models for dispersion of contaminants in rivers. The proposed models include non-uniform coefficients in any functional form that vary in the vertical and transverse direction. A hybrid numerical-analytical solution is obtained by making use of the so-called Generalized Integral Transform Technique – GITT, yielding analytical expressions for the space dependence of the concentration fields, Cotta (1993). This approach is aided by employing mixed symbolic-numerical computations (Mathematica platform), Wolfram (1999). The goal here is to improve and complement existing solution implementations to study the dispersion of waste materials in rivers, User’s Guide for RIVRISK (2000). RIVRISK is a computational tool, constructed by EPRI and Tetra Tech, Inc., which based on the input data describing the chemical and physical characteristics of the relevant power plant and industrial facility releases and of the receiving river, predicts probable risks associated with the release of such pollutants. The solution methodology is also based on the integral transform method, and the analytical nature of the solutions is preferred for robustness and computational speed. This philosophy is maintained throughout our joint developments, as illustrated along the present contribution in advancing this hybrid computational tool towards the solution of two-dimensional and three-dimensional steady-state dispersion models.

2. Two-Dimensional Problem

A horizontal two-dimensional model is used to formulate the typical situation to be considered here. The contaminant is released continuously into a river, with a variable depth \( p(x) \) and average width \( W \). The velocity of the river is given by \( u(x,y) \) and \( v(x,y) \), longitudinal and transversal components respectively, and varies in any arbitrary functional form along the transversal, \( y \), and the longitudinal, \( x \), directions. It is assumed for the horizontal two-dimensional model that the mass concentration gradients in the transversal direction are more significant than in the vertical direction and that the riverbanks are not dispersive. The model also allows a gradual variation of the depth of the river and the dissolved pollutant has density approximately equal to the density of the receiving fluid, so no buoyancy effects are considered. The discharge velocity of the contaminant is neglected in comparison with the river flow rate. Another important consideration is the assumption that the longitudinal turbulent diffusion effects are small when compared with the longitudinal advective term. Assuming steady-state and that we are dealing with shallow rivers, we have:

\[
U(X,Y) \frac{\partial C}{\partial X} + V(X,Y) \frac{\partial C}{\partial Y} = \frac{\partial}{\partial Y} \left[ \varepsilon_{y}(X,Y) \frac{\partial C}{\partial Y} \right] - \lambda C
\]

(1)

\[
\frac{\partial C}{\partial Y} \bigg|_{y=0} = 0; \frac{\partial C}{\partial Y} \bigg|_{y=1} = 0 \text{ and } C(0,Y) = F(Y)
\]

(2)

where the dimensionless groups are defined as

\[
C = \frac{C^*}{C_0}; \quad X = \frac{x}{W}; \quad Y = \frac{y}{W}; \quad U(X,Y) = \frac{u(x,y)}{u_{av}}; \quad V(X,Y) = \frac{v(x,y)}{u_{av}};
\]

\[
\varepsilon_{y}(X,Y) = \frac{D_{yy}(x,y)}{u_{av} W}; \quad \lambda = \frac{k W}{u_{av}}; \quad F(Y) = \frac{f(y)}{C_0}
\]

(3)

and \( C \) is the dimensionless concentration, \( C_0 \) is the initial concentration, \( C^* \) is the dimensional concentration \( (M/L^3) \), \( W \) is the width of the river \( (L) \), \( x \) is the distance along the flow direction \( (L) \), \( y \) is the distance in the transverse direction \( (L) \), \( u(x,y) \) is the flow velocity profile in the longitudinal direction \( (L/T) \), \( v(x,y) \) is the flow velocity profile in the transversal direction \( (L/T) \), \( u_{av} \) is the average velocity \( (L/T) \), \( D_{yy}(x,y) \) is the lateral turbulent diffusion coefficient \( (L^2/T) \), \( \varepsilon_{y}(x,y) \) is the dimensionless lateral turbulent diffusion coefficient and \( k \) is the decay term constant \( (L^3) \). To solve the problem stated in equations (1) and (2), the GITT methodology will be used. This approach offers a more flexible hybrid numerical-analytical structure for both linear and non-linear convection-diffusion problems and the solution methodology details can be found in Cotta (1993). The following eigenvalue problem is chosen to offer a basis to expand the dimensionless concentration solution:
\[
\frac{d^2 \psi_i(Y)}{dY^2} + \beta_i^2 \psi_i(Y) = 0 \quad \text{with} \quad \left. \frac{d\psi_i(Y)}{dY} \right|_{Y=0} = 0 \quad \text{and} \quad \left. \frac{d\psi_i(Y)}{dY} \right|_{Y=1} = 0
\]  

(4)

and the solution of equations (4) are called eigenfunctions:

\[
\psi_i(Y) = \cos(\beta_i Y)
\]

(5)

and the eigenvalues of the Sturm-Liouville problem above are given below together with the norm \( N_i \):

\[
\beta_i = i\pi \quad \text{and} \quad N_i = \int_{Y=0}^{Y=1} \psi_i^2(Y) \, dY
\]

(6)

for \( i = 0, 1, 2, \ldots \). The integral transform pair (transform and inversion) can be written as:

\[
\overline{C}_i(X) = \int_{Y=0}^{Y=1} \psi_i(Y) \sqrt{N_i} C(X,Y) \, dY
\]

(7)

\[
C(X,Y) = \sum_{i=0}^{\infty} \frac{\psi_i(Y)}{\sqrt{N_i}} \overline{C}_i(X)
\]

(8)

One then proceeds towards the process of integral transformation, making use of the proposed eigenfunction expansion to obtain the following system of ordinary differential equations, Cotta (1993):

\[
\sum_{j=0}^{\infty} A_j(X) \frac{d\overline{C}_j(X)}{dX} = \sum_{j=0}^{\infty} B_j(X) \overline{C}_j(X) - \lambda \overline{C}_j(X)
\]

(9)

with the following inlet condition for \( X = 0 \):

\[
\overline{C}_j(0) = \frac{1}{N_{i+2}} \int_{Y=0}^{Y=1} \psi_i(Y) F(Y) \, dY
\]

(10)

where the coefficients are defined by

\[
A_j(X) = \frac{1}{\sqrt{N_i N_j}} \int_{Y=0}^{Y=1} U(X,Y) \psi_j(Y) \psi_i(Y) \, dY
\]

(11)

\[
B_j(X) = \frac{1}{\sqrt{N_i N_j}} \left[ \int_{Y=0}^{Y=1} \psi_j(Y) \left( \frac{\partial}{\partial Y} \left( \frac{\partial \psi_i(Y)}{\partial Y} \right) \right) \, dY - \int_{Y=0}^{Y=1} V(X,Y) \psi_j(Y) \frac{d\psi_i(Y)}{dY} \, dY \right]
\]

(12)

The system of ordinary differential equations presented in equations (9) and (10) was solved in the Mathematica platform, Wolfram (1999), by making use of the built in function \texttt{NDSolve}, with a user prescribed relative error control. Once the solution is obtained for the transformed potentials, the inversion formula, equation (8), is used to evaluate the original concentration field.

Now, let us suppose that the mass flux in the vertical direction predominates over the transversal flux and that the river bed and the river surface are not dispersive. These assumptions will lead to the vertical two-dimensional model, Yeh et al. (1979) and Nokes et al. (1984), and the mathematical formulation is very similar to equations (1) and (2). Following the nomenclature and model found in the literature, with the exception that the present formulation accounts for the variability of the river width and longitudinal variations for the velocity and vertical eddy diffusivity fields, we have:

\[
U(X,Z) \frac{\partial C}{\partial X} + \omega(X,Z) \frac{\partial C}{\partial Z} = \frac{\partial}{\partial Z} \left( \varepsilon_i(X,Z) \frac{\partial C}{\partial Z} \right) - \lambda C
\]

(13)

\[
\frac{\partial C}{\partial Z} \bigg|_{Z=0} = 0 \quad ; \quad \frac{\partial C}{\partial Z} \bigg|_{Z=1} = 0 \quad \text{and} \quad C(0,Z) = F(Z)
\]

(14)

where the dimensionless groups are defined below:

\[
C = \frac{C'}{C_o} \quad ; \quad X = \frac{x}{d} \quad ; \quad Z = \frac{z}{d} \quad ; \quad U(X,Z) = \frac{u(x,z)}{u_w} \quad ; \quad \omega(X,Z) = \frac{w(x,z)}{u_w} \quad ; \quad \varepsilon_i(X,Z) = \frac{D_{e_i}(x,z)}{u_w W} \quad ; \quad \lambda = \frac{k W}{u_w} \quad ; \quad F(Z) = \frac{f(z)}{C_o}
\]

(15)

while \( f(z) \) is an arbitrary function and \( d \) is the river’s average depth. The subscript \( z \) indicates the vertical direction and \( \omega \) is the vertical velocity component. The same procedure will be followed and since the
mathematical formulation is identical to the previous model, the deductive steps will not be shown. The final transformed system is given by:

$$\sum_{j=0}^{N_y} A_j(X) \frac{d\overline{C}_j(X)}{dX} = \sum_{j=0}^{N_y} B_j(X) \overline{C}_j(X) - \lambda \overline{C}_j(X)$$  \hspace{1cm} (16)

$$\overline{C}_j(0) = \frac{1}{N_i^{1/2}} \int_{Z=0}^{\infty} \Omega_i(Z) F(Z) dZ$$  \hspace{1cm} (17)

where the coefficients \( A_j \) and \( B_j \) are written as

$$A_j(X) = \frac{1}{\sqrt{N_y}} \int_{Z=0}^{\infty} U(X,Z) \Omega_j(Z) \Omega_j(Z) dZ$$  \hspace{1cm} (18)

$$B_j(X) = \frac{1}{\sqrt{N_y}} \int_{Z=0}^{\infty} \Omega_j(Z) \frac{\partial}{\partial Z} \left[ \varepsilon_i(X,Z) \frac{d\Omega_j(Z)}{dZ} \right] dZ - \int_{Z=0}^{\infty} \omega(X,Y) \Omega_i(Z) \frac{d\Omega_j(Z)}{dZ} dZ$$  \hspace{1cm} (19)

\( \Omega_i \)'s are the eigenfunctions in the inverse formula. The system of equations (16) and (17) is again solved within the Mathematica software.

3. Three-Dimensional Problem

A steady-state three-dimensional formulation is now considered for mass transport in rivers and channels. It is considered that the riverbank, the riverbed and the river’s surface are not dispersive and these boundaries will be modeled with second type boundary conditions. Another important aspect to be considered is that the density of the pollutant is approximately equal to the density of the receiving fluid. It is also assumed that the transport in the longitudinal direction is mainly due to advection. The chosen problem formulation in dimensionless form is:

$$U(X,Y,Z) \frac{\partial C}{\partial X} + \zeta V(X,Y,Z) \frac{\partial C}{\partial Y} + \omega(X,Y,Z) \frac{\partial C}{\partial Z} = \zeta \frac{\partial}{\partial Y} \left[ \varepsilon_i(X,Y,Z) \frac{\partial C}{\partial Y} \right]$$  \hspace{1cm} (20)

subject to the following boundary conditions

$$\frac{\partial C}{\partial Y} = 0 \text{, for } Y = 0 \text{ and for } Y = 1; \quad \frac{\partial C}{\partial Z} = 0 \text{, for } Z = 0 \text{ and for } Z = 1; \quad C(X = 0, Y, Z) = F(Y, Z)$$  \hspace{1cm} (21)

\( F(Y, Z) \) is an arbitrary function for the inlet condition. The dimensionless groups are defined below:

$$X = \frac{x}{d}; \quad Y = \frac{y}{W}; \quad U(X,Y,Z) = \frac{u(x,y,z)}{u_{av}}; \quad V(X,Y,Z) = \frac{v(x,y,z)}{u_{av}}; \quad \omega(X,Y,Z) = \frac{w(x,y,z)}{u_{av}};$$

$$\frac{C}{C_*} \varepsilon_i(X,Y,Z) = \frac{D_{yy}(x,y,z)}{u_{av} W}; \quad \frac{\varepsilon_i(X,Y,Z)}{C_*} = \frac{D_{zz}(x,y,z)}{u_{av} d}; \quad \lambda = \frac{k_e d}{u_{av}}; \quad F(Y, Z) = \frac{f(y,z)}{C_*};$$

$$\zeta = \frac{d}{W}$$  \hspace{1cm} (22)

where \( d \) is the river’s average depth (L), \( W \) is the width (L), \( u_{av} (L/T) \) is the average velocity, \( C_* \) is the discharge concentration \( (M/L^3) \), \( D_{yy}(x,y,z) \) and \( D_{zz}(x,y,z) \) are the dimensional eddy diffusivities \( (L^2/T) \) in the transverse and vertical directions, \( f(y,z) \) is the inlet condition \( (x = 0) \), \( k_e \) is the dimensional chemical reaction parameter \( (T^{-1}) \) and \( u(x,y,z), v(x,y,z), \) and \( w(x,y,z) \) are the variable velocity field components, \( \zeta \) is the aspect ratio, \( \varepsilon_i(X,Y,Z) \) and \( \varepsilon_i(X,Y,Z) \) are the dimensionless eddy diffusivities, \( \lambda \) is the dimensionless chemical reaction parameter, \( U(X,Y,Z), V(X,Y,Z) \) and \( \omega(X,Y,Z) \) are the dimensionless velocity field components, and \( C_* \) is the dimensional concentration \( (M/L^3) \). The transform-inverse formulae are now obtained from the double integral transformation and inversion:

$$\overline{C}_n(X) = \frac{1}{\sqrt{N_y N_z}} \int_{0}^{\infty} \int_{0}^{\infty} \overline{C}_n(X,Y,Z) \psi_i(Y) \Omega_i(Z) dYdZ$$  \hspace{1cm} (23)

$$C(X,Y,Z) = \frac{1}{\sqrt{N_y N_z}} \int_{0}^{\infty} \int_{0}^{\infty} \overline{C}_n(X) \psi_i(Y) \Omega_i(Z) dYdZ$$  \hspace{1cm} (24)
and the eigenvalue problems which shall provide the basis for the expansion of the original potential, $C(X,Y,Z)$, are similar to the previous two-dimensional case and shall not be repeated here (for details in de Barros 2004). The eigenvalues $(\gamma, \beta)$ and eigenfunctions $(\psi, \Omega)$ and norms for the vertical and transverse directions are also of a similar nature. Operating the partial differential equation, equation (20), with the integral transform operator and transforming all of the possible terms with the aid of the inverse formula, equation (24), we obtain the following system of ordinary differential equations:

$$
\sum_{p=0}^{\infty} \sum_{j=0}^{\infty} \theta^*_i p_n j (X) \frac{d \overline{C}_{p j} (X)}{dX} = \sum_{p=0}^{\infty} \sum_{j=0}^{\infty} \phi^*_i p_n j (X) \overline{C}_{p j} (X) - \lambda \overline{C}_n (X)
$$

(25)

$$
\overline{C}_n (0) = \overline{F}_n = \frac{1}{\sqrt{N_y N_z}} \int_0^1 \int_0^1 \int_0^1 \psi_i (Y) \Omega_n (Z) F (Y,Z) dYdZ
$$

(26)

where:

$$
\theta^*_i p_n j (X) = \frac{1}{\sqrt{N_y N_z}} \int_0^1 \int_0^1 \int_0^1 \psi_i (Y) \Omega_n (Z) \gamma \Omega_j (Z) \frac{\partial}{\partial Y} \left[ \psi_j (X,Y,Z) \frac{d\psi_i (Y)}{dY} \right] dYdZ
$$

(27)

$$
\phi^*_i p_n j (X) = \frac{1}{\sqrt{N_y N_z}} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \psi_i (Y) \Omega_n (Z) \psi_p (Y) \frac{\partial}{\partial Z} \left[ \psi_j (X,Y,Z) \frac{d\Omega_j (Z)}{dZ} \right] dYdZ
$$

(28)

The related coefficients given in equations (27) and (28), are analytically handled through the symbolic manipulation package Mathematica, Wolfram (1999), and details in this implementation can be found in de Barros (2004).

4. Results and Discussions

In order to illustrate the present hybrid approach for the solution of the contaminant dispersion equation with variable coefficients, we take as an example, a fairly general transversally variable velocity profile, defined in Mazumder et al. (1994) and Wang et al. (1978), here modified to allow for gradual longitudinal variation:

$$
u (x,y) = p_o u_o \left[ 1 - \frac{y}{W} \right] e^{-\alpha \frac{y}{W}}
$$

(29)

where $u_o$ is the maximum velocity and $\alpha$ is an empirical parameter. The depth, $p$, of the river or channel varies linearly with $x$ and is constant within the $y$ direction from the initial pollutant discharge position $x_o$ to a final position $x_f$ (de Barros, 2004). The subscripts $o$ and $f$ indicate the initial position of discharge and the final position of interest. The parameter $\alpha$ thus governs the degree of asymmetry in the flow model considered. A example of chlorine dispersion is taken from the literature, Lew et al. (1999) and User’s guide for RIVRISK (2000), previously employed for co-validation with the RIVRISK model results for constant coefficients, de Barros and Cotta (2003). This example illustrates a power plant with a medium size generating capacity that chlorinates its cooling water to prevent biofouling of its heat exchangers. It is located along a 100 m wide river and its depth varies from 6 m, position where the pollutant is being discharged continuously, to 4 m, located 5 km downstream with an average flow rate of 100 m$^3$/s. The total residual chlorine concentration is nominally taken as 1 mg/l and it is being discharged through a diffuser. The polluting source is located 5 m into the river from the shore. Figure 1 illustrates the longitudinal velocity component profiles and the effect of introducing a variable depth along the river, equation (29). The relevant data for the considered application are: $W$ (m)=100; $W_d$ (m)=5; $h$ (m)=0; $e_{w_y}$ (m$^2$/s)= 0.05; $u_o$ (m/s)=0.17; $k_e$ (1/day)= 10; $C_o$ (mg/l)=1; $p_o$ (m)=6; $p_f$ (m)=4.
where $u_{av}$ is the mean velocity of the river at $x = 0$. Our first concern was to analyze the convergence rates in the proposed eigenfunction expansion for the variable coefficients model. Table 1 demonstrates the convergence characteristics of the expansions for the two-dimensional model with non-uniform coefficients, for the longitudinal plane at $Y = 0.05$, identifying dimensionless positions close to the river shore that are more affected by the contaminant plume. The convergence progress can be observed on the table through the increase on the system truncation order, denoted by the letter $M$. A maximum of 100 ordinary differential equations were simultaneously solved. As expected and typical of eigenfunction expansions, the convergence rate of the solution closer to the polluting source is slower. As the value of $X$ increases, the convergence rate is improved. Nevertheless, it can be observed that three converged digits are obtained in all cases for low truncation orders.

Table 1 - Convergence analysis for variable coefficients formulation (Dimensionless concentration at $Y = 0.05$, for $\alpha = 2$ and $X=1, 10$ and 30)

<table>
<thead>
<tr>
<th>Concentration</th>
<th>$M = 5$</th>
<th>$M = 10$</th>
<th>$M = 15$</th>
<th>$M = 20$</th>
<th>$M = 25$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (1, 0.05)</td>
<td>0.292685</td>
<td>0.147150</td>
<td>0.149458</td>
<td>0.150140</td>
<td>0.150312</td>
</tr>
<tr>
<td>C (10, 0.05)</td>
<td>0.0355545</td>
<td>0.0202583</td>
<td>0.0202758</td>
<td>0.0202874</td>
<td>0.0202916</td>
</tr>
<tr>
<td>C (30, 0.05)</td>
<td>0.00408241</td>
<td>0.00405925</td>
<td>0.00406134</td>
<td>0.00406272</td>
<td>0.00406323</td>
</tr>
<tr>
<td>Concentration</td>
<td>$M = 30$</td>
<td>$M = 35$</td>
<td>$M = 40$</td>
<td>$M = 45$</td>
<td>$M = 50$</td>
</tr>
<tr>
<td>C (1, 0.05)</td>
<td>0.150345</td>
<td>0.150325</td>
<td>0.150299</td>
<td>0.150284</td>
<td>0.15028</td>
</tr>
<tr>
<td>C (10, 0.05)</td>
<td>0.0202924</td>
<td>0.0202919</td>
<td>0.0202913</td>
<td>0.0202910</td>
<td>0.0202909</td>
</tr>
<tr>
<td>C (30, 0.05)</td>
<td>0.00406332</td>
<td>0.00406327</td>
<td>0.00406320</td>
<td>0.00406316</td>
<td>0.00406315</td>
</tr>
<tr>
<td>Concentration</td>
<td>$M = 55$</td>
<td>$M = 60$</td>
<td>$M = 65$</td>
<td>$M = 70$</td>
<td>$M = 75$</td>
</tr>
<tr>
<td>C (1, 0.05)</td>
<td>0.150283</td>
<td>0.150288</td>
<td>0.150291</td>
<td>0.150292</td>
<td>0.150291</td>
</tr>
<tr>
<td>C (10, 0.05)</td>
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<td>0.0202911</td>
<td>0.0202912</td>
<td>0.0202912</td>
<td>0.0202912</td>
</tr>
<tr>
<td>C (30, 0.05)</td>
<td>0.00406315</td>
<td>0.00406317</td>
<td>0.00406318</td>
<td>0.00406318</td>
<td>0.00406318</td>
</tr>
<tr>
<td>Concentration</td>
<td>$M = 80$</td>
<td>$M = 85$</td>
<td>$M = 90$</td>
<td>$M = 95$</td>
<td>$M = 100$</td>
</tr>
<tr>
<td>C (1, 0.05)</td>
<td>0.150290</td>
<td>0.150289</td>
<td>0.150288</td>
<td>0.150289</td>
<td>0.150289</td>
</tr>
<tr>
<td>C (10, 0.05)</td>
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<td>0.0202911</td>
<td>0.0202911</td>
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<td>0.0202911</td>
</tr>
<tr>
<td>C (30, 0.05)</td>
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<td>0.00406317</td>
<td>0.00406317</td>
<td>0.00406317</td>
<td>0.00406317</td>
</tr>
</tbody>
</table>

For the steady-state vertical two-dimensional model, represented by equations (13)-(14), a validation against experimental results will be presented. The test case consists of a 0.05 m deep channel with an average velocity of 0.281 m/s. The Reynolds number, $Re$, is equal to 10700 and von Karman’s constant has a value of 0.34 and was experimentally determined. The vertical eddy diffusivity and velocity profile are taken from literature, Nokes et al. (1984) and Nokes et al. (1988), as well as the experimental input data, Nokes et al. (1988). The discharge is a point source located at the dimensionless coordinates, $Z = 0.24$ and $Y = 5.59$, Nokes et al. (1988). The friction velocity, $u_f^*$, is taken as 0.055 m/s. The employed velocity component and diffusivity are given as:

$$U(Z) = 1 + \frac{u_f^*}{u_{av}} [1 + \ln(Z)] \quad \text{and} \quad \varepsilon(Z) = \frac{u_{av} \kappa}{u_f} Z (1 - Z)$$

Figure 2 illustrates the good agreement between the experimental results, Nokes et al. (1988), and the hybrid solution here advanced. As expected, the major differences are located near the source, $X = 0$. This seems very reasonable since the mass transport phenomenon near the source tends to be three-dimensional. Table 2 demonstrates the excellent GITT solution convergence behavior, with four fully converged significant digits at fairly low system truncation orders.
Experimental Results
Nokes et al. (1988)

Figure 2: Validation with experimental results obtained by Nokes et al. (1988). $C_{eq}$ represents the average concentration.

Table 2: Convergence analysis for the vertical two-dimensional dispersion model with variable coefficients
(Dimensionless concentration distribution for $Z = 0.25$).

<table>
<thead>
<tr>
<th>Concentration</th>
<th>$M = 10$</th>
<th>$M = 20$</th>
<th>$M = 30$</th>
<th>$M = 40$</th>
<th>$M = 50$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C ($X = 10$)</td>
<td>0.1659</td>
<td>0.16837</td>
<td>0.1682</td>
<td>0.16847</td>
<td>0.1684</td>
</tr>
<tr>
<td>C ($X = 30$)</td>
<td>0.12002</td>
<td>0.12169</td>
<td>0.12156</td>
<td>0.12176</td>
<td>0.12171</td>
</tr>
<tr>
<td>C ($X = 60$)</td>
<td>0.09944</td>
<td>0.10076</td>
<td>0.10068</td>
<td>0.10083</td>
<td>0.10079</td>
</tr>
</tbody>
</table>

Concentration $M = 60$

<table>
<thead>
<tr>
<th>Concentration</th>
<th>$M = 60$</th>
<th>$M = 70$</th>
<th>$M = 80$</th>
<th>$M = 90$</th>
<th>$M = 100$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C ($X = 10$)</td>
<td>0.1685</td>
<td>0.1685</td>
<td>0.1685</td>
<td>0.16848</td>
<td>0.16851</td>
</tr>
<tr>
<td>C ($X = 30$)</td>
<td>0.12177</td>
<td>0.12175</td>
<td>0.12178</td>
<td>0.12176</td>
<td>0.12178</td>
</tr>
<tr>
<td>C ($X = 60$)</td>
<td>0.10084</td>
<td>0.10082</td>
<td>0.10085</td>
<td>0.10083</td>
<td>0.10085</td>
</tr>
</tbody>
</table>

For the three-dimensional situation, we have based our test-case on a RIVRISK example found in User’s Guide for RIVRISK (2000), together with velocity and diffusivity profiles taken from Yeh et al. (1979). We consider a river with an average depth of 17 m and width of 80 m with the following velocity and diffusivity profiles:

$$u(z) = a_1 z^n$$
$$D_{zz}(z) = a_2 z^n$$

and

$$a_i = \frac{u_{av} d (q_i + 1)}{d^{n+1}}$$
$$D_{yy} = \frac{D_{zzav}}{d^{n+1}}$$

where $a_1$, $a_2$, $q_1$ and $q_2$ are constant parameters that depend on the friction of the river bed and the Reynolds number. $D_{zzav}$ and $D_{yyav}$ are average values for the turbulent diffusion coefficients. For high Reynolds number we have $q_1 = \frac{1}{7}$ and $q_2 = \frac{6}{7}$, Yeh et al. (1979). The average velocity is 0.3 m/s and the discharge is continuous and limited by the spatial coordinates $y_1 = 0$, $y_2 = 10$ m in the horizontal plane and $z_1 = 10$ m and $z_2 = 12$ m in the vertical plane. The input data are: $W (m) = 80$; $D (m) = 17$; $\zeta = 0.2125$; $z_1 (m) = 10$; $z_2 (m) = 12$; $y_1 (m) = 0$; $y_2 (m) = 10$; $D_{zzav} (m^2/s) = 0.017$; $D_{yyav} (m^2/s) = 0.05$; $C_0$ (mg/l) = 1. Table 3 again confirms the excellent convergence behavior.

Table 3: Convergence analysis for three-dimensional test-case (dimensionless concentration values).

<table>
<thead>
<tr>
<th>M</th>
<th>X = 1</th>
<th>X = 3</th>
<th>X = 5</th>
<th>X = 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.150232</td>
<td>0.139694</td>
<td>0.130784</td>
<td>0.119716</td>
</tr>
<tr>
<td>50</td>
<td>0.423289</td>
<td>0.302061</td>
<td>0.232775</td>
<td>0.173629</td>
</tr>
<tr>
<td>100</td>
<td>0.537064</td>
<td>0.322450</td>
<td>0.236308</td>
<td>0.173875</td>
</tr>
<tr>
<td>150</td>
<td>0.586768</td>
<td>0.324446</td>
<td>0.236253</td>
<td>0.173836</td>
</tr>
<tr>
<td>200</td>
<td>0.593726</td>
<td>0.324390</td>
<td>0.236211</td>
<td>0.173816</td>
</tr>
<tr>
<td>250</td>
<td>0.595112</td>
<td>0.324447</td>
<td>0.236267</td>
<td>0.173848</td>
</tr>
<tr>
<td>300</td>
<td>0.595896</td>
<td>0.324428</td>
<td>0.236244</td>
<td>0.173833</td>
</tr>
<tr>
<td>350</td>
<td>0.595542</td>
<td>0.324450</td>
<td>0.236259</td>
<td>0.173842</td>
</tr>
<tr>
<td>400</td>
<td>0.595227</td>
<td>0.324462</td>
<td>0.236267</td>
<td>0.173846</td>
</tr>
</tbody>
</table>

4. Conclusions

The Generalized Integral Transform Technique (G.I.T.T.) is employed to solve the transport of dissolved substances in rivers, streams and channels, proving itself as a useful hybrid numerical-analytical method for handling partial differential equations with variable coefficients, while maintaining a global error control.
sole numerical task is associated with the solution of a system of ordinary differential equations in one of the space variables, in our case the longitudinal variable. The proposed model can be useful as a practical tool for analyzing water quality in rivers when the velocity profile and the turbulent diffusion coefficients need to be represented, and are available, as transversally and/or longitudinally varying functions.

References


IMSL Library, 1991, MATH/LIB, Houston, TX.


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