IMPROVED LUMPED PARAMETER FORMULATIONS FOR THE SOLUTION OF CONTAMINANT TRANSPORT PROBLEMS

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Abstract. *This work is aimed at proposing improved lumped differential approaches for the solution of solute transport problems in porous media. The results obtained by the proposed technique were tested for a one-dimensional contaminant transport problem and compared against those obtained by a previously reported classical lumped differential solution. Numerical results obtained through a built in function from the MATHEMATICA software system are utilized to verify the proposed solutions in the cases of dispersion and advection dominated transport problems. Finally, a third example is chosen to show the behavior of the proposed approaches in the case of time-dependent mass injection considering a possible leaching scenario.*

Keywords*: Lumped Parameters, Contaminant Transport, Porous Media, CIEA, Lumped Formulations*

1. Introduction

Purely numerical methods, like finite differences or finite elements, have been widely used in safety assessments of landfills and radioactive waste repositories. Such techniques allow for the prediction of groundwater contamination in a wide range of situations, where several phenomena can be considered in addition to the advection-dispersion mass transport equation.

However, such accurate approaches are too costly to perform uncertainty analysis of soil contamination, when several simulations are required, and to model complex interacting systems. In such cases, the use of simple approximate formulations of the mass transport equation, like lumped differential formulations, become imperative. Classical lumped formulations have been applied in the literature to predict aquifer contamination (Gelhar and Wilson, 1974; Fryberger and Bellis, 1977 and Mercado, 1976) and complex chemical systems (Maeda and Bergstrom, 2000; Sardin *et al.*, 1991; Sparks, 1991; Villermaux, 1981 and Villermaux, 1987).

Recently the ideas of lumped formulations have been systematically extended to the so-called coupled integral equations approach (CIEA). The CIEA is a formulation technique used to simplify parabolic and elliptic, linear and nonlinear, partial differential equations. A mixed lumped differential formulation is obtained through the use of improved lumping procedures, such as Hermite-type approximations for integrals, on the independent variables selected to be removed. Such approach allows for considering the effects of axial dispersion between successive cells. This technique, recently reviewed by Cotta and Mikhailov (1997), has been already employed for the solution of different classes of linear and nonlinear (Cotta *et al.*, 2001 and Ruperti *et al.*, 2004) heat transfer problems.

This work is aimed at proposing improved lumped differential approaches, or formally CIEAs, previously used in the case of ablative thermal protection systems (Ruperti *et al.*, 2004), to solve the one-dimensional solute transport in groundwater pathway. Numerical results obtained by using the Mathematica software system (Wolfram, 1996) of symbolic manipulation are utilized to verify the proposed solutions for several values of the involved parameters, such as the pore water velocity, and the dispersion and distribution coefficients. A one-dimensional migration problem of a radionuclide in soil with time-dependent injection, corresponding to a leaching case, is chosen to show the accuracy of the proposed solutions.

2. Problem formulation

The one-dimensional linearized Burgers equation (Cotta *et al.*, 1998; Pontedeiro *et al.*, 2000; Heilbron *et al.*, 2002 and Javandel *et al.*, 1984) provides the simplest mathematical model for the convection-diffusion class of problems that models the migration of radionuclides in porous media. The problem in dimensionless form is described by the following mathematical formulation (Javandel *et al.*, 1984):

$$\frac{\partial C(x,t)}{\partial t} = \Delta \frac{\partial^2 C(x,t)}{\partial x^2} - \sigma \frac{\partial C(x,t)}{\partial x} - \gamma C(x,t), \quad 0 < x < 1, \quad t > 0 \tag{1}$$

with the boundary and initial conditions, respectively, given by:

$$-\frac{\Delta}{\sigma}\frac{\partial C(x,t)}{\partial x} + C(x,t) = \phi(t), \quad x = 0, \quad t > 0 \tag{2}$$

$$\frac{\partial C(x,t)}{\partial x} = 0, \quad x = 1, \quad t > 0 \tag{3}$$

$$C(x,t) = 0, \quad 0 < x < 1, \quad t = 0 \tag{4}$$

where the following non-dimensional groups have been used:

$$t = \frac{D_0\, t^*}{L^{*2}};\ x = \frac{x^*}{L^*};\ C = \frac{C^*}{C_0};\ \Delta = \frac{D_x^*}{R_d D_0};\ \sigma = \frac{L^*\, q^*}{R_d D_0\, \varepsilon};\ \gamma = \frac{\lambda L^{*2}}{D_0} \tag{5}$$

where the asterisks denote dimensional values of the parameters, λ is the decay rate constant, D_0 is a reference value for the dispersion coefficient, C_0 is a reference value for the concentration, L^* is the domain length, q^* is the Darcy velocity, ε is the porosity and $\phi(t)$ is a mass injection function. The dispersion coefficient D_x^* [m^2/yr], and the dimensionless retardation factor R_d are defined, respectively, by:

$$D_x = \alpha_L V_{aq} \tag{6}$$

$$R_d = 1 + \frac{\rho_s K_d}{\varepsilon} \tag{7}$$

The longitudinal dispersivity is represented by α_L, ρ_s is the soil bulk density; K_d is the distribution coefficient and V_{aq} is the pore water velocity in the aquifer, given by:

$$V_{aq} = \frac{q^*}{\varepsilon} \tag{8}$$

3. Lumped differential solutions

We seek an approximation for the partial differential system, Eqs. (1-4), through elimination of the spatial dependence, offering an ordinary differential system for the spatially averaged concentration. Two improved lumped differential approaches are herein proposed and compared with the classical one. The resulting systems of ordinary differential equations and all the CIEA results were obtained through mixed symbolic-numerical computation by using the MATHEMATICA software system (Cotta and Mikhailov, 1997; Wolfram, 1996).

3.1. Classical lumped differential solution

The same classical approach utilized in (Sardin *et al.*, 1991) is herein presented. In this case, the integral that defines the average concentration within the aquifer is written as:

$$C_{av}(t) = \int_0^1 C(x,t)dx \tag{9}$$

which is adopted as the concentration at the right boundary:

$$C(1,t) = C_{av}(t) \tag{10}$$

The concentration at the left boundary is given by:

$$C(0,t)=\phi(t) \tag{11}$$

Equation (1) is integrated within the region $0 \le x \le 1$, to yield, after utilization of the boundary conditions and Eqs. (9-11):

$$\frac{\partial C_{av}(t)}{\partial t}=\sigma\,\phi(\mathrm{t})-(\gamma+\sigma)C_{av}(t) \tag{12}$$

with the initial condition:

$$C_{av}(0)=0 \tag{13}$$

3.2. Improved lumped differential solutions (CIEA)

In this section one recalls some already reported CIEA analysis for heat transfer problems (10). The ordinary differential systems for the spatially averaged concentration are obtained through improved approximations. For this purpose, the integrals that define the average concentration and concentration gradient within the aquifer are written as:

$$C_{av}(t)=\int_0^1 C(x,t)dx \tag{14}$$

$$C(1,t)-C(0,t)=\int_0^1 \frac{\partial C(x,t)}{\partial x}dx \tag{15}$$

The CIEA solutions are based on Hermite-type approximations for the integrals in Eqs. (14) and (15). Different degrees of approximation can be achieved, with increasing analytical involvement but also increasing overall accuracy depending on the order of approximation for each Hermite integration of Eqs. (14) and (15):

3.2.1. $H_{0,0}/H_{0,0}$ Solution

The integrals in Eqs. (14) and (15) are approximated, both, through the trapezoidal rule ($H_{0,0}$ formula) to yield:

$$C_{av}(t)\cong\frac{1}{2}[C(0,t)+C(1,t)] \tag{16}$$

$$C(1,t)-C(0,t)\cong\frac{1}{2}\left[\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}+\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=1}\right] \tag{17}$$

Equations (16) and (17) are solved through symbolic manipulation yielding a solution for $C(0,t)$, $C(1,t)$, and $\partial C(0,x)/\partial x$ with respect to $C_{av}(t)$ and $\phi(t)$:

$$C(0,t)=\frac{\sigma\,\phi(\mathrm{t})+4\Delta\,C_{av}(t)}{4\Delta+\sigma} \tag{18}$$

$$C(1,t)=\frac{-\sigma\,\phi(\mathrm{t})+2\,(2\Delta+\sigma)C_{av}(t)}{4\Delta+\sigma} \tag{19}$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}=-\frac{4\sigma(\phi(t)-C_{av}(t))}{4\Delta+\sigma} \tag{20}$$

Following the formalism in the use of the CIEA for the approximate formulation of heat transfer problems (Cotta and Mikhailov, 1997), Eq. (1) is integrated within the whole domain, to yield, after utilization of the above solution:

$$\frac{\partial C_{av}(t)}{\partial t}=\frac{2\sigma(2\Delta+\sigma)}{4\Delta+\sigma}\phi(\mathrm{t})-\frac{[2\sigma(2\Delta+\sigma)+\gamma(4\Delta+\sigma)]}{4\Delta+\sigma}C_{av}(t) \tag{21}$$

with the initial condition given by Eq. (13).

3.2.2. $H_{1,1}/H_{0,0}$ Solution

The corrected trapezoidal rule ($H_{1,1}$ formula) is employed in approximating the average concentration integral, Eq. (14), and maintaining the $H_{0,0}$ formula for the average concentration gradient expression, Eq. (17):

$$C_{av}(t) \cong \frac{1}{2}[C(0,t)+C(1,t)]+\frac{1}{12}\left[\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}-\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=1}\right] \tag{22}$$

The same procedure adopted above is followed resulting in the ODE system:

$$\frac{\partial C_{av}(t)}{\partial t}=\sigma\,\phi(t)-\gamma\,C_{av}(t)+\sigma\,\frac{[\sigma\,\phi(t)-3(2\Delta+\sigma)C_{av}(t)]}{2(3\Delta+\sigma)} \tag{23}$$

with the initial condition given by Eq. (13).

The concentrations and derivatives at the left and right boundaries are given in this case by:

$$C(0,t)=\frac{\sigma\,\phi(t)+3\Delta\,C_{av}(t)}{3\Delta+\sigma} \tag{24}$$

$$C(1,t)=\frac{-\sigma\,\phi(t)+3(2\Delta+\sigma)C_{av}(t)}{2(3\Delta+\sigma)} \tag{25}$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}=-\frac{3\sigma(\phi(t)-C_{av}(t))}{3\Delta+\sigma} \tag{26}$$

The ODEs (12), (21) and (23) are solved through the built in function NDSolve from *MATHEMATICA* (Wolfram, 1996), starting from the initial condition given by Eq. (13).

4. Analysis

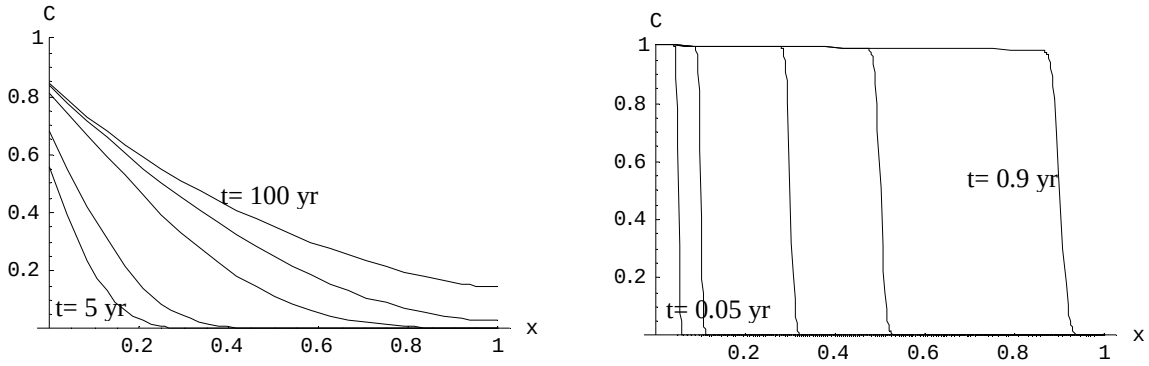
The present methodology was investigated for three different cases. The first and second test-cases consider the extreme situations of dispersion and advection dominated problems, respectively, with the aim at analyzing the behavior of the lumped formulations. In both cases, a local solution was obtained by numerically solving the complete problem, given by Eqs. (1-4), for the following parameters: retardation factor: 1 (K_d=0); domain length: L=100 m; decay rate constant: λ=0.02 1/yr; mass injection function: $\phi(t)$=1. The other parameters are given in Tab. 1.

Table 1. Parameters chosen for the dispersion and advection dominated test-cases.

	DISPERSION	**ADVECTION**
α [m]	10	0.01
Vaq [m/yr]	1	100
Δ	0.1	0.01
σ	1	100
γ	2	2

The numerical solution was obtained by using the NDSolve built in function of the MATHEMATICA software (Wolfram, 1996), which uses the method of lines as solution methodology. Figure 1 shows the migration effect of the contaminant for the two extreme cases at given times (5, 10, 30, 50 and 100 yr for Fig. 1.a, and 0.05, 0.10, 0.30, 0.50 and 0.90 yr for Fig. 1.b). The shape of the contaminant front shown in fig 1.b is typical of an advection dominated problem, where a fine initial step size of 0.1 yr was used in the numerical solution, with a resulting processing time more expensive than that of the dispersive case, as expected. Of course, the advance of the contaminant front is faster

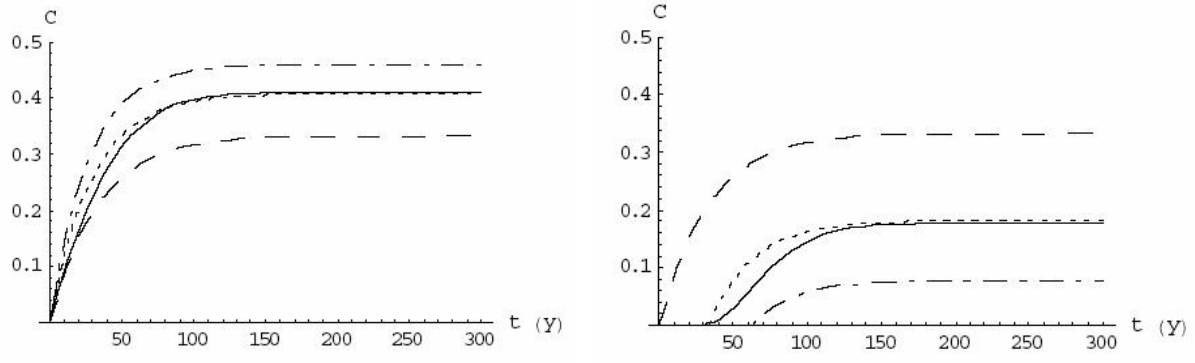
for the advective case, when the plume reaches the out boundary condition in less than 1 yr, while in the dispersive case the plume reaches the boundary in approximately 50 yr.



(a) Dispersion dominated case (b) Advection dominated case

Figure 1. Concentration profiles at given times.

The $H_{0,0}/H_{0,0}$ (dashed-dotted line) and $H_{1,1}/H_{0,0}$ (dotted line) solutions were compared against the classical lumped formulation (dashed line) and the numerical results obtained by the local solution (solid line), as shown in Fig. 2.a for the average concentration, and in Fig. 2.b for the concentration at x=1. Clearly the $H_{1,1}/H_{0,0}$ solution is closer to the "exact" curve, showing an "equilibrated" and good behavior with respect to the classical lumped and $H_{0,0}/H_{0,0}$ approaches. The simulations were made by using the MATHEMATICA software (Wolfram, 1996), while the present approach could be implemented in another computational language, as Fortran. The processing time for the lumped approaches is minimum because there is only one independent variable and only one ordinary differential equation for each lumped approach. Depending on the situations considered it is possible to obtain explicit analytical solutions for the lumped formulations.

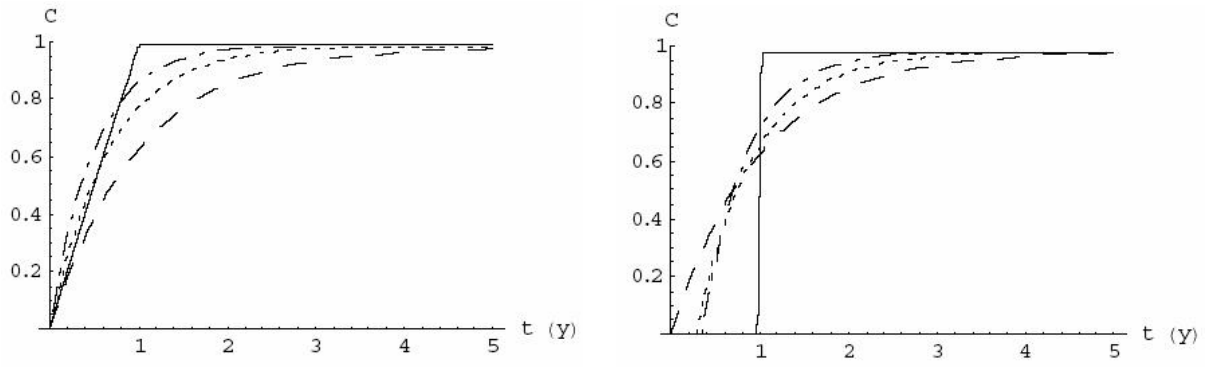


(a) Average concentration (b) Concentration at boundary x=1

Figure 2. Behavior of the concentration for the dispersive case: $H_{0,0}/H_{0,0}$ (dashed-dotted line), $H_{1,1}/H_{0,0}$ (dotted line), classical lumped (dashed line) and numerical (solid line) solutions.

The effect of the considerations used in the formulation of the three different approaches can be observed in Fig. 2.b. The curve corresponding to the classical lumped formulation is exactly the same as that presented in Fig. 2.a, because the concentration at x=1 was imposed to be equal to the average concentration, Eq. (10). The approach $H_{0,0}/H_{0,0}$ already considers some information of the boundary and show an expected dislocated curve from the origin, due to the time of travel of the contaminant to reach the boundary at x=1, but with underestimated values of the concentration along the time. In the case of the $H_{1,1}/H_{0,0}$ approach, in addition to the dislocated curve, the values are very close to the "exact" solution, which can be expected due to the increased overall accuracy of this formulation.

The results of the advection dominated case are presented comparatively in Fig. 3. In this case the $H_{1,1}/H_{0,0}$ approach is also "equilibrated", but a little less accurate with respect to the dispersive case. This behavior can be explained due to the influence of the Hermite approximations of the balance integral on the advective term.



(a) Average concentration (b) Concentration at boundary x=1

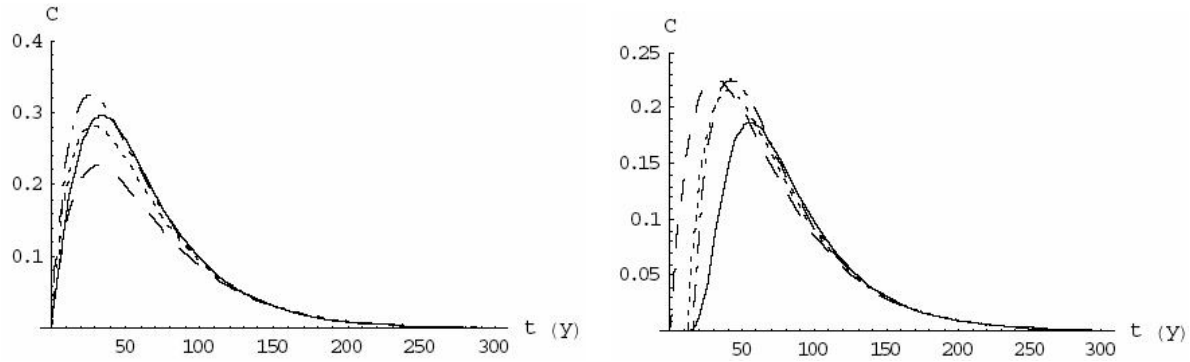
Figure 3. Behavior of the concentration for the advective case: $H_{0,0}/H_{0,0}$ (dashed-dotted line), $H_{1,1}/H_{0,0}$ (dotted line), classical lumped (dashed line) and numerical (solid line) solutions.

One can observe that for times greater than 3 yr the agreement between the $H_{1,1}/H_{0,0}$ approach and the numerical solution is evident, whereas that, for t< 1 yr the results are more conservative.

A third case was considered where a dispersive-advective migration problem of a radionuclide in soil was simulated with a time-dependent mass injection representing a possible leaching scenario. The following parameters were used: retardation factor: 10; domain length: L=100 m; decay rate constant: λ=0.0231 1/yr (half-life= 30 yr); mass injection function: $\phi(t)$=Exp(-b t). The other parameters are given in Tab. 2. The approach $H_{1,1}/H_{0,0}$ is in more agreement with respect to the numerical solution, such as shown in Fig. 4, being "equilibrated" too. For larger times the values of the three approaches converge to the numerical results, whereas at other times more conservative results are obtained.

Table 2. Parameters chosen for the dispersive-advective test-case.

	VALUE
α [m]	10
Vaq [m/yr]	20
Δ	0.2
σ	2
γ	2.31
b	0.0231438



(a) Average concentration (b) Concentration at boundary x=1

Figure 4. Radionuclide contamination due to a leaching scenario.

5. Conclusions

The proposed CIEA $H_{1,1}/H_{0,0}$ approach, based on a more involved Hermite-type approximation for integrals, showed be the best lumped formulation analyzed at the present work. The results showed a good accuracy for the examples chosen, with a better agreement in the case of dispersion dominated problems. The classical lumped approach was not competitive with the proposed CIEA approaches due to its inherent formulation, where the average concentration is imposed at the right boundary.

These formulations can be extended for multidimensional linear or non-linear problems and combined with other numerical or hybrid techniques. The effects of the proposed solutions on the axial dispersion between successive cells will be studied as a further extension of the present work.

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