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A quasi-analytical approach to the advection–diffusion–reaction problem, using operator splitting

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ABSTRACT

Solutions of the combined advection–diffusion–reaction (ADR) transport equation are generally restricted to numerical methods. However, each subprocess, advection, diffusion and reaction can all be solved individually using analytical techniques for a variety of situations. We present a simple numerical technique that uses the split operator method, and the Semi-Lagrangian scheme, to combine these analytical solutions. The result is a coherent, quasi-analytical solution to the combined ADR transport equation.

1. Introduction

The advection–diffusion–reaction (ADR) equation is important in a wide variety of fields. From air pollution modelling, to groundwater transport, to biological processes, and beyond [1], the solution of this equation plays a fundamental role. Indeed, its analogue also plays a critical role in areas such as finance (as the Black–Scholes equation) and semiconductor physics (as the drift-diffusion equation). As such, solving the ADR equation accurately and efficiently is important to many areas of study.

Typically, when solving the ADR equation, numerical methods (such as finite difference or finite element [2]) are the default option, because for most practical problems, that is, multi-dimensional problems, the ADR equation is too difficult to solve analytically beyond the primary simplifying restriction of uniform flow. Analytical solutions that do overcome the above limitation are typically special cases that transform uniform flow solutions to a specific form of non-uniform flow field (for example, [3,4]). The difficulty (and non-generality) of this approach make numerical methods seem all the more attractive, despite fundamental problems associated with these techniques when applied to the ADR equation [5]. However, quasi-analytical techniques, for example, [6,7], combine aspects of both analytical and numerical methods, and provide a viable alternative by utilising the best aspects of each.

This paper presents a novel quasi-analytical technique to solve the ADR equation for non-uniform flow fields. In the field of hydrology, analytical solutions of the flow field for arbitrary flow domains [8,9] have led to quasi-analytical solutions for the pure advection simplification of the ADR equation [10,11]. These provide a fast, yet accurate alternative to numerical methods for dealing with variable velocities and non-parallel streamlines. Likewise, pure diffusion can be solved analytically for flow fields too complicated for combined advection–diffusion-reaction, see for example [12]. Finally, the reaction subprocess of the ADR

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equation has always been the most amenable to analytic solutions, and can be solved for a wide variety of cases. Therefore, the advection, diffusion and reaction equations can all be solved either quasi-analytically or analytically when they are separated, in domains where the combined ADR equation is currently insoluble. As such, a natural question to ask is "Can we accurately combine these analytical solutions?"

In this paper we present a split operator (SO) technique to combine analytical solutions of advection, diffusion and reaction. SO methods are a commonly used approach for combining numerical solutions of interacting physical phenomena, such as in groundwater transport. These methods replace a complicated model with a group of appropriately chosen subprocesses, described by the model, and solved successively in time [13]. The decoupled subprocesses, being simpler to solve than the original system, allow for the solution of otherwise intractable problems. Over the years three basic classes of SO methods [14] have arisen in environmental transport problems: sequential SO (SSO); alternating SO; and iterative SO. As the type of SO method is not the salient aspect of our methodology, we restrict ourselves to the simplest and most common, the SSO, to demonstrate how to combine analytical solutions of advection, diffusion and reaction.

The SSO method divides a problem into two or more subproblems which are solved sequentially, with the solution of each subproblem used as the initial condition for the following subproblem. The most common approach is to split the whole problem into K $(k = 1 \dots K)$ discrete time intervals (Δt), where each group of subproblems is solved for $t^k = k\Delta t$, and the solution of the final subproblem is used as the initial condition of the first subproblem of $t^{k+1} = (k+1)\Delta t$.

This paper is organised as follows. In the next section we provide a mathematical description of the problem to be solved. Section 3 presents the analytical solution technique required to solve each decoupled subprocess, and the method used to combine these is proffered in Section 4. Section 5 examines potential sources of error in the SSO methodology, and the results of the combined technique, along with comparative solutions, are presented in Section 6. Finally, in Section 7 we present a discussion and conclusions.

2. Mathematical description of the problem

As stated in Section 1, the problem to be solved is that of combined advection–diffusion–reaction, with the technique described in Section 4 applicable to a wide range of physical situations. In its general form, the governing ADR equation is

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) - \nabla \cdot (\mathbf{u}C) + R \tag{1}$$

where C is the concentration (of whatever solute is being modelled), D is the diffusion coefficient, $\mathbf{u}$ is the bulk velocity of the solvent, and R is the reaction term (that is, a source or sink of solute). Note that each of the terms, D, $\mathbf{u}$ and R may vary with space, time, or the concentration C.

However, in this paper, for the purposes of clarity and simplicity, we restrict ourselves to the relatively simple case of a one-dimensional (1D) velocity field, $u_* = \mathbf{u}(y)$, equal and constant latitudinal and longitudinal diffusion, $D_{x_*} = D_{y_*} = D_*$, and a simple linear decay term for reaction, $\lambda_* C_*$, where λ_* is a constant. The dimensionalised form of the ADR equation to be solved is then

$$\frac{\partial C_*}{\partial t_*} = D_* \frac{\partial}{\partial x_*}\left(\frac{\partial C_*}{\partial x_*}\right) + D_* \frac{\partial}{\partial y_*}\left(\frac{\partial C_*}{\partial y_*}\right) - u_* \frac{\partial C_*}{\partial x_*} - \lambda_* C_* \tag{2}$$

with the asterisk subscripts representing the dimensionalised parameters of equation (1). Non-dimensionalising the above equation (refer to (Eqs A.1–A.7) in Appendix A for details) results in the specific form of the ADR equation to be solved throughout this paper,

$$\frac{\partial C}{\partial t} = \nabla \cdot (\nabla C) - \mathbf{u}(y)\frac{\partial C}{\partial x} - \lambda C. \tag{3}$$

Finally, we define an initial two-dimensional (2D) Gaussian distribution of solute,

$$C(x, y, 0) = \bar{c} e^{-\left(\frac{(x-x_0)^2}{2\sigma_x^2} + \frac{(y-y_0)^2}{2\sigma_y^2}\right)} \tag{4}$$

(with the peak concentration $\bar{c} = 1$). This domain is seen in Fig. 1, with s and d the lengths of the x and y axes respectively, and the domain scaled for the length of the y-axis, that is, $d = 1$. For convenience we will use a square domain, $s = 1$. All boundary conditions are Dirichlet (first-type) and set to $C = 0$.

3. Analytical solutions of the decoupled subprocesses

The SSO method can be viewed as an approximate technique to integrate equation (3) over an arbitrary time interval Δt [15]. The method is perhaps clearer when presented in the notation of Tompson and Dougherty [16],

$$\Delta C = C(\mathbf{x}, t+\Delta t) - C(\mathbf{x}, t) = \int_t^{t+\Delta t} \nabla \cdot (\nabla C) dt - \int_t^{t+\Delta t} \mathbf{u}(y)\frac{\partial C}{\partial x} dt - \int_t^{t+\Delta t} \lambda C dt. \tag{5}$$

Solving the first integral gives a trial solution, henceforth $C^{(1)}(\mathbf{x}, t+\Delta t)$, which acts as the initial condition of the second integral. The solution of the second integral, henceforth $C^{(2)}(\mathbf{x}, t+\Delta t)$, acts as the initial condition of the third integral, the solution of which gives the final result $C(\mathbf{x}, t+\Delta t)$.