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Internal layers of a transient convection-diffusion problem by perturbation methods†

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A transient convection-diffusion problem with moving sharp fronts is studied by using perturbation methods. A uniformly valid approximate solution is obtained for two cases: shock layer and angular layer. It is shown that the shock layer function can be described by the complementary error function, while the angular layer function can be described by the first iterated integral of the complementary error function.

1 INTRODUCTION

Understanding pollutant transport mechanisms in water bodies, including surface and subsurface flow, is essential for risk assessment, pollutant cleanup, monitoring network design, and various other related activities. A typical transport mechanism involving time-dependent convection-diffusion, with convection being the dominant process, can be expressed as

$$\phi \frac{\partial c}{\partial t} - \nabla \cdot (D \nabla c) + V \cdot \nabla c = F$$

This equation is widely used in soil science, chemical, environmental, and petroleum reservoir engineerings, and water resources. Some of the known applications include the movement of ammonium or nitrate in soils (Gardner,[10] Misra & Mishra,[22] Reddy *et al.*[24]), pesticide movement (Kay & Elrick,[16] van Genuchten & Wierenga,[31]), the transport of radioactive waste materials (Arnett *et al.*,[2] Duguid & Reeves[9]), the fixation of certain iron and zinc chelates (Lahav & Hochberg[19]), the precipitation and dissolution of gypsum (Glas *et al.*,[11] Keisling *et al.*,[17] Kemper *et al.*[18]) or other salts (Melamed *et al.*[21]), saltwater intrusion problems in coastal aquifers (Shamir & Harleman[25]), thermal and contaminant pollution of rivers, lakes, and estuaries (Baron & Wajc,[3] Cleary,[7] DiToro,[8] Thomann[30]), and convective heat transfer problems (Carslaw & Jaeger,[6] Lykov & Mikhailov[20]).

To clearly understand the phenomena of moving sharp fronts of this equation and the techniques of singular perturbation, we consider the following one-dimensional transient convection-diffusion equation

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} + V(t)\frac{\partial c}{\partial x} = 0 \tag{1.1}$$

defined in $\Omega = \{(x,t) : 0 < x < \infty,\ 0 < t < \infty\}$, where $c(x,t)$ is a resident solute concentration at the position x and time t; D is a positive-valued diffusion coefficient; and $V(t)$ is the mean solute velocity, which could be a function of time. In many applications, the values of D are very close to zero. Equation (1.1) is subject to initial condition

$$c(x,0) = f(x) \tag{1.2}$$

for $0 < x < \infty$, Dirichlet boundary condition at $x = 0$

$$c(0,t) = g(t) \tag{1.3}$$

and boundary condition at infinity

$$\lim_{x\uparrow\infty} c(x,t) = 0 \tag{1.4}$$

for $0 < t < \infty$, where $f(x)$ and $g(t)$ are functions to be determined by the physical conditions of the specific application. In subsurface flow, description of the flow physics is often augmented by chemical and/or biological considerations. This generally leads to convective–diffusive–reactive transport equations. When multiple species are present in the aqueous phase, the governing equations form a set of partial differential equations that are coupled through reaction terms. These equations generally need to be solved numerically. In all these cases, the most dominant factor is still the convection.

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The main objective of this study is to propose a reasonable approximate solution to a solute transport process using singular perturbation procedures. The accuracy of the approximate solution is examined and its relative performance can be used to compare with other solution techniques. Furthermore, the proposed solution allows one to investigate the effect of uncertainties in model parameters, initial and boundary conditions on the pollutant concentration level.

The solution to a singularly perturbed problem is said to possess *boundary layer behavior* if it exhibits rapid variations within some small region along the *boundary* of the domain under consideration and the width of the region goes to zero as the small parameter of the problem tends to zero. The solution to a singularly perturbed problem is said to possess *internal layer behavior* if it exhibits rapid variations within some small region along a curve *internal* to the domain and the width of the region goes to zero as the small parameter of the problem tends to zero. In this study we are interested in two types of internal layers arising from the propagation of singularity emanating from the inflow corner of the domain:

- *shock layer* if the solution of the reduced problem, by letting the small parameter be zero, is discontinuous along the internal curve;
- *angular layer* if the solution of the reduced problem has discontinuous first-derivatives along the internal curve.

Each type of internal layer is considered as a combination of two *related* boundary layers located on two sides of the internal curve, respectively, so that the non-smoothness of the solution to the reduced problem can be removed.

It is known that the layer structure of many problems having boundary layer behavior can be described by virtue of the exponential function (exp). In this work, two types of moving fronts are explicitly found in terms of the complementary error function (erfc) and its first iterated integral (ierfc). Due to the fact that the functions erfc(s), ierfc(s) decay faster than the function $\exp(-s)$ as s tends to infinity, we are led to require more stable, accurate numerical methods to approximate moving fronts than boundary layer functions. For example, numerical papers Stynes and O'Riordan,[29] and Guo and Stynes[12] are for singularly perturbed linear time-dependent convection-diffusion problems which have boundary layer behavior without the types of internal layers studied in this work.

Works that are related to the present work are Isakova,[14] Bobisud,[4] and Shih[26,27,28] for the internal layers caused by the rough initial data. The internal layers under this investigation are due to the corner singularity and they are more complicated than those generated by the rough initial data. One such related work for a linear parabolic problem with corner singularity is by Howes[13] who gives some exponential upper bound for the angular layer function.

2 PERTURBATION METHODS

In this study, the technique of singular perturbation is applied to the given problem (1.1), (1.2), (1.3), (1.4). Specifically, we first construct the *outer solution*, a solution to eqn (1.1) with $D = 0$. The outer solution provides a good approximation to the concentration of solute transport for the entire domain except along a neighborhood of a characteristic curve of the first-order hyperbolic differential operator. Along this characteristic curve the outer solution changes abruptly and is not *uniformly* valid for all intended values of the independent variables. It gives rise to determine another type of solution, the *inner solution*, in this narrow region by employing a stretched variable along the curve of nonuniform approximation. The inner solution satisfies a parabolic partial differential equation without a small parameter after scaling the original independent variables. The initial and boundary conditions for the inner solution are imposed in such a way that a matching principle between outer and inner solutions is valid and this inner function is important only near this curve. The inner solution is used to supplement the outer solution along the characteristic curve and their sum provides an approximation to the solute concentration for the *entire* domain.

For a constant diffusion $0 < D \ll 1$, the solute concentration $c(x,t)$ defined by eqns (1.1), (1.2), (1.3), and (1.4) can be approximated by a solution $u(x,t)$ to the first-order hyperbolic partial differential equation, obtained from eqn (1.1) by putting $D = 0$

$$\frac{\partial u}{\partial t} + V(t)\frac{\partial u}{\partial x} = 0 \tag{2.1}$$

defined in Ω. With the positive mean solute velocity $V(t)$, the reduced eqn (2.1) is subject to the inflow auxiliary conditions: initial condition (1.2) and boundary condition (1.3). From the theory of hyperbolic partial differential equations, eqn (2.1) has the characteristic curve

$$x = P(t) := \int_0^t V(\tau)\,\mathrm{d}\tau \tag{2.2}$$

emanating from the origin and the function u is found to be of the form

$$u(x,t) = \begin{cases} f(x - P(t)) & x > P(t) \\ g(P^{-1}(P(t) - x)) & x < P(t) \end{cases} \tag{2.3}$$

where P^{-1} is the inverse function of P. Indeed, the change of variables $\xi = x - P(t)$, $\eta = t$ reduces the hyperbolic eqn (2.1) to the differential equation $\partial u/\partial \eta = 0$, which has a solution of the form

$u(\xi,\eta) = \phi(\xi)$ for some function ϕ. In terms of the original variables (x,t), we then have $u(x,t) = \phi(x - P(t))$. The desired result (2.3) follows from the auxiliary conditions (1.2) and (1.3). Note that the existence of P^{-1} is guaranteed by $V(t) > 0$.

Although $u(x,t)$ provides a good approximation to the solute concentration $c(x,t)$ in most of the domain Ω for a small diffusion coefficient D, there is a discrepancy between $u(x,t)$ and $c(x,t)$ along the characteristic curve $x = P(t)$. From

$$u(P(t)+,t) := \lim_{x\downarrow P(t)} u(x,t) = f(0)$$

$$u(P(t)-,t) := \lim_{x\uparrow P(t)} u(x,t) = g(0)$$

the function $u(x,t)$ is not continuous along the characteristic curve $x = P(t)$ unless the equality $f(0) = g(0)$ holds. Moreover, even if the relation $f'(0) = g'(0)$ is valid, the function $u(x,t)$ is not differentiable along the curve $x = P(t)$ as shown below.

$$\frac{\partial u}{\partial x}(P(t)+,t) := \lim_{x\downarrow P(t)} \frac{\partial u}{\partial x}(x,t) = f'(0)$$

$$\frac{\partial u}{\partial x}(P(t)-,t) := \lim_{x\uparrow P(t)} \frac{\partial u}{\partial x}(x,t) = -\frac{g'(0)}{V(0)}$$

$$\frac{\partial u}{\partial t}(P(t)+,t) := \lim_{x\downarrow P(t)} \frac{\partial u}{\partial t}(x,t) = -f'(0)V(t)$$

$$\frac{\partial u}{\partial t}(P(t)-,t) := \lim_{x\uparrow P(t)} \frac{\partial u}{\partial t}(x,t) = \frac{g'(0)}{V(0)}V(t)$$

Thus the function $u(x,t)$ is differentiable along the curve $x = P(t)$ only if the condition $g'(0) + V(0)f'(0) = 0$ is true. The internal layer function is usually required to supplement the outer function $u(x,t)$ along the characteristic curve $x = P(t)$ so that their sum gives an approximation to the solute concentration on the *entire* domain Ω when the diffusion D is small. Note that the internal layer function is important in a neighborhood of the characteristic curve $x = P(t)$ and it is very close to zero outside a neighborhood of the curve $x = P(t)$.

Define the stretched variable ξ along the characteristic curve $x = P(t)$ by

$$\xi = \frac{x - P(t)}{\sqrt{D}}$$

With the variables ξ and t, eqn (1.1) becomes the heat equation

$$\frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial \xi^2} = 0 \tag{2.4}$$

defined in $-\infty < \xi < \infty$, $0 < t < \infty$. Note that, after using the stretched variable ξ, eqn (2.4) does not depend on the small parameter D anymore.

For the sake of convenience, denote $v(\xi,t)$ by $v^+(\xi,t)$ and $v^-(\xi,t)$ for $0 < \xi < \infty$ and $-\infty < \xi < 0$, respectively. To specify some initial and boundary conditions for eqn (2.4), we have two different cases as follows.

2.1 Shock layer function

First assume that $f(0) \neq g(0)$. Then we have

$$u(P(t)+,t) = f(0) \neq g(0) = u(P(t)-,t)$$

and the proposed internal layer function $v(\xi,t)$ is to overcome the discontinuity of $u(x,t)$ along $x = P(t)$. In other words, the sum $u(x,t) + v(\xi,t)$ is constructed to be continuous along the curve $x = P(t)$. In particular, we impose

$$u(P(t)+,t) + v^+(0,t) = \tfrac{1}{2}[u(P(t)+,t) + u(P(t)-,t)] = u(P(t)-,t) + v^-(0,t)$$

Consequently, the function $v^+(\xi,t)$ is subject to the initial condition

$$v^+(\xi,0) = 0 \tag{2.5}$$

and boundary conditions

$$v^+(0,t) = \tfrac{1}{2}[u(P(t)-,t) - u(P(t)+,t)] = \tfrac{1}{2}[g(0) - f(0)] \tag{2.6}$$

$$\lim_{\xi\uparrow\infty} v^+(\xi,t) = 0$$

when $0 < \xi < \infty$. Similarly, the function $v^-(\xi,t)$ is subject to the initial condition

$$v^-(\xi,0) = 0 \tag{2.7}$$

and boundary conditions

$$v^-(0,t) = \tfrac{1}{2}[u(P(t)+,t) - u(P(t)-,t)] = \tfrac{1}{2}[f(0) - g(0)] \tag{2.8}$$

$$\lim_{\xi\downarrow-\infty} v^-(\xi,t) = 0$$

when $-\infty < \xi < 0$. It then follows that

$$v^-(\xi,t) = -v^+(-\xi,t) \qquad \xi < 0$$

and thus it is sufficient to find the function $v^+(\xi,t)$. The theory of heat equation (Carslaw & Jaeger[6] (p. 63) or Cannon[5] (p, 50)) implies that the function $v^+(\xi,t)$ defined by eqn (2.4) subject to initial condition (2.5) and boundary condition (2.6) can be expressed as

$$v^+(\xi,t) = \int_0^t \frac{\partial G}{\partial \eta}(\xi,0,t-\tau)v^+(0,\tau)\,d\tau$$

where $G(\xi,\eta,t)$ is Green's function of the heat operator in the quarter plane defined by

$$G(\xi,\eta,t) = K(\xi-\eta,t) - K(\xi+\eta,t)$$

with the fundamental solution of the heat operator $K(\xi,t)$ (Carslaw & Jaeger[6] (p. 62) or Cannon[5] (p. 33)) defined by

$$K(\xi, t) = \frac{1}{2\sqrt{\pi t}} \exp\left(-\frac{\xi^2}{4t}\right) \quad (2.9)$$

From

$$\frac{\partial G}{\partial \eta}(\xi, 0, t) = -2\frac{\partial K}{\partial \xi}(\xi, t) = \frac{\xi}{2\sqrt{\pi}t^{3/2}} \exp\left(-\frac{\xi^2}{4t}\right)$$

we have

$$\begin{aligned}\int_0^t \frac{\partial G}{\partial \eta}(\xi, 0, t-\tau)\,\mathrm{d}\tau &= \int_0^t \frac{\partial G}{\partial \eta}(\xi, 0, s)\,\mathrm{d}s \\ &= \frac{2}{\sqrt{\pi}}\int_{\frac{\xi}{2\sqrt{t}}}^{\infty} \exp(-\rho^2)\,\mathrm{d}\rho \\ &= \operatorname{erfc}\left(\frac{\xi}{2\sqrt{t}}\right)\end{aligned}$$

where erfc is the complementary error function defined by

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^{\infty} \exp(-s^2)\,\mathrm{d}s$$

with the following properties

$$\operatorname{erfc}(0) = 1 \qquad \operatorname{erfc}(-x) = 2 - \operatorname{erfc}(x) \quad (2.10)$$

$$\operatorname{erfc}(x) \sim \frac{1}{\sqrt{\pi}x}\exp(-x^2) \qquad \text{as } x \uparrow \infty \quad (2.11)$$

Thus, we obtain

$$v^+(\xi, t) = \tfrac{1}{2}[g(0) - f(0)]\operatorname{erfc}\left(\frac{\xi}{2\sqrt{t}}\right)$$

According to eqn (2.10), the function $v^-(\xi, t)$ defined by eqn (2.4) subject to initial condition (2.7) and boundary condition (2.8) can be found as

$$v^-(\xi, t) = \tfrac{1}{2}[f(0) - g(0)]\operatorname{erfc}\left(-\frac{\xi}{2\sqrt{t}}\right)$$

The internal layer function

$$v(\xi, t) = \begin{cases} \tfrac{1}{2}[g(0) - f(0)]\operatorname{erfc}\left(\dfrac{\xi}{2\sqrt{t}}\right) & \xi > 0 \\ \tfrac{1}{2}[f(0) - g(0)]\operatorname{erfc}\left(\dfrac{-\xi}{2\sqrt{t}}\right) & \xi < 0 \end{cases}$$

is called a *shock layer* function, which is discontinuous along the curve $\xi = 0$ such that the discontinuity of $u(x, t)$ along the characteristic curve $x = P(t)$ is eliminated.

Based on the techniques of singular perturbation, one has obtained an asymptotic approximation $C := u + v$ given by

$$C(x,t) = \begin{cases} f(x - P(t)) + \tfrac{1}{2}[g(0) - f(0)]\operatorname{erfc}\left(\dfrac{x - P(t)}{2\sqrt{Dt}}\right) & x \geqslant P(t) \\ g(P^{-1}(P(t) - x)) + \tfrac{1}{2}[f(0) - g(0)]\operatorname{erfc}\left(\dfrac{P(t) - x}{2\sqrt{Dt}}\right) & x \leqslant P(t) \end{cases} \quad (2.12)$$

which is continuous along $x = P(t)$, and this approximation to $c(x, t)$ is uniformly valid in Ω.

As an illustrative example, for $f(x) = 0$, $g(t) = 1$, and $V(t) = 2$, we have $P(t) = 2t$ and the function $C(x, t)$ given by (2.12) becomes

$$C(x, t) = \tfrac{1}{2}\operatorname{erfc}\left(\frac{x - 2t}{2\sqrt{Dt}}\right)$$

by using (2.10). This function satisfies the initial boundary value problem

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + 2\frac{\partial C}{\partial x} = 0 \qquad \text{in } \Omega$$

$$C(x, 0) = 0 \qquad C(0, t) = 1 - \operatorname{erfc}(\sqrt{t/D})$$

$$\lim_{x \uparrow \infty} C(x, t) = 0$$

It then follows that the function $\psi(x, t) := c(x, t) - C(x, t)$ satisfies the problem

$$\frac{\partial \psi}{\partial t} - D\frac{\partial^2 \psi}{\partial x^2} + 2\frac{\partial \psi}{\partial x} = 0$$

$$\psi(x, 0) = 0 \qquad \psi(0, t) = \operatorname{erfc}(\sqrt{t/D})$$

$$\lim_{x \uparrow \infty} \psi(x, t) = 0$$

The maximum principle (Protter & Weinberger[23] (p. 183)) states

$$\min\{0, \psi(x, 0), \psi(0, t)\} \leqslant \psi(x, t) \leqslant \max\{0, \psi(x, 0), \psi(0, t)\}$$

and, thus, we obtain

$$c(x, t) = C(x, t) + \mathcal{O}(\operatorname{erfc}(\sqrt{t/D})) = C(x, t) + \mathcal{O}(\sqrt{D})$$

in Ω. Figure 1 is for the function $C(x, t)$ when $D = 0{\cdot}01$ (solid curve), $0{\cdot}1$ (dashed curve), $0{\cdot}2$ (dotted curve) and $t = 1, 2, 3$.

The exact solution of this example can be written as

$$c(x, t) = \tfrac{1}{2}\operatorname{erfc}\left(\frac{x - 2t}{2\sqrt{Dt}}\right) + \tfrac{1}{2}\exp\left(\frac{2x}{D}\right)\operatorname{erfc}\left(\frac{x + 2t}{2\sqrt{Dt}}\right)$$

whose derivation is given in the Appendix. This result also appears in van Genuchten and Alves,[32] and Jury

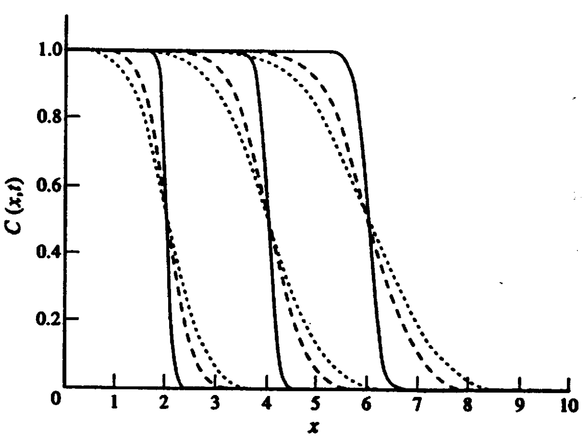

Fig. 1. Shock layer behavior.

and Roth[15] (p. 158). We conclude that the asymptotic solution $C(x,t)$ is an excellent approximation to the exact solution $c(x,t)$ due to the fact that

$$\tfrac{1}{2}\exp\left(\frac{2x}{D}\right)\operatorname{erfc}\left(\frac{x+2t}{2\sqrt{Dt}}\right) \sim \frac{1}{x+2t}\sqrt{\frac{Dt}{\pi}} \times \exp\left[-\frac{(x-2t)^2}{4Dt}\right] \qquad \text{as } D \downarrow 0$$

by virtue of eqn (2.11).

2.2 Angular layer function

In the case of $f(0) = g(0)$, we have

$$u(P(t)+,t) = f(0) = g(0) = u(P(t)-,t)$$

$$\frac{\partial u}{\partial x}(P(t)+,t) = f'(0) \neq -\frac{g'(0)}{V(0)} = \frac{\partial u}{\partial x}(P(t)-,t)$$

$$\frac{\partial u}{\partial t}(P(t)+,t) = -f'(0)V(t) \neq \frac{g'(0)}{V(0)}V(t) = \frac{\partial u}{\partial t}(P(t)-,t)$$

and the proposed internal layer function $v(\xi,t)$ is to overcome the discontinuity in the first derivatives of $u(x,t)$ along $x = P(t)$. In other words, the sum $u(x,t) + \sqrt{D}v(\xi,t)$ is not only continuous along $x = P(t)$ but also differentiable in both x and t along $x = P(t)$. In particular,

$$v^+(0,t) = v^-(0,t)$$

$$\frac{\partial u}{\partial x}(P(t)+,t) + \frac{\partial v^+}{\partial \xi}(0,t) = \frac{1}{2}\left[\frac{\partial u}{\partial x}P(t)+,t) + \frac{\partial u}{\partial x}(P(t)-,t)\right] = \frac{\partial u}{\partial x}(P(t)-,t) + \frac{\partial v^-}{\partial \xi}(0,t)$$

$$\frac{\partial u}{\partial t}(P(t)+,t) + \sqrt{D}\frac{\partial v^+}{\partial t}(0,t) = \frac{1}{2}\left[\frac{\partial u}{\partial t}(P(t)+,t) + \frac{\partial u}{\partial t}(P(t)-,t)\right] = \frac{\partial u}{\partial t}(P(t)-,t) + \sqrt{D}\frac{\partial v^-}{\partial t}(0,t)$$

Consequently, the function $v^+(\xi,t)$ is subject to an initial condition

$$v^+(\xi,0) = 0 \tag{2.13}$$

and boundary conditions

$$\frac{\partial v^+}{\partial \xi}(0,t) = \frac{1}{2}\left[\frac{\partial u}{\partial x}(P(t)-,t) - \frac{\partial u}{\partial x}(P(t)+,t)\right] = -\frac{1}{2}\left[f'(0) + \frac{g'(0)}{V(0)}\right] \tag{2.14}$$

$$\lim_{\xi\uparrow\infty} v^+(\xi,t) = 0$$

when $0 < \xi < \infty$. Similarly, the function $v^-(\xi,t)$ is subject to the intial condition

$$v^-(\xi,0) = 0 \tag{2.15}$$

and boundary conditions

$$\frac{\partial v^-}{\partial \xi}(0,t) = \frac{1}{2}\left[\frac{\partial u}{\partial x}(P(t)+,t) - \frac{\partial u}{\partial x}(P(t)-,t)\right] = \frac{1}{2}\left[f'(0) + \frac{g'(0)}{V(0)}\right] \tag{2.16}$$

$$\lim_{\xi\downarrow-\infty} v^-(\xi,t) = 0$$

when $-\infty < \xi < 0$. It then follows that

$$v^-(\xi,t) = v^+(-\xi,t) \qquad \xi < 0 \tag{2.17}$$

and, thus, it is sufficient to find the function $v^+(\xi,t)$. From the theory of the heat equation (Carslaw & Jaeger[6] (p. 76) or Cannon[5] (p. 55)), the function $v^+(\xi,t)$ defined by eqn (2.4) subject to initial condition (2.13) and boundary condition (2.14) can be expressed as

$$v^+(\xi,t) = -\int_0^t N(\xi,0,t-\tau)\frac{\partial v^+}{\partial \xi}(0,\tau)\,d\tau$$

where $N(x,\eta,t)$ is Neumann's function (Cannon[5] (p. 43)) of the heat operator in the quarter plane given by

$$N(x,\eta,t) = K(x-\eta,t) + K(x+\eta,t)$$

with the fundamental solution of the heat operator given by (2.9). Thus, we have

$$v^+(\xi,t) = \frac{1}{2}\left[f'(0) + \frac{g'(0)}{V(0)}\right]\int_0^t N(\xi,0,t-\tau)\,d\tau$$

A computation gives

$$\int_0^t N(\xi,0,t-\tau)\,d\tau = 2\sqrt{\frac{t}{\pi}}\exp\left(-\frac{\xi^2}{4t}\right) - \xi\operatorname{erfc}\left(\frac{\xi}{2\sqrt{t}}\right) = 2\sqrt{t}\operatorname{ierfc}\left(\frac{\xi}{2\sqrt{t}}\right)$$

where ierfc is the first iterated integral of the complementary error function defined by (Abramowitz & Stegun[1] (p. 299))

$$\operatorname{ierfc}(x) = \int_x^\infty \operatorname{erfc}(s)\,ds = \frac{1}{\sqrt{\pi}}\exp(-x^2) - x\operatorname{erfc}(x) \tag{2.18}$$

with the following properties

$$\operatorname{ierfc}(x) \sim -2x \qquad \text{as } x \downarrow -\infty$$

$$\operatorname{ierfc}(x) \sim \frac{1}{2x^2}\exp(-x^2) \qquad \text{as } x \uparrow \infty \tag{2.19}$$

$$\operatorname{ierfc}(0) = \frac{1}{\sqrt{\pi}} \qquad \operatorname{ierfc}'(0) = -1$$

$$\operatorname{ierfc}(-x) = 2x + \operatorname{ierfc}(x) \tag{2.20}$$

Thus, we get

$$v^{+}(\xi,t)=\left[f'(0)+\frac{g'(0)}{V(0)}\right]\sqrt{t}\,\mathrm{ierfc}\left(\frac{\xi}{2\sqrt{t}}\right)$$

Furthermore, by eqn (2.17), we obtain

$$v^{-}(\xi,t)=\left[f'(0)+\frac{g'(0)}{V(0)}\right]\sqrt{t}\,\mathrm{ierfc}\left(\frac{-\xi}{2\sqrt{t}}\right)$$

The internal layer function

$$v(\xi,t)=\begin{cases}\left[f'(0)+\frac{g'(0)}{V(0)}\right]\sqrt{t}\,\mathrm{ierfc}\left(\frac{\xi}{2\sqrt{t}}\right) & \xi>0\\ \left[f'(0)+\frac{g'(0)}{V(0)}\right]\sqrt{t}\,\mathrm{ierfc}\left(\frac{-\xi}{2\sqrt{t}}\right) & \xi<0\end{cases}$$

is called an *angular layer* function, which is continuous along $\xi=0$ but is discontinuous in its ξ-derivatives along the curve $\xi=0$ so that the discontinuity in the first derivatives of $u(x,t)$ along $x=P(t)$ is eliminated.

An asymptotic approximation $C:=u+\sqrt{D}v$ given by

$$C(x,t)=\begin{cases}f(x-P(t))+\left[f'(0)+\frac{g'(0)}{V(0)}\right]\sqrt{Dt}\,\mathrm{ierfc}\left(\frac{x-P(t)}{2\sqrt{Dt}}\right) & x\geqslant P(t)\\ g(P^{-1}(P(t)-x))+\left[f'(0)+\frac{g'(0)}{V(0)}\right]\sqrt{Dt}\,\mathrm{ierfc}\left(\frac{P(t)-x}{2\sqrt{Dt}}\right) & x\leqslant P(t)\end{cases}\tag{2.21}$$

is not only continuous but also differentiable along $x=P(t)$. This approximation to $c(x,t)$ is uniformly valid in Ω.

For an illustration with $f(x)=x$, $g(t)=t$, $V(t)=2$, we have $P(t)=2t$ and the asymptotic approximation given by eqn (2.21) becomes

$$C(x,t)=(x-2t)+\tfrac{3}{2}\sqrt{Dt}\,\mathrm{ierfc}\left(\frac{x-2t}{2\sqrt{Dt}}\right)\tag{2.22}$$

with the use of eqn (2.20). The function $C(x,t)$ defined by eqn (2.22) satisfies the initial boundary value problem

$$\frac{\partial C}{\partial t}-D\frac{\partial^2 C}{\partial x^2}+2\frac{\partial C}{\partial x}=0 \qquad \text{in } \Omega$$

$$C(x,0)=x \qquad C(0,t)=t-\frac{3}{2}\sqrt{Dt}\,\mathrm{ierfc}(\sqrt{t/D})$$

The maximum principle implies that

$$c(x,t)=C(x,t)+\mathcal{O}(\sqrt{Dt}\,\mathrm{ierfc}(\sqrt{t/D}))$$
$$=C(x,t)+\mathcal{O}(D^{3/2})$$

holds in Ω. Figure 2 is for the function $C(x,t)$ when $D=0{\cdot}01$ (solid curve), $0{\cdot}1$ (dashed curve), $0{\cdot}2$ (dotted curve) and $t=1$.

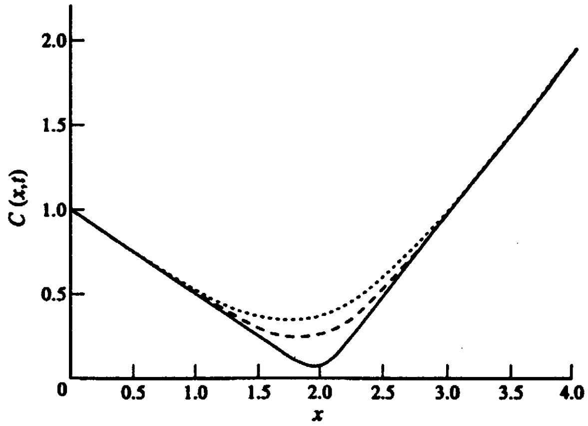

Fig. 2. Angular layer behavior.

The exact solution of this example derived in the Appendix is

$$c(x,t)=x-2t+\tfrac{3}{2}\sqrt{Dt}\left\{\mathrm{ierfc}\left(\frac{x-2t}{2\sqrt{Dt}}\right)-\exp\left(\frac{2x}{D}\right)\mathrm{ierfc}\left(\frac{x+2t}{2\sqrt{Dt}}\right)\right\}\tag{2.23}$$

It then follows from eqn (2.19) that the asymptotic solution $C(x,t)$ gives an excellent approximation to the exact solution $c(x,t)$ due the fact that

$$c(x,t)\sim C(x,t)+\frac{3(Dt)^{3/2}}{(x+2t)^2}\exp\left[-\frac{(x-2t)^2}{4Dt}\right] \qquad \text{as } D\downarrow 0$$

by virtue of eqn (2.19).

3 SUMMARY AND CONCLUSIONS

The significance of the asymptotic results presented in this paper for the transient convection-diffusion prob-(lems by using perturbation methods is the following. First, the function $C(x,t)$ defined by eqn (2.12) or eqn (2.21) provides an excellent approximation to the solute concentration $c(x,t)$ for a small diffusion coefficient D. It offers a way to measure the accuracy of other solution techniques including numerical methods. Second, the results yield functional relationships for the time-distribution of pollutant concentration in water bodies when the diffusion coefficient D is small. These functional relations allow one to examine the sensitivity of model output with respect to model parameter values and initial/boundary conditions. Information obtained from the sensitivity analysis can further be incorporated into uncertainty analysis. Moreover, the identification of the shock (or angular) layer function as a complementary error function (or the first iterated integral of the complementary error function) gives a foundation to design a highly *accurate, stable* numerical method for the general problem. For example, those who are interested in local grid refinement in numerical computations may find the variable $[x - P(t)]/2\sqrt{Dt}$ of erfc and ierfc useful in choosing mesh size and location of refined meshes. Finally, from the mathematical viewpoint, the layer structure of solute concentration shown in this paper may play an important role in obtaining error estimates for reliable numerical methods.

The uniformly valid approximate solutions (2.12), (2.21) for the shock and angular layers which are of the zeroth order in D can be generalized to higher orders in D in principle. Specifically, an asymptotic expansion of the order n for the shock layer case is of the form $\Sigma_{k=0}^{n} D^k u_k(x, t) + \Sigma_{k=0}^{2n} D^{k/2} v_k(\xi, t)$; while an asymptotic expansion of the order n for the angular layer case is given by $\Sigma_{k=0}^{n} D^k u_k(x, t) + \Sigma_{k=1}^{2n} D^{k/2} v_k(\xi, t)$, where the outer solutions $u_k(x, t)$ are defined by the first-order hyperbolic partial differential operator given in eqn (2.1) and the internal layer functions $v_k(\xi, t)$ are defined by the heat operator given by eqn (2.4). The moving sharp fronts studied in this paper are due to the corner singularity of the inflow auxiliary conditions. The analysis can be applied to other types of moving sharp fronts caused by non-smoothness of the inflow initial/boundary data or the sign-change of the mean velocity. Furthermore, the results presented here can be extended to eqn (1.1) with the velocity $V(x, t)$ depending on both spatial and temporal variables. The internal layer functions are then governed by a parabolic differential equation which can be reduced to the heat equation by a change of independent variables (Shih[28]).

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APPENDIX

From Cannon[5] (p. 50), we have the following theorem.
Theorem A.1: The diffusion equation

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} = 0 \tag{A1}$$

in Ω with a positive diffusion coefficient D subject to the initial condition

$$c(x,0) = f(x) \qquad 0 < x < \infty$$

and the Dirichlet boundary condition

$$c(0,t) = g(t) \qquad 0 < t < \infty$$

is given by

$$c(x,t) = \int_0^\infty G(x,\eta,t)f(\eta)\,d\eta + D\int_0^t \frac{\partial G}{\partial \eta}(x,0,t-\tau)g(\tau)\,d\tau$$

where $G(x,\eta,t)$ is Green's function of the diffusion operator, given in (A1), over the quarter plane defined by

$$G(x,\eta,t) = K(x-\eta,t) - K(x+\eta,t) \tag{A2}$$

with the fundamental solution $K(x,t)$ of the diffusion operator given by

$$K(x,t) = \frac{1}{2\sqrt{\pi D t}}\exp\left(-\frac{x^2}{4Dt}\right)$$

Moreover, the above result can be extended to a convention-diffusion problem.
Theorem A.2: The convection-diffusion equation

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} + V\frac{\partial c}{\partial x} = 0 \tag{A3}$$

in Ω with a positive diffusion coefficient D and a constant V subject to the initial condition

$$c(x,0) = f(x) \qquad 0 < x < \infty \tag{A4}$$

and the Dirichlet boundary condition

$$c(0,t) = g(t) \qquad 0 < t < \infty \tag{A5}$$

is given by

$$c(x,t) = \left\{\int_0^\infty G(x,\eta,t)f(\eta)\exp\left(-\frac{V\eta}{2D}\right)d\eta + D\int_0^t \frac{\partial G}{\partial \eta}(x,0,t-\tau)g(\tau)\exp\left(\frac{V^2\tau}{4D}\right)d\tau\right\} \times \exp\left(\frac{Vx}{2D} - \frac{V^2 t}{4D}\right)$$

where $G(x,\eta,t)$ is Green's function of the diffusion operator, given in (A1) over the quarter plane defined by (A2).

Proof: The substitution

$$c(x,t) = v(x,t)\exp\left(\frac{Vx}{2D} - \frac{V^2 t}{4D}\right)$$

converts the initial boundary value problem (A3), (A4), (A5) to

$$\frac{\partial v}{\partial t} - D\frac{\partial^2 v}{\partial x^2} = 0$$

$$v(x,0) = f(x)\exp\left(-\frac{Vx}{2D}\right)$$

$$v(0,t) = g(t)\exp\left(\frac{V^2 t}{4D}\right)$$

The desired integral representation of $c(x,t)$ follows from Theorem A.1.

From Theorem A.2, we are ready to obtain the explicit repsentations of $c(x,t)$ with two sets of input data. We state some preliminary results on integration.

Lemma A.1.

$$\int_{-\infty}^x \frac{1}{2\sqrt{\pi D t}}\exp\left[-\frac{(s-Vt)^2}{4Dt}\right]ds = 1 - \tfrac{1}{2}\operatorname{erfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) \tag{A6}$$

$$\int_x^\infty \frac{1}{2\sqrt{\pi D t}}\exp\left[-\frac{(s+Vt)^2}{4Dt}\right]ds = \tfrac{1}{2}\operatorname{erfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right) \tag{A7}$$

$$\int_{-\infty}^x \frac{x-s}{2\sqrt{\pi D t}}\exp\left[-\frac{(s-Vt)^2}{4Dt}\right]ds = x - Vt + \sqrt{Dt}\,\operatorname{ierfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) \tag{A8}$$

$$\int_x^\infty \frac{x-s}{2\sqrt{\pi D t}}\exp\left[-\frac{(s+Vt)^2}{4Dt}\right]ds = -\sqrt{Dt}\,\operatorname{ierfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right) \tag{A9}$$

Proof: Equations (A6), (A8) follow by using substitution

$$\frac{s - Vt}{2\sqrt{Dt}} = \rho$$

and eqn (2.18); while eqns (A7), (A9) are obtained with the substitution

$$\frac{s + Vt}{2\sqrt{Dt}} = \sigma$$

and (2.18).

Lemma A.2

$$\int_0^t \frac{x}{2\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right] \quad \text{(A10)}$$

$$\int_0^t \frac{x(t - s)}{2\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s = \frac{\sqrt{Dt}}{V}\left\{\operatorname{ierfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) - \exp\left(\frac{Vx}{D}\right)\operatorname{ierfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right\} \quad \text{(A11)}$$

Proof: Split the given integral of (A10) as

$$\int_0^t \frac{x}{2\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s = \int_0^t \frac{x + Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s + \int_0^t \frac{x - Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s$$

Equation (A10) follows after using substitutions

$$\frac{x - Vs}{2\sqrt{Ds}} = \rho \qquad \frac{x + Vs}{2\sqrt{Ds}} = \sigma \quad \text{(A12)}$$

for two resultant integrals, respectively. For (A11), we have

$$\int_0^t \frac{x(t - s)}{2\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s = \int_0^t \frac{xt}{2\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s - \int_0^t \frac{xs}{2\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s$$

$$= t\left\{\int_0^t \frac{x + Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s + \int_0^t \frac{x - Vs}{4\sqrt{\pi D s^3}} \times \exp\left[\frac{-(x - Vs)^2}{4Ds}\right] \mathrm{d}s\right\}$$

$$- \frac{x}{V}\left\{\int_0^t \frac{x + Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s - \int_0^t \frac{x - Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s\right\}$$

$$= \left(t - \frac{x}{V}\right) \int_0^t \frac{x + Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s + \left(t + \frac{x}{V}\right) \int_0^t \frac{x - Vs}{4\sqrt{\pi D s^3}} \exp\left[-\frac{(x - Vs)^2}{4Ds}\right] \mathrm{d}s$$

The desired result follows after using substitution (A12) and (2.18).

Theorem A.3: The convection–diffusion eqn (A3) in Ω with a positive diffusion coefficient D and a constant V subject to the initial condition

$$c(x, 0) = c_i \qquad 0 < x < \infty$$

with a constant c_i and the Dirichlet boundary condition

$$c(0, t) = c_b \qquad 0 < t < \infty$$

with a constant c_b is given by

$$c(x, t) = c_i + \frac{c_b - c_i}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right) \times \operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

Proof: The initial data gives the contribution

$$\exp\left(\frac{Vx}{2D} - \frac{V^2 t}{4D}\right) \int_0^\infty [K(x - \eta, t) - K(x + \eta, t)] \times \exp\left(-\frac{V\eta}{2D}\right) \mathrm{d}\eta = \exp\left(-\frac{V^2 t}{4D}\right) \int_{-\infty}^x K(s, t) \exp\left(\frac{Vs}{2D}\right) \mathrm{d}s$$

$$- \exp\left(\frac{Vx}{D} - \frac{V^2 t}{4D}\right) \int_x^\infty K(s, t) \exp\left(-\frac{Vs}{2D}\right) \mathrm{d}s$$

$$= \int_{-\infty}^x \frac{1}{2\sqrt{\pi D t}} \exp\left[\frac{(s - Vt)^2}{4Dt}\right] \mathrm{d}s - \exp\left(\frac{Vx}{D}\right) \times \int_x^\infty \frac{1}{2\sqrt{\pi D t}} \exp\left[-\frac{(s + Vt)^2}{4Dt}\right] \mathrm{d}s$$

$$= 1 - \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

after using (A6), (A7). The boundary data yields the integral

$$D\exp\left(\frac{Vx}{2D}\right)\int_0^t \frac{\partial G}{\partial \eta}(x,0,s)\exp\left(-\frac{V^2s}{4D}\right)\mathrm{d}s$$
$$= -2D\exp\left(\frac{Vx}{2D}\right)\int_0^t \frac{\partial K}{\partial x}(x,s)\exp\left(-\frac{V^2s}{4D}\right)\mathrm{d}s$$
$$= \int_0^t \frac{x}{2\sqrt{\pi D s^3}}\exp\left[-\frac{(x-Vs)^2}{4Ds}\right]\mathrm{d}s$$
$$= \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right)+\exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right)\right]$$

by using (A10). Thus **Theorem A.2** gives the desired result.

Theorem A.4: The convection-diffusion eqn (A3) in Ω with a positive diffusion coefficient D and a constant V subject to the initial condition

$$c(x,0) = c_i x, \qquad 0 < x < \infty$$

with a constant c_i and the Dirichlet boundary condition

$$c(0,t) = c_b t \qquad 0 < t < \infty$$

with a constant c_b is given by

$$c(x,t) = c_i(x - Vt) + \left(c_i + \frac{c_b}{V}\right)\sqrt{Dt}\left\{\operatorname{ierfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) - \exp\left(\frac{Vx}{D}\right)\operatorname{ierfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right)\right\}.$$

Proof: The initial data yields

$$\exp\left(\frac{Vx}{4D}\right)\int_0^\infty \eta[K(x-\eta,t)-K(x+\eta,t)]\exp\left(-\frac{V\eta}{2D}\right)\mathrm{d}\eta$$
$$= \exp\left(-\frac{V^2t}{4D}\right)\int_{-\infty}^x (x-s)K(s,t)\exp\left(\frac{Vs}{2D}\right)\mathrm{d}s$$
$$+\exp\left(\frac{Vx}{D}-\frac{V^2t}{4D}\right)\times\int_x^\infty (x-s)K(s,t)\exp\left(-\frac{Vs}{2D}\right)\mathrm{d}s$$
$$= \int_{-\infty}^x \frac{x-s}{2\sqrt{\pi Dt}}\exp\left[-\frac{(s-Vt)^2}{4Dt}\right]\mathrm{d}s$$
$$+\exp\left(\frac{Vx}{D}\right)\int_x^\infty \frac{x-s}{2\sqrt{\pi Dt}}\exp\left[-\frac{(s+Vt)^2}{4Dt}\right]\mathrm{d}s$$
$$= x - Vt + \sqrt{Dt}\left[\operatorname{ierfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) - \exp\left(\frac{Vx}{D}\right)\times\operatorname{ierfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right)\right]$$

with the use of (A8), (A9). Next, the boundary data gives

$$D\exp\left(\frac{Vx}{2D}\right)\int_0^t (t-s)\frac{\partial G}{\partial \eta}(x,0,s)\exp\left(-\frac{V^2s}{4D}\right)\mathrm{d}s$$
$$= -2D\exp\left(\frac{Vx}{2D}\right)\int_0^t (t-s)\frac{\partial K}{\partial x}(x,s)\exp\left(\frac{-V^2s}{4D}\right)\mathrm{d}s$$
$$= \int_0^t \frac{x(t-s)}{2\sqrt{\pi D s^3}}\exp\left[-\frac{(x-Vs)^2}{4Ds}\right]\mathrm{d}s$$
$$= \frac{\sqrt{Dt}}{V}\left\{\operatorname{ierfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) - \exp\left(\frac{Vx}{D}\right)\operatorname{ierfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right)\right\}$$

by virtue of (A11). Thus **Theorem A.2** gives rise to

$$c(x,t) = c_i(x - Vt) + \left(c_i + \frac{c_b}{V}\right)\sqrt{Dt}\times\left\{\operatorname{ierfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) - \exp\left(\frac{Vx}{D}\right)\operatorname{ierfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right)\right\}$$