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SHORT COMMUNICATIONS

CONVERGENCE CHARACTER OF A SOLUTION TO THE TRANSPORT EQUATION WITH POLYNOMIAL INITIAL CONDITIONS

I. P. E. KINNMARK*

Department of Civil Engineering, Princeton University, Princeton, NJ 08544, U.S.A.

AND

M. F. N. MOHSEN†

University of Petroleum and Minerals, Dhahran, Saudi Arabia.

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I. INTRODUCTION

Mohsen and Pinder[1] presented a solution to the transport equation

$$D\frac{\partial^2 c}{\partial x^2} - V\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \tag{1}$$

where

$c(x, t)$ is the concentration of the migrating species $[M/L^3]$
D is the diffusion coefficient $[L^2/T]$
V is the fluid velocity $[L/T]$
x is the spatial co-ordinate $[L]$
t is the time $[T]$

solved under the initial condition

$$c(x,0) = g(x) = \begin{cases} a_0 + a_1x^1 + a_2x^2 + \cdots + a_px^p, & 0 \leqslant x \leqslant l_1 \\ 0, & l_1 < x \leqslant l \end{cases}$$

and the following two sets of boundary conditions

$$\left.\begin{aligned} c(0,t) &= c_1 \\ c(l,t) &= c_2 \end{aligned}\right\} \quad \text{(Dirichlet)} \tag{2}$$

* Graduate Student, (Current address: Department of Civil Engineering, University of Notre Dame, Notre Dame, IN 46556, U.S.A.)
† Associate Professor of Civil Engineering. (Currently a Visiting Fellow at Princeton University, Princeton, NJ 08544, U.S.A.)

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$$\left.\begin{aligned} c(0,t)&=c_1\\ \frac{\partial c}{\partial x}(l,t)&=0\end{aligned}\right\}\quad \text{(Neumann)} \tag{3}$$

$c(x, t)$ was normalized as shown below:

$$\theta(x,t)=\frac{c(x,t)}{c_1}=\begin{cases}\phi(x,t) \text{ for Dirichlet condition } c(l,t)=c_2\\ \psi(x,t) \text{ for Neumann condition } c'(l,t)=0\end{cases} \tag{4}$$

A combined form of the general solution was shown to be

$$\theta(x,t)=\bar{\bar{\theta}}(x)+\mathrm{e}^{PX/2}\sum_{n=1}^{\infty}\omega[B_n-B_n^0]\sin(\xi_n X)\mathrm{e}^{-[\xi_n^2+(P/2)^2]T} \tag{5}$$

where

P = Peclet number = Vl/D
T = Non-dimensional time = Dt/l^2
X = Non-dimensional distance = x/l
ωB_n = Fourier coefficients for polynomial initial condition
ωB_n^0 = Fourier coefficients for '0' initial condition
$\xi_n = n\pi$ for Dirichlet and Z_n for Neumann b.c., respectively
Z_n = non-zero roots of $Z_n \cot(Z_n) + P/2 = 0$
$\bar{\bar{\theta}}$ = the solution to the steady state part of (1) under the given non-homogeneous boundary conditions (2) or (3).

For a more detailed description of the solution and various parameters therein see Reference 1.

Numerical evaluation of the solution at large and small values of T is difficult. At small T the solution is a slowly decaying sine series and, therefore, requires many terms for convergence. At large T, evaluation of even the first term of the series may cause machine underflow, even though the solution may not have converged. Thus it is helpful to know a range of T and P for which computer evaluation of the solution is possible. In the following section the convergence of the solution is investigated and a region of applicability (for the governing parameters T and P) is established, in which the solution may be computer evaluated.

REGION OF APPLICABILITY OF THE SOLUTION

Two different factors limit the applicability of the analytical solution presented in the previous section, when numerical evaluations are desired. At small times the convergence is less rapid, owing to the fact that the magnitude of the argument in the exponential function in (5) is small. A small time T_l is derived which guarantees that the sum of the first k terms in the series deviate less than an arbitrary small number ε from the sum of the infinite series for different Peclet-numbers, P. Secondly, at sufficiently large times even the first term in the series is too small to be represented on a given computer, i.e. underflow occurs. For a given underflow limit ε_M and Peclet number P the largest possible time T_s, which does not cause underflow in the first term, is derived. We assume that the following properties hold for $g(x)$.

$$0 \leqslant G(x)=\frac{g(x)}{c_1}\leqslant \bar{\bar{\theta}} \leqslant 1 \tag{6}$$

To evaluate the series in (5) k terms are used. We want to determine a minimum time T_l such that the remainder of the series is less than ε, that is

$$S_k(T_l) < \varepsilon \tag{7}$$

where

$$S_k(T) = \sum_{n=k+1}^{\infty} e^{PX/2} \omega (B_n^0 - B_n) \sin(\xi_n X) e^{-[\xi_n^2 + (P/2)^2]T} \tag{8}$$

$$B_n = \int_0^l G(x) e^{-PX/2} \sin(\xi_n X) dx \tag{9}$$

$$B_n^0 = \int_0^l \bar{\bar{\theta}}(x) e^{-PX/2} \sin(\xi_n X) dx \tag{10}$$

We start by obtaining an estimate of $|B_n^0 - B_n|$ using (6), (9) and (10)

$$|B_n^0 - B_n| \leqslant \frac{2l}{P}[1 - e^{-P/2}] \tag{11}$$

We are now in a position to estimate $S_k(T_l)$ using (8) and (11)

$$S_k(T_l) \leqslant \frac{2l}{P}[e^{P/2} - 1] \sum_{n=k+1}^{\infty} \omega e^{-[\xi_n^2 + (P/2)^2]T_l}, \quad 0 \leqslant X \leqslant 1 \tag{12}$$

Now we need an estimate of the two different ω's, ω^{ψ} and ω^{ϕ}. The values for the ω's were derived by Mohsen and Pinder.[1]

$$\omega^{\psi} = \frac{2}{l}\left[\frac{2Z_n}{2Z_n - \sin(2Z_n)}\right] \tag{13}$$

Here we use the fact that $Z_n \geqslant \pi/2$ and $P > 0$, thus

$$\omega^{\psi} \leqslant \frac{2}{l}\frac{2Z_n}{2Z_n - 1}$$

Now apply the inequality $Z_{n+1} > Z_n$

$$\omega^{\psi} \leqslant \frac{2}{l}\frac{2Z_1}{2Z_1 - 1} \leqslant \frac{2}{l}\frac{\pi}{\pi - 1}$$

$$\omega^{\phi} = \frac{2}{l} \tag{14}$$

Thus (12), (13) and (14) yield:

$$S_k(T_l) \leqslant \frac{4\pi}{\pi - 1}\frac{e^{P/2} - 1}{P} e^{-(P/2)^2 T_l} \sum_{n=k+1}^{\infty} e^{-\xi_n^2 T_l} \tag{15}$$

Application of the fact that $\xi_n > \pi(n - \frac{1}{2})$ together with some simple inequalities and summation of a geometric series yield

$$S_k(T_l) \leqslant \frac{4\pi}{\pi - 1}\frac{e^{P/2} - 1}{P}\frac{e^{-[(P/2)^2 + \pi^2(k+\frac{1}{2})^2]T_l}}{1 - e^{-\pi^2(2k+1)T_l}} \tag{16}$$

For all T_l satisfying the following relation

$$T_l > \eta(k) = \frac{\ln(11/10)}{\pi^2(2k + 1)} \tag{17}$$

we can find a lower limit for the denominator in the last expression in (16) and thus find an upper bound for the last expression in (16)

$$S_k(T_l) < \frac{44\pi}{\pi - 1} \frac{e^{P/2} - 1}{P} e^{-[(P/2)^2 + \pi^2(k+\frac{1}{2})^2]T_l} \tag{18}$$

If we now impose the condition that $S_k(T_l)$ be less than ε, equation (18) allows a simple calculation of a lower limit for T_l, as long as the assumption (17) holds

$$T_l > \frac{\ln\left(\dfrac{44\pi}{\pi - 1}\right) + \ln\left(\dfrac{e^{P/2} - 1}{P}\right) - \ln \varepsilon}{(P/2)^2 + \pi^2(k + \frac{1}{2})^2} \tag{19}$$

This is a lower time limit for which we can evaluate the series and limit the error to ε.

With a very similar derivation to the above we can show that an upper time limit at which the solution can be evaluated without risking underflow in the first term is

$$T_s < \frac{\ln\left(\dfrac{4\pi}{\pi - 1}\right) + \ln\left(\dfrac{e^{P/2} - 1}{P}\right) - \ln(\varepsilon_M)}{(P/2)^2 + Z_1^2} \tag{20}$$

Equation (19) holds for all k. For small values of k equation (19) may however be too conservative. The emphasis of the current study is however on high accuracy evaluations, thus, necessitating larger k values.

In Figure 1 we find equations (17), (19) and (20) plotted for the case of

$$\varepsilon = 10^{-20} \tag{21}$$

$$\varepsilon_M = 10^{-70} \tag{22}$$

$$k = 50 \tag{23}$$

First we notice that T_l is everywhere greater than $\eta(k)$ which is necessary for the region of

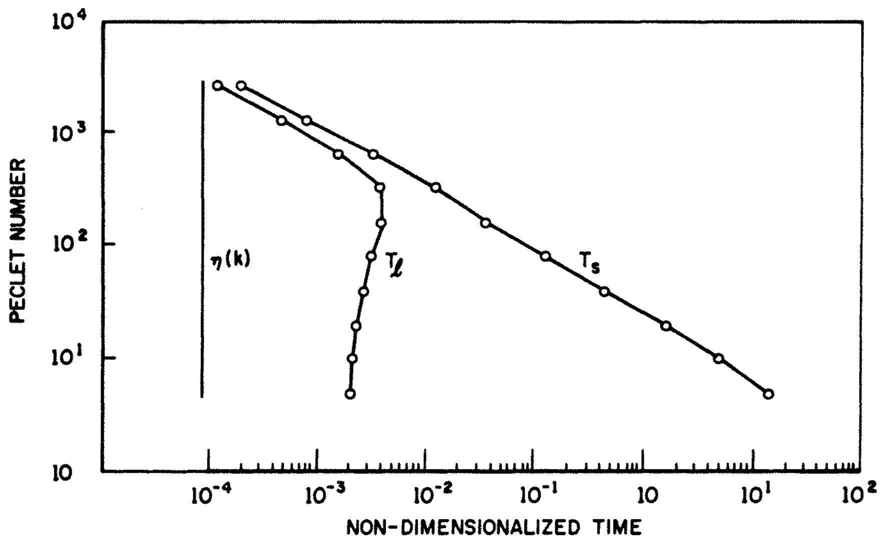

Figure 1. Region of applicability for numerical evaluation of the analytical solution to the transport equation ($\varepsilon = 10^{-20}$, $\varepsilon_M = 10^{-70}$, $k = 50$)

applicability to be bounded by T_l and T_s. Therefore the region in which the analytical solution can be used is bounded below by T_l and above by T_s. When studying this region we see that for Peclet numbers above approximately 300 the T_l and T_s curves come so close together that the region of applicability virtually vanishes. Therefore a Peclet number of approximately 300 seems to be an upper limit for the applicability of the solution.

CONCLUSION

A certain region of parameters is shown to generate satisfactory numerical evaluation of an analytical solution to the convective-dispersive equation with polynomial initial condition. A lower time limit is established, above which the error due to truncation of the infinite series is within a prescribed limit. An upper time limit is determined below which evaluation of the first term in the series does not cause underflow.

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REFERENCE

1. M. F. N. Mohsen and G. F. Pinder, 'Analytical solution of the transport equation using a polynomial initial condition for verification of numerical simulators', *Int. j. numer. methods fluids*, **4**, 701–707 (1984).