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SHORT COMMUNICATION

ANALYTICAL SOLUTION OF THE TRANSPORT EQUATION USING A POLYNOMIAL INITIAL CONDITION FOR VERIFICATION OF NUMERICAL SIMULATORS

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INTRODUCTION

To establish the accuracy of numerical solutions to the convective-diffusive transport equation

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

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 coordinate $[L]$
t is time, $[T]$.

One normally seeks a comparison with an analytical solution. Difficulties arise, however, where the initial condition $c(x, 0) = 0$, $0 < x \leq l$, normally imposed upon the analytical solution, is incompatible with the initial condition expressed by the numerical approximation. For example, the finite element method employing linear 'chapeau' basis functions, of necessity generates a ramp function initial condition at the upstream boundary of a one-dimensional domain. The objective of this paper is to provide an analytical solution compatible with those initial conditions most commonly encountered in finite element and collocation approximations.

The paper consists of three parts. We begin with the problem specification wherein a general polynomial initial condition is assumed. This section is followed by a presentation of

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the solution, which is derived in detail in an appendix. Finally the solution is presented graphically and the significance of the specific form of the initial condition is discussed.

PROBLEM FORMULATION

Equation (1) requires an initial condition and two boundary conditions for proper specification. The initial condition can be written in general as

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

The case of $a_0\neq 0$, $a_1\neq 0$, $a_2,\ldots,a_p=0$ corresponds to a linear initial condition such as illustrated in Figure 1. Higher degree polynomial initial conditions are illustrated in Figures presented later.

The boundary condition at $x=0$ is given as

$$c(0,t)=c_1 \tag{3}$$

Because the boundary condition at $x=l$ is somewhat controversial, we consider both the Dirichlet case

$$c(l,t)=c_2 \tag{4}$$

and the Neumann case

$$\frac{\partial c}{\partial x}(l,t)=0 \tag{5}$$

We assume in the derivation that $c_1\geq c_2$ and that $g(x)\leq c_s(x)$ where $c_s(x)$ is the steady state solution.

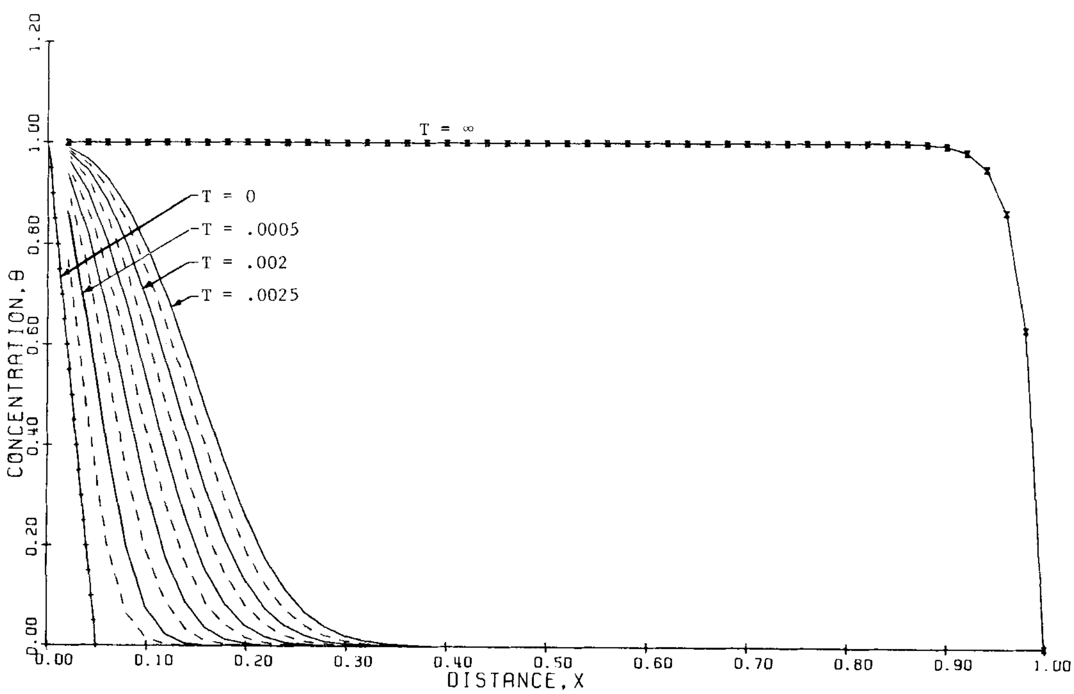

Figure 1. Solutions generated by a step initial condition (– – – –), a ramp initial condition (———) with $l_1=0{\cdot}05$. The ramp initial condition is shown by (+ + +); the steady-state solution (✕✕✕).

SOLUTION

Let $\theta(x, t)$ be a normalized form of $c(x, t)$, as shown below:

$$\theta(x,t)=\frac{c(x,t)}{c_1}=\begin{cases}\phi(x,t) \text{ for Dirichlet condition } c(l,t)=c_2\\ \psi(x,t) \text{ for Neumann condition } \dfrac{\partial c}{\partial x}(l,t)=0\end{cases} \tag{6}$$

Employing a methodology detailed in Appendix I, a combined form of the general solution may be written as

$$\theta(x,t)=\bar{\bar{\theta}}(x)+e^{PX/2}\sum_{n=1}^{\infty}\omega[B_n-B_n^0]\sin(\xi_n X)e^{-[\xi_n^2+(P/2)^2]T} \tag{7}$$

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 (3), (4), or (5).

Table I completes the description of the solution. Note that the following definitions pertain to Table I.

$$A_q=\frac{a_q}{c_1} \tag{8}$$

and

$$I_q(\xi_n)=e^{-Pl_1/2l}\sum_{r=0}^{q}\left\{\frac{(-1)^r q!\, l_1^{q-r}}{\rho^{r+1}(q-r)!}\sin\left[\frac{\xi_n l_1}{l}-(r+1)\alpha\right]\right\}-\frac{(-1)^q q!}{\rho^{q+1}}\sin[-(q+1)\alpha] \tag{9}$$

$$\rho=\sqrt{\left[\left(\frac{P}{2l}\right)^2+\frac{n^2\pi^2}{l^2}\right]} \tag{10}$$

$$\alpha=\cos^{-1}\left(-\frac{P}{2l\rho}\right) \tag{11}$$

Table I

Boundary condition at $X=1$	Solution $\theta(x,t)$	Steady-state Part $\bar{\bar{\theta}}(x)$	Fourier coefficients		
			ω	B_n	B_n^0
Dirichlet $c(l,t)=c_2$	$\phi(x,t)$	$\bar{\bar{\phi}}(x)=A+Be^{PX}$†	$\omega^{\phi}=\frac{2}{l}$	$B_n^{\phi}=\sum_{q=0}^{p}A_q I_q(n\pi)$	$B_n^{0\phi}=\left[\frac{n\pi/l}{n^2\pi^2/l^2+(P/2l)^2}\right]\times\left[1-\left(\frac{c_2}{c_1}\right)(-1)^n e^{-P/2}\right]$
Neumann $\frac{\partial c}{\partial x}(l,t)=0$	$\psi(x,t)$	$\bar{\bar{\psi}}(x)=1$	$\omega^{\psi}=\frac{2}{l}\left[\frac{2Z_n}{2Z_n-\sin(2Z_n)}\right]$	$B_n^{\psi}=\sum_{q=0}^{p}A_q I_q(Z_n)$	$B_n^{0\psi}=\left[\frac{Z_n/l}{Z_n^2/l^2+(P/2l)^2}\right]$

† $A=\dfrac{c_2/c_1-e^P}{1-e^P}$ and $B=\dfrac{1-c_2/c_1}{1-e^P}$

Special case 1

For the more common case of $c_1 = 1$ and $c_2 = 0$, the expression for $\omega(B_n^{\phi} - B_n^{0\phi})$ simplifies to

$$\omega(B_n - B_n^0) = \frac{2}{l}\left\{\left(\sum_{q=0}^{p} A_q I_q(n\pi)\right) - \frac{n\pi/l}{n^2\pi^2/l^2 + \left(\frac{P}{2l}\right)^2}\right\}$$

Special case 2

If further $g(x) \equiv 0$, we get the solution for '0' initial condition for which

$$\omega(B_n - B_n^0) = -\omega B_n^0 = -\frac{2}{l}\frac{n\pi/l}{n^2\pi^2/l^2 + (P/2l)^2}$$

A different form of the solution in an unintegrated form for an arbitrary initial condition was derived by Carslaw and Jaeger.[1] Two FORTRAN codes for the Dirichlet and Neuman boundary conditions have been developed.*

DISCUSSION

Let us now consider the practical significance of using an analytical solution that employs an initial condition totally compatible with a numerical approximation under investigation. Figure 1 illustrates the difference between the commonly used step function initial condition and the ramp function initial condition that is consistent with a finite element approximation using linear chapeau basis functions and a grid spacing of 0·05, $x \in [0, 1]$. It is observed that the front delineated by the solid line and representing the correct analytical solution is always ahead of the front determined by the step function initial condition. The importance of this observation is highlighted in Figure 2 where a larger spatial increment of 0·20, $x \in [0, 1]$ is employed. In this instance the deviation between the two solutions is even more pronounced.

In Figure 3 we present a comparison between solutions obtained with a cubic initial condition, such as encountered using Hermite polynomial basis functions, and the step-function initial condition presented in the preceding discussion. Here, as in the previous ramp-function case, the correct analytical solution precedes that obtained using the step initial condition.

As a final example, consider a quintic polynomial that is compatible with a collocation or finite element approximation defined on a net with spacing 0·20, $x \in [0, 1]$. This solution is compared with the standard step-function initial condition in Figure 4. In this case one observes not only a difference in the locations of the fronts obtained using the different initial conditions, but also a difference in their shape. The 'hump', clearly evident in the quintic initial condition, is apparent only in the compatible analytical solution.

The differences between the solutions generated using the step-functions and polynomial initial conditions are important when the accuracies of various numerical approximations of the convective-diffusive transport equation (1) are being evaluated. Error norms usually require an exact solution for their determination. Thus, where numerical schemes of high order accuracy are being examined, an analytical solution compatible with the numerical auxiliary conditions can be very important.

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* The listing of the computer codes may be obtained from the authors upon request.

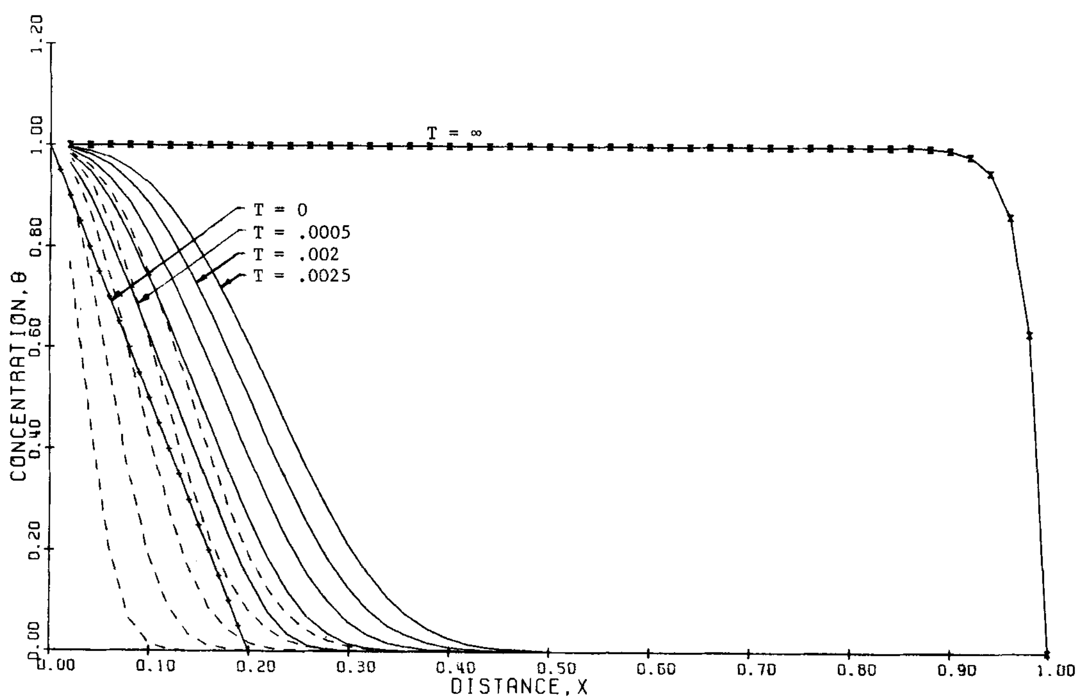

Figure 2. Solutions generated by a step initial condition (– – –) and a ramp initial condition with $l_1 = 0{\cdot}2$. The initial condition is shown by (+++++); the steady-state solution by (-x-x-x-), $P = 50$.

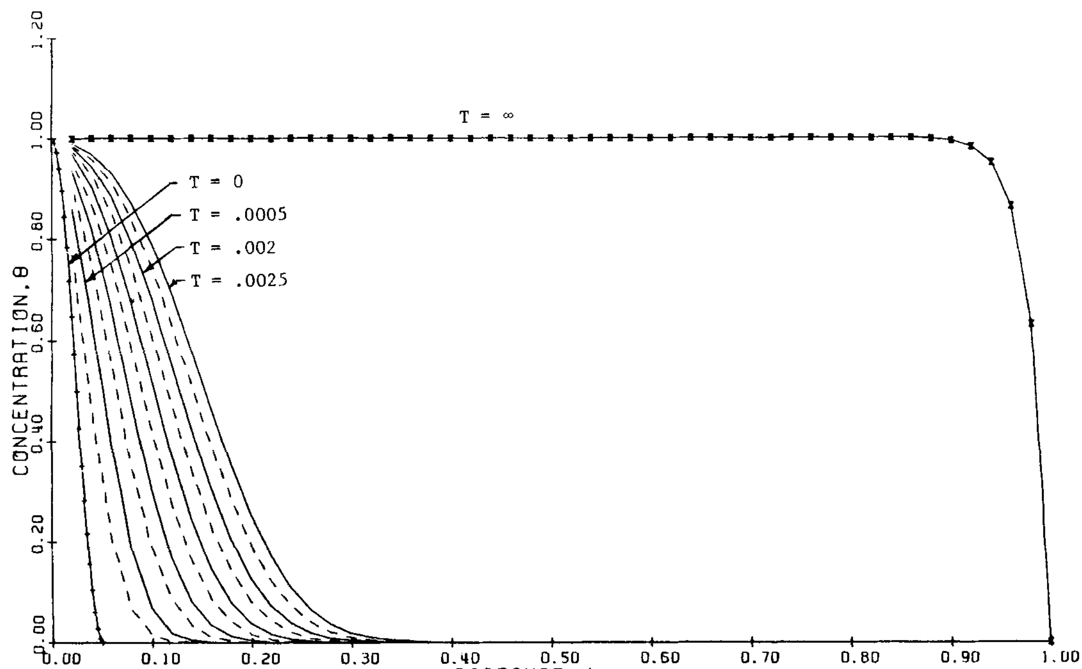

Figure 3. Solutions generated by a step initial condition (– – – –), and a cubic Hermitian initial condition (———) with $l_1 = 0{\cdot}05$. The initial condition is shown by (+ + +); the steady-state solution by (-x-x-x-x-), $P = 50$.

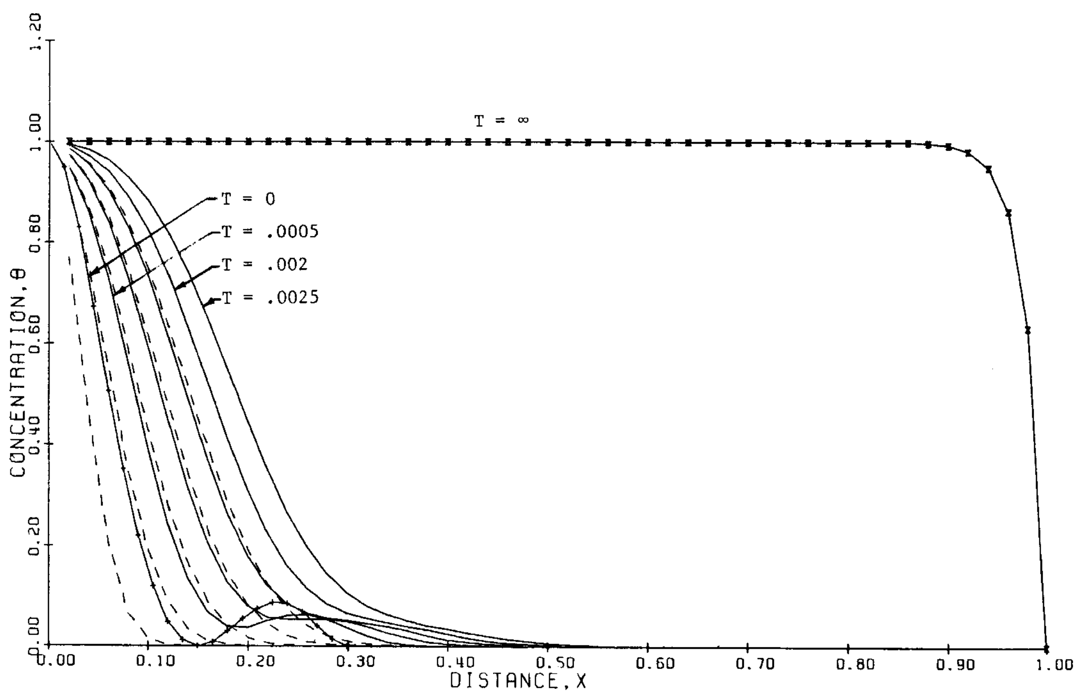

Figure 4. Solutions generated by a step initial condition (- - - -), a quintic Hermitian initial condition (———), for $l_1 = 0{\cdot}03$. The initial condition is shown by (+ + + + +); the steady-state solution by (-×-×-×-), $P = 50$.

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APPENDIX I: DETAILS OF DERIVATION

Case I Dirichlet boundary condition at $x = l$, i.e. $c(l, t) = c_2$

The steady-state part $\bar{\bar{\phi}}(x)$ of the solution may be obtained as

$$\bar{\bar{\phi}}(x) = \frac{c_2/c_1 - e^P}{1 - e^P} + \frac{1 - c_2/c_1}{1 - e^P} e^{PX}, \quad 0 < \bar{\bar{\phi}}(x) < 1 \tag{12}$$

The transient part of the solution under homogeneous boundary conditions $\bar{\phi}(0, t) = 0$ and $\bar{\phi}(l, t) = 0$ and an initial condition $\bar{\phi}(x, 0) = \phi(x, 0) - \bar{\bar{\phi}}(x)$, may be obtained by separation of variables as

$$\bar{\phi}(x, t) = e^{PX/2} \sum_{n=1}^{\infty} E_n^{\phi} \sin(n\pi X) e^{-[n^2\pi^2 + (P/2)^2]T} \tag{13}$$

E_n^{ϕ} may be evaluated by satisfying the initial condition

$$\bar{\phi}(x, 0) = e^{PX/2} \sum_{n=1}^{\infty} E_n^{\phi} \sin(n\pi X) \equiv G(x) - \bar{\bar{\phi}}(x)$$

where

$$G(x)=\begin{cases}\sum_{q=0}^{p} A_q x^q, & 0\le x\le l_1\\ 0, & l_1<x\le l\end{cases}$$

or

$$[G(x)-\bar{\bar{\phi}}(x)]e^{-PX/2}=\sum_{n=1}^{\infty} E_n^{\phi}\sin(n\pi x) \tag{14}$$

Multiplying both sides of (14) by $\sin(m\pi X)$ and integrating over 0 to l

$$E_m^{\phi}=\omega(B_m^{\phi}-B_m^{0\phi}) \tag{15}$$

where

$$B_m^{\phi}=\int_0^l G(x)e^{-PX/2}\sin(m\pi X)\,dx \tag{16}$$

and

$$B_m^{0\phi}=\int_0^l \bar{\bar{\phi}}(x)e^{-PX/2}\sin(m\pi X)\,dx \tag{17}$$

$$\omega^{\phi}=2/l \tag{18}$$

The definite integral on the right hand size of (15) may be evaluated using the following result[2]

$$\int x^q e^{ax}\sin(bx)\,dx=e^{ax}\sum_{r=0}^{q}\frac{(-1)^r q!\,x^{q-r}}{[\sqrt{a^2+b^2}]^{r+1}(q-r)!}\sin\left[bx-(r+1)\cos^{-1}\left(\frac{a}{\sqrt{(a^2+b^2)}}\right)\right] \tag{19}$$

Carrying out the integration in (16) and (17) using (19), the Fourier coefficients in Table I may be obtained.

Case II: Neuman boundary condition at $x=l$; i.e. $\partial c/\partial x(l,t)=0$

The approach here is similar to Case I. The steady-state part $\bar{\bar{\psi}}(x)$ may be shown to be

$$\bar{\bar{\psi}}(x)=1 \tag{20}$$

The transient part is

$$\bar{\psi}(x,t)=e^{PX/2}\sum_{n=1}^{\infty} E_n^{\psi}\sin(Z_n X)e^{-[Z_n^2+(P/2)^2]T} \tag{21}$$

The rest of the derivation is analogous to that of case I.

APPENDIX II: TESTED DOMAIN OF THE COMPUTER CODES

The developed FORTRAN codes were tested for a range of values of the governing parameters. For $T>5\times10^{-3}$, fifty-term convergence was achieved in a series of numerical experiments carried out to test the codes. The initial conditions assumed in these experiments were polynomials of order ranging from 0 to 5. The range of Peclet number considered was between 5 and 100. For $T<5\times10^{-3}$, oscillatory results were obtained.

REFERENCES

1. H. S. Carlaw and J. C. Jaeger, *Conduction of Heat in Solids*, 2nd edn., Oxford University Press, 1959, p. 144.
2. *Standard Mathematical Tables*, Twenty-second Edition, CRC, 1974, pp. 454–455.