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Simulation of Advection Diffusion Equation Based on Lumped Parameter Model

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Abstract

This study aims to produce numerical solution of one-dimensional advection-diffusion equation generated from lumped parameter model of lung channel. The numerical scheme FTBSCS is employed to solve the model. The effect of inductive time constant from 0 to 3s is computed numerically and presented graphically. Computed results show that advection exits in oscillation and transition mode. The stability condition of the scheme leads to determine the range of inductive time constant.

Keywords: Lumped model, Oscillatory flow, Inductive time constant, Advection-diffusion equation, Finite difference scheme.

Introduction

Water pollution in oceans, rivers, lakes or groundwater and pollution in atmospheretake place continually in surroundings. It is essential to know the contaminant or pollutant concentration or the salinity or temperature distribution in the water for safety of the environment [1]. This type of problem describes transport and diffusion process can be modeled using one dimensional advection diffusion equation (ADE). ADE illustrates many quantities such as mass, velocity, vorticity, heat and energy [2].Many authors are involved in solving ADE by using finite difference method (FDM).The mathematical model of water pollution is solved using implicit centered difference scheme in space and forward difference method in time by [3]. Aral and Liao [4] solved for two-dimensional transport equation with time dependent dispersion coefficients analytically. Kumar et al. [5] presented analytical solution of one dimensional ADE with variable coefficients in a finite domain using Laplace transformation. The ADE has been used as a model equation in many engineering problems such as dispersion of tracers in porous media [6,7], pollutant transport in rivers and streams [8], thermal pollution in river systems [9]. Stability analysis of finite difference scheme for solving ADE isstudied by [10-13]. As stated above, most of the works has been done for open channel. But ADE has

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wide applications in other disciplines too, like biosciences, soil physics, petroleum engineering and chemical engineering. In vivo, fluid (liquid or gas) moves along closed channel and flow might be transported to downstream by advection or spread out by diffusion when unidirectional flow is weaken. For example, a complete cycle of respiration in human lung channel is a consequence of oscillatory flow (advection)and stagnation in transition (diffusion) in nature. A patient who is unable to perform respiration, artificial high frequency oscillatory ventilation (HFOV) helps to survive in the world. HFOV controls the constant oscillatory flow along human lung channel and flows in lung channel faces resistance and compliance effects. Oscillatory flow and mass transport was studied along model channel of human lung by [14, 15]. They simulated governing equations with boundary conditions to show effective diffusion along straight tube. Laminar, turbulent and oscillatory dispersion along a circular channel is calculated by [16]. He established a relation between channel radius and diffusion coefficient. Tanaka et al. [17] examined that a secondary flow during HFOV method ensures effective diffusion in bent and bifurcated tubes than in straight tube. A lamped-parameter model has been developed to study airflow distribution by Elad et al. [18] .The authors also derived the modified time-dependent expressions of resistance and compliance of a single compartment. Numerical analysis of air flow along lung channel with asymmetric compliance was examined experimentally and numerically by Hirahara et al. [19]. We found that the flow for inhomogeneous compliance ratio leads to irreversible flow along lung model. This type of flow effect might be the result of diffusion.

In the current paper, a transport equation of lung model channel is produced from lumped parameter model [18] and is solved by FTBSCS scheme of explicit finite difference method. The inductive time constant leads the rate of diffusion for oscillatory mode and at the transition mode. The numerical results are presented graphically.

Formation of Mathematical Model

A model channel of human lung with compliance C (flexibility) and resistance R is taken under consideration. An oscillatory flow with fluid velocity u is passing along the model channel and inertial effect L raise. If

$q(t)$ is the flow rate and ΔP is the driving force then the lumped parameter model by Elad et al. [18] is

$$L_i \frac{dq_i}{dt} + R_i q_i + \frac{1}{C_i} \int q_i dt = \Delta p \tag{1}$$

Where the flow rate, resistance, inertance and compliance of i-th channel are q_i, R_i, L_i and C_i respectively, $\Delta P = P_0 \sin(\omega t + \varphi)$ is the driving force for the pressure amplitude, P_0 and $\omega = 2\pi f$ where f is the number of oscillation at the inlet of channel.

Differentiating Eqn. (1) and executing some algebra, a second order ODE is obtained which exhibits time varying effect of flow only. It is a crying need to have a flow simulation for spatial and temporal quantities such that $q = q(x,t)$. The following substitutions are integrated for space-time equation of the model.

$$\begin{aligned} \frac{dq}{dt} &= uq_x + q_t \\ \frac{d^2q}{dt^2} &= u^2 q_{xx} + q_{tt} + 2uq_{tx} \end{aligned} \tag{2}$$

In absence of driving force (during transition), Eqn.(2) contributes

$$Lq_{tt} + 2Luq_{tx} + Lu^2 q_{xx} = -q / C - Rq_t - Ruq_x \tag{3}$$

Disregarding the compliance of channel (rigid model), Eqn.(3) becomes

$$aq_{tt} + bq_{tx} + cq_{xx} = dq_t + eq_x \tag{4}$$

Where $a = L, b = 2Lu, c = Lu^2, d = -R$ and $e = -Ru$.

Here $b^2 = 4ac$ confirms that Eqn.(4) is parabolic. Moreover, it befalls parabolic after ignoring mixed term and the rate of flow rate whose effect is unimportant in the system. Since the resistive force is opposite to the main flow, d is always positive. According to the above mentioned considerations, the governing equation of the dynamical problem is:

$$\begin{aligned} &q_t + uq_x = Dq_{xx} \\ &D = Lu^2 / R \end{aligned} \tag{5}$$

which is a one dimension advection-diffusion equation with inductive time constant. The first term is local accumulation, the second term is movement by carrying fluid and the last term is movement by random motions in the fluid.

Peclet Number and Inductive Time Constant

If an instantaneous point mass is released at the center of a channel of length l and the downstream flow speed along x-direction is u. Then the advection time is $t_a = l/u$ and the diffusion time is $t_d = l^2 / D$. The Peclet number is a dimensionless parameter with ratio of diffusive time to advection time scales is defined as $Pe = t_d / t_a = ul / D$.

For $Pe \ll 1$ (in practice, if $Pe < 0.1$), diffusion is dominant. Spreading occurs almost symmetrically despite the directional bias of the flow. For $Pe \gg 1$ (in practice, if $Pe > 10$), spreading is almost inexistent and mass is simply moved along the flow.

In flow dynamics, the inductive time constant is the ratio of inertia to resistance such that $t_L = L / R$ where L represents the inertia [$\mathrm{Pa.s^2/m^3}$] for fluid flow and R is the resistive force [$\mathrm{Pa.s/m^3}$] by channel. As in Eqn.(5), the rate of diffusion is proportional to inductive time constant and can be defined as:

$$D = Lu^2 / R \Rightarrow D \propto t_L \tag{6}$$

Where u^2 is a proportionality constant and t_L controls the rate of diffusion.

Analytic Solution

The exact solution corresponding to instantaneous and localized release of the 1D transport Eqn. (5) with initial condition $q(x,0) = q_0(x)$ is given [20]

$$q(x,t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x - x_c - ut)^2}{4Dt} \right) \tag{7}$$

Where the center of mass traces the trajectory, $x = x_0 + ut$.

Computational Model for ADE

The unsteady incompressible flow along a rigid channel without driving force and compliance effect is an advection-diffusion Eqn.(5). In physical domain of channel length ($0 \le x \le l$), thisone-dimensional transport equation as initial boundary problem can be written as

$$\begin{aligned} &q_t + uq_x = Dq_{xx} \\ &q(x,0) = q_0(x), \quad 0 \le x \le l \\ &q(0,t) = g(t), \quad q(l,t) = h(t), \quad 0 < t \le T \end{aligned} \tag{8}$$

In order to obtain computational scheme by finite difference method (FDM), we discretize the space-time plane with mesh size $\Delta x \times \Delta t$. Space size and time steps are taken equal individually. The spatial and temporal coordinate at the grid point $q(x_i, t_j)$ is defined as

$$\begin{aligned} x_i &= x_0 + i\Delta x;\ i = 0,1,2,\cdots,m \\ t_j &= t_0 + j\Delta t;\ j = 0,1,2,\cdots,n \end{aligned}$$

The approximate solution at grid points $q(x_i, t_j)$ is $q_{i,j} \in R^n$ so that $q_{i,j} \approx q(x_i, t_j)$.

Computational Technique for ADE

To solve the computational model (8), the forward time difference formula is

$$q_t = \frac{q_{i,j+1} - q_{i,j}}{\Delta t} + o(\Delta t) \tag{9}$$

The backward space difference formula becomes

$$q_x = \frac{q_{i,j} - q_{i-1,j}}{\Delta x} + o(\Delta x) \tag{10}$$

The symmetric space difference formula is

$$q_{xx} = \frac{q_{i+1,j} - 2q_{i,j} + q_{i-1,j}}{\Delta x^2} + o(\Delta x^2) \tag{11}$$

Substituting Eqns.(9-11) into Eqn. (8)to get

$$\frac{q_{i,j+1} - q_{i,j}}{\Delta t} + \frac{q_{i,j} - q_{i-1,j}}{\Delta x} = \frac{q_{i+1,j} - 2q_{i,j} + q_{i-1,j}}{\Delta x^2} + o(\Delta t, \Delta x, \Delta x^2) \tag{12}$$

Dropping the truncation error terms and rearranging, we can explicitly solve for time level that implies

$$\begin{aligned} & q_{i,\,j+1} = sq_{i+1,\,j} + (1 - r - 2s)q_{i,\,j} + (r+s)q_{i-1,\,j} \\ & \text{for } 1 \le i \le m-1,\, 0 \le j \le n-1 \\ & \text{where },\, r = u\frac{\Delta t}{\Delta x},\, s = \frac{D\Delta t}{\Delta x^2} \end{aligned} \tag{13}$$

which is an explicit finite difference scheme by **FTBSCS** technique.

Stability Condition for the Scheme

Stability is a property that concerns the growth or decay of errors introduced at any stage during the computation and strongly governs the numerical solution. For advection-diffusion problem, we calculate von Neumann stability condition $e^{a\Delta t} \le \cos(k_m \Delta x) - iC\sin k_m \Delta x) \le 1$, where a is a constant, k_m is the wave number and C is the CFL condition. The von Neumann simultaneous stability condition for the scheme [21] is $r + s \ge 0$ and $1 - r - 2s \ge 0$ which correspond to

$0 \le s \le 1/2$ and $-s \le r \le 1 - 2s$. This condition controls the time increment by $\Delta t \le \frac{\Delta x^2}{u\Delta x + 2D}$ where D for rate of mass diffusion and u is the flow speed. It is mentionable that when $u = 0$ the Eqn.(8) becomes pure diffusion and satisfies the stability limit. Also, for $D = 0$, the problem reduces to pure advection and gives the well-known stability limit.

Results and Discussions

Validation of Numerical Scheme

The time marching scheme for Gaussian curve along the model channel as a test case is taken for

$$q(x,t) = e^{-200(x-x_c-ut)^2} \tag{14}$$

The advection-diffusion (for $D \neq 0, u \neq 0$), pure advection (for $D = 0, u \neq 0$) and pure diffusion (for $D \neq 0, u = 0$) equations are respectively

$$q_t + uq_x = Dq_{xx} \tag{15}$$

$$q_t + uq_x = 0 \tag{16}$$

$$q_t = Dq_{xx} \tag{17}$$

The Eqns. (15-17) with initial condition from Eqn. (14) is solved numerically.

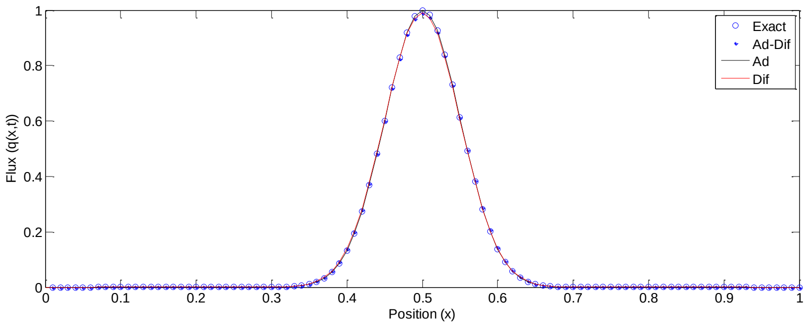

Figure 1: AD effect for $t_L = 0.1$s with $u = 0.5$ cm/s.

For our model channel of length $l = 1$ cm , $u = 0.5$ cm/s and $D = 0.025\,\text{cm}^2/\text{s}$ in (8), the distribution of Gaussian pulse at $t = 1$s is computed and compared with the flux obtained using explicit finite difference method for three cases (advection-diffusion, advection and diffusion) as shown in Figure 1. It is seen that result of (16) is exactly accurate with the exact distribution (14). And diffusion is negligible for (15) and (17). This result is carried out for various values of x with

$\Delta t = 0.001, Cr = 0.05$, $Pe = 20$ and $t_L = 0.1$ The numerical value of Pe ensures the dominance of advection for slow motion along small dimension of biological model channel. As depicted in Figure 2, $\Delta t = 0.001, \mathrm{Cr} = 0.05$ and $Pe = 0.67$ for the change in $t_L = 3$. Due to increase the inductive time constant the diffusion becomes dominant and mass spreads out faster than the flow moves. The convergence of the solution is found for $0 \le t_L < 4$.

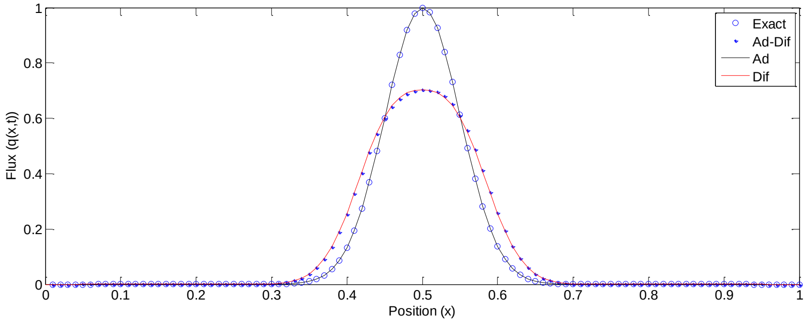

Figure 2: AD effect for $t_L = 3\text{s}$ with $u = 0.5$ cm/s.

Simulation for Parallel and Oscillatory Flows

Respiration in human lung is the consequence of oscillatory flow in which parrel flow condition exits in transition of cycle change. So, parrel and ossilatory flow is simulated applying numerical scheme FTBSCS. If $u = 0.5$ cm/s, $Pe = 2000$ and advective time constant is $t_L = 0.001\text{s}$, the numerical scheme represents the advection and diffusion effects as in Figures 3 and 4.

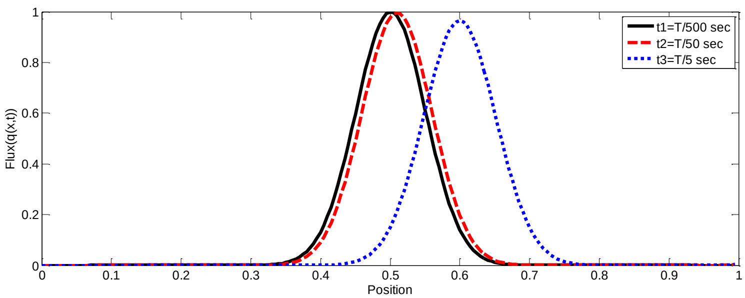

Figure 3: AD effect for $t_L = 0.001\text{s}$ with $u = 0.5$ cm/s for transition phase ($\varphi = 0$).

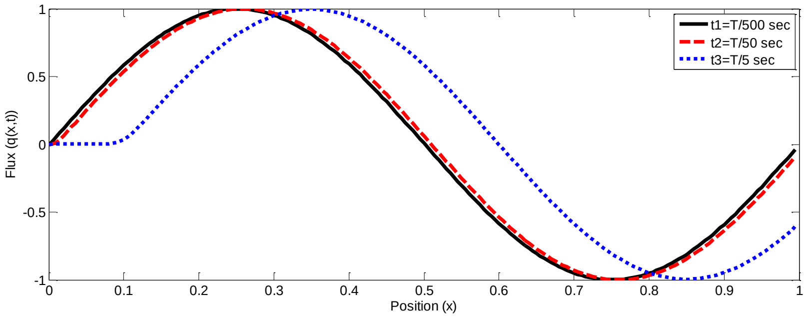

Figure 4: AD effect for $t_L = 0.001$s with $u = 0.5$ cm/s for oscillatory phase ($\varphi \neq 0$).

This section represents the effect of inductive time constant for parallel and oscillatory flow in alveolus zone of lung channel where flow rate is very low. In this area, oscillatory flow occurs due to the mutual driving force. It is very difficult to measure the real effect of flow in this region. So, the inductive time constant may infer the movements of O_2 particles by advection. Moreover, the distribution of particles is at rest in time of phase transition such that pure diffusion may occur. As shown in Figure 3, for a momentary time $t = 0.002$s (solid curve) and $t = 0.02$s (dash curve), the advection and diffusion effect is measured for $t_L = 0.001$ s. The diffusion effect is almost negligible and advection effect is growing. At the eleventh of time, $t = 0.2$s (dot curve) the advection effect is found dominant on diffusion where $Cr = 0.1$ and $Pe = 2000$. As depicted in Figure 4, the oscillatory phase is taken in which no diffusion effect is found. This experiment is conducted for inlet condition stated in [22]. The advection is dominant entire the experiment for $T = t = 1$s. It may occur due to small dimension of channel and for regaining of driving force along the channel.

Error Estimation and Convergence

The explicit finite difference scheme FTBSCS is employed to compute the result for transition and oscillatory condition in this experiment. The relative error estimated in L_1-norm is defined by $err = \frac{\|q_e - q_a\|_1}{\|q_e\|}$

Where q_e is the exact and q_a is the approximate solution computed for $t \in [0,10]$s.

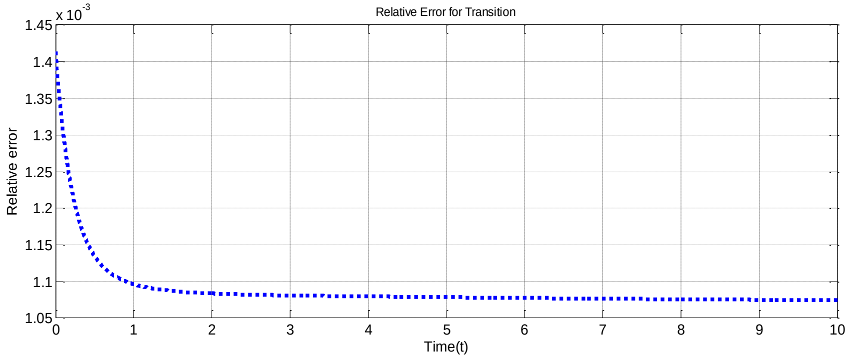

Figure 5: Rate of convergence at transition phase ($\varphi = 0$)

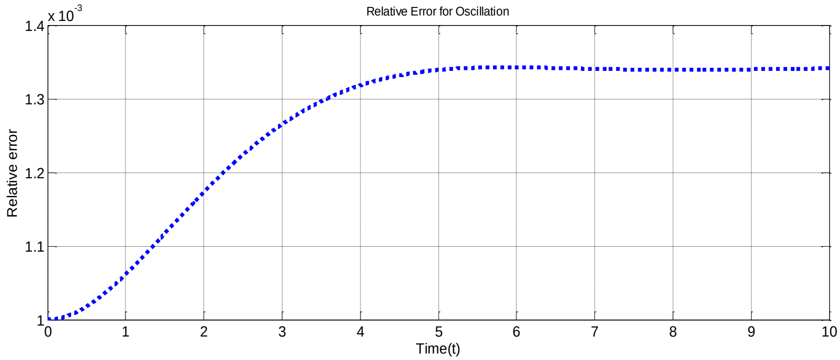

Figure 6: Rate of convergence at oscillatory phase ($\varphi \neq 0$)

Error estimation is essential enough in support of accuracy of numerical result. For this, the analytical result is used for code validation as well as error estimation of transition and oscillatory phases. The scheme is the same but flow condition is different. Figure 5 shows that initially the error is much and within a few second it becomes steady and the solution is convergent with a small error, $err = 1.07 \times 10^{-3}$. On the contrary, the rate of convergence for oscillatory state is gained with $err = 1.35 \times 10^{-3}$ as shown in Figure 6.

Conclusion

This paper modify lumped parameter model to 1D advection-diffusion transportation equation as IBVP. The inductive time constant is introduced to this new model that plays a significant role of advection-diffusion effect. The numerical model is solved for estimation of flux distribution during transition and oscillatory phase along human lung model channel by explicit FTBSCS technique. In transition phase, advection dominates the diffusion whereas in oscillatory flow, no diffusion effect exists even for $Pe < 0.1$. Relative errors of both flow phases is calculated and found convergent within a small error 0.001.

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