Numerical Study on Advection Diffusion Equation for Human Lung Model Channel

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Abstract

An advection-diffusion equation (AD) based on lumped parameter model for O_2 transportation along human lung channel is presented and solved numerically with three explicit finite difference schemes FTFSCS (forward time forward space and centered space), FTBSCS (forward time backward space and centered space) and FTCSCS (forward time centered space in first order and second order). The stability conditions are obtained and implemented in numerical solution to present the AD effects entire the flow experiment. The role of inductive time constant within $t_L \in [0.01, 0.1]$ is investigated which dominates the rate of diffusion in the flow. Error comparisons with analytical solutions of ADE are also presented graphically to show the accuracy of the schemes.

Keywords— Lumped model, Lung model channel, Inductive time constant, Advection-diffusion equation, Finite difference scheme.

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1 Introduction

Most of the transportation of fluid in physical problem to biological system occur in advection and diffusion process according to the model $q_t + uq_x = Dq_{xx}$, where $q(x,t) =$ flux, D = the rate of diffusion and u= the mean flow velocity. Water pollution in oceans, rivers, lakes or ground water and pollution in atmosphere take place continually in surroundings. It is essential to know the contaminant 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, 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 is studied by [10-13]. As stated above, most of the works has been done for open channel. But ADE has 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.

With the above discussions, in this paper, a transport equation of lung model channel is produced from lumped parameter model [18]. The numerical study on stability with FTFSCS, FTBSCS and FTCSCS techniques are discussed for solving the AD problem. A relation between inductive time constant and the rate of diffusion is introduced. The AD effect and relative errors for numerical solutions are presented graphically. The variations of relative error of lung model equation for each scheme are also presented graphically.

2 Mathematical Model

A lumped parameter model with resistance (R), inertance (L) and Compliance (C) for incompressible fluid flow in absence of driving force along human lung model channel may be modeled from

$$L\frac{dq}{dt}+Rq+\frac{1}{C}\int q\,dt=0 \tag{1}$$

where $q=q(t)$ is the flow rate of fluid to

$$\frac{\partial q}{\partial t}+u\frac{\partial q}{\partial x}=\frac{Lu^2}{R}\frac{\partial^2 q}{\partial x^2} \tag{2}$$

where $q=q(x,t)$ is the flux. This is an advection-diffusion equation (ADE) of lung model. Using Fourier transform, convolution theorem and Dirac delta function, the analytic solution of Eqn.(2) is [20]

$$q(x,t)=\frac{M}{A_{yz}\sqrt{4\pi Dt}}\exp\ -\frac{(x-ut)^2}{4Dt} \tag{3}$$

Where, $D=Lu^2/R \Rightarrow D\propto t_L$ and the inductive time constant , $t_L=L/R$

Where, u is the constant velocity, M is the mass volume along the model channel, and $q(x,0)=M\delta(x)$ is the initial condition of IBVP.

3 Numerical Technique for Model Equation

The unsteady incompressible flow along a rigid channel without driving force and compliance effect is an ADE (2) for physical domain of channel length ($0\le x\le l$), is

$$\begin{aligned}
&q_t+uq_x=Dq_{xx}\\
&q(x,0)=q_0(x),\quad 0\le x\le l\\
&q(0,t)=g(t),\quad q(l,t)=h(t),\quad 0<t\le T
\end{aligned} \tag{4}$$

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

$$x_i=x_0+i\Delta x;\ i=0,1,2,\cdots,m$$

$$t_j=t_0+j\Delta t;\ j=0,1,2,\cdots,n$$

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

The forward time (FT) difference formula

$$\frac{\partial q}{\partial t} \approx \frac{q_i^{j+1} - q_i^j}{\Delta t} \qquad (5)$$

The forward space (FS) difference formula

$$\frac{\partial q}{\partial x} \approx \frac{q_{i+1}^j - q_i^j}{\Delta x} \qquad (6)$$

The backward space (BS) difference formula

$$\frac{\partial q}{\partial x} \approx \frac{q_i^j - q_{i-1}^j}{\Delta x} \qquad (7)$$

The first order centered space difference formula

$$\frac{\partial q}{\partial x} \approx \frac{q_{i+1}^j - q_{i-1}^j}{2\Delta x} \qquad (8)$$

The second order centered space difference formula

$$\frac{\partial^2 q}{\partial x^2} \approx \frac{q_{i+1}^j - 2q_i^j + q_{i-1}^j}{(\Delta x)^2} \qquad (9)$$

are employed to have the following computational schemes.

3.1 Explicit Scheme by FTFSCS Techniques

Substituting (5), (6) and (9) into (4) and rearranging according to the time level, implies to

$$q_i^{j+1} = \lambda\, q_{i-1}^j + (1 - 2\lambda + \gamma)\, q_i^j + (\lambda - \gamma)\, q_{i+1}^j \qquad (10)$$

3.2 Explicit Scheme by FTBSCS Techniques

Inserting (5), (7) and (9) into (4) and rearranging, the scheme implies to

$$q_i^{j+1} = (\lambda + \gamma)\, q_{i-1}^j + (1 - 2\lambda - \gamma)\, q_i^j + \lambda\, q_{i+1}^j \qquad (11)$$

3.3 Explicit Scheme by FTCSCS Techniques

Finally (5), (8) and (9) into (4) becomes

$$q_i^{j+1} = (\lambda + \frac{\gamma}{2})\, q_{i-1}^j + (1 - 2\lambda)\, q_i^j + (\lambda - \frac{\gamma}{2})\, q_{i+1}^j \qquad (12)$$

Where (3.1 to 3.3), $\lambda = \frac{D\Delta t}{(\Delta x)^2}$, $\gamma = \frac{\mathrm{u}\Delta \mathrm{t}}{\Delta \mathrm{x}}$

3.4 Stability Conditions

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. The von Neumann stability condition may be developed by $e^{a\Delta t} \le \cos(k_m \Delta x) - i\gamma \sin k_m \Delta x) \le 1,$ where a is a constant, k_m is the wave number and γ is the CFL condition. We develop simultaneous stability condition for the schemes (10) to (12) and perform numerical simulation by implementing the schemes for various parameters. The stability conditions are Shown in Table 1.

TABLE 1
STABILIY CONDITIONS FOR THE VARIOUS SCHEMES

Conditions for the schemes	
Explicit Schemes	Stability Conditions
FTFSCS	$\frac{1}{2} \le \lambda \le 1$ and $2\lambda - 1 \le \gamma \le \lambda$
FTBSCS	$0 \le \lambda \le 1$ and $-\lambda \le \gamma \le 1 - 2\lambda$
FTCSCS	$0 \le \lambda \le \frac{1}{2}$ and $-2\lambda \le \gamma \le 2(1-\lambda)$

4 NUMERICAL RESULTS AND DISCUSSIONS

4.1 Problem Description

An incompressible fluid flow along human lung model channel of length, l=4 mm is passed for fluid velocity, u=60 mm/s on a second. The inductive time constant, $t_L = 0.1$ is calculated from lab experimental value of L and R so that the inductive time constant based diffusion rate is D=3600 mm²/s. The computed time step and grid width are $\Delta t = 2 \times 10^{-4}$ and $\Delta x = 0.04$.

Solutions:

The numerical experiment for the problem is investigated for the schemes FTFSCS in Fig.1, FTBSCS in Fig.2 and FTCSCS in Fig.3 for several distinct times within the experimental time. The time constant, $t_L = 0.1$ is taken for the entire simulation where the accepted value for $t_L \in [0.01, 0.1]$ is found within the stability condion. The effect of advection-diffusion (AD) is compared at a time, $t = T/50$ for all three schemes. It is seen that AD effect is minimum for FTFSCS scheme and maximum for FTBSCS scheme and moderate for FTCSCS.

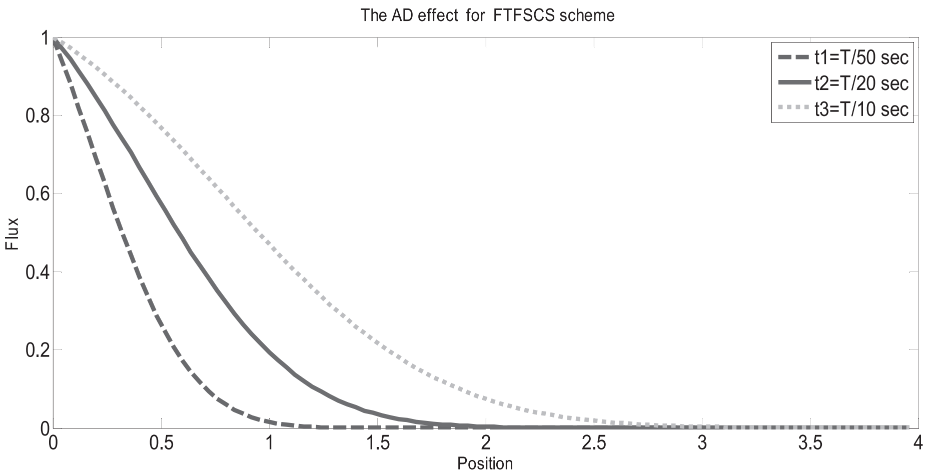

Figure 1: AD effect for FTFSCS Scheme.

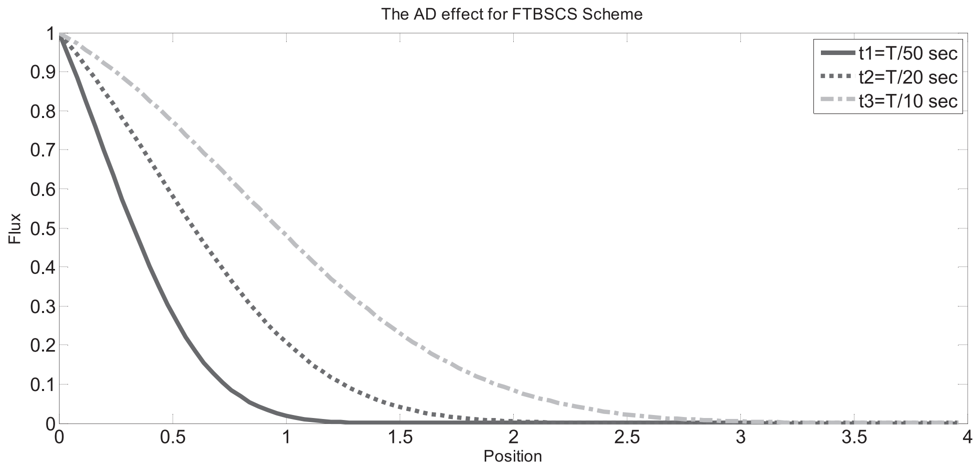

Figure 2: AD effect for FTBSCS Scheme.

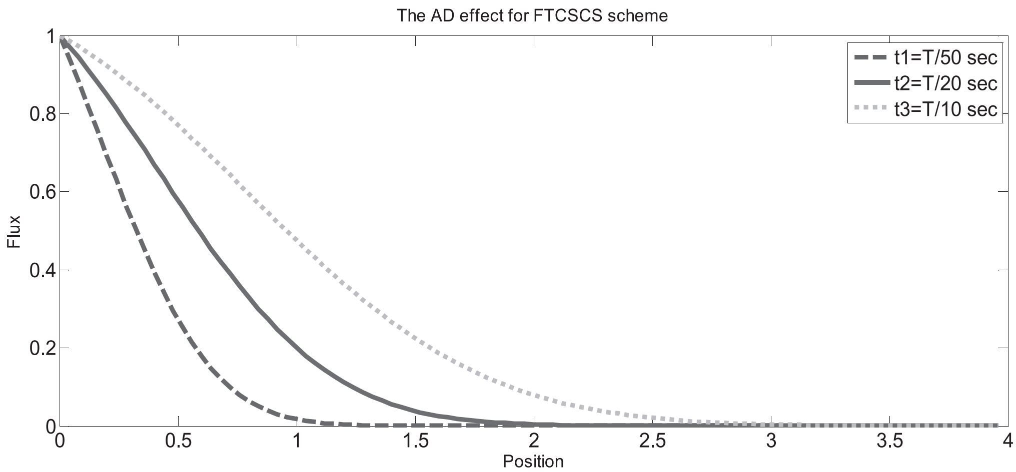

Figure 3: AD effect for FTCSCS Scheme.

4.2 Error Estimation and Convergence

The explicit finite difference schemes FTFSCS, FTBSCS and FTCSCS is employed to compute the results of the model problem for t=1s. 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 $t \in [0,1]$ s.

As depicted in Fig.5, the curves marked by dot line (red) shows the relative error for the FTFSCS scheme, the solid line (green) shows the relative error for the FTBSCS scheme and the dash line (blue) shows the relative error for the FTCSCS scheme in the same numerical conditions. It is evident that FTBSCS has minimum relative error in comparison with FTFSCS and FTCSCS scheme.

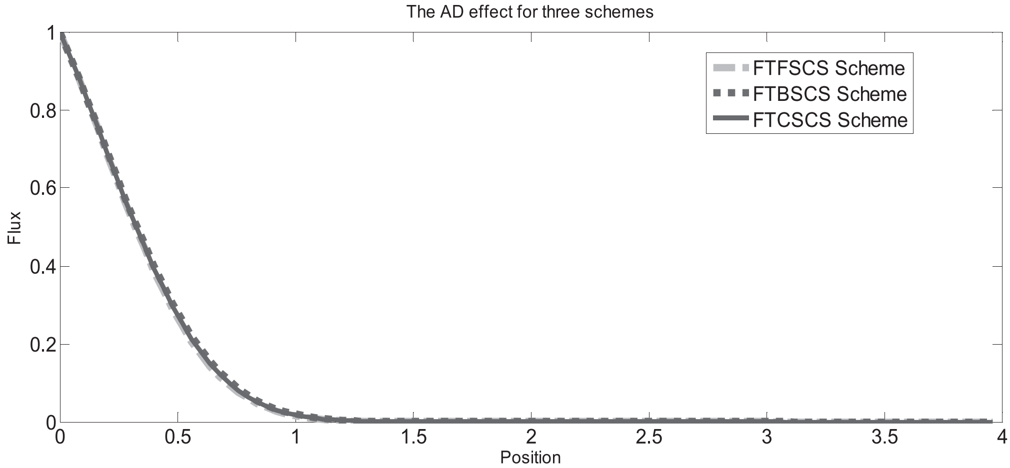

Figure 4: AD effect for FTFSCS, FTBSCS and FTCSCS scheme in time $t = T/50$ s

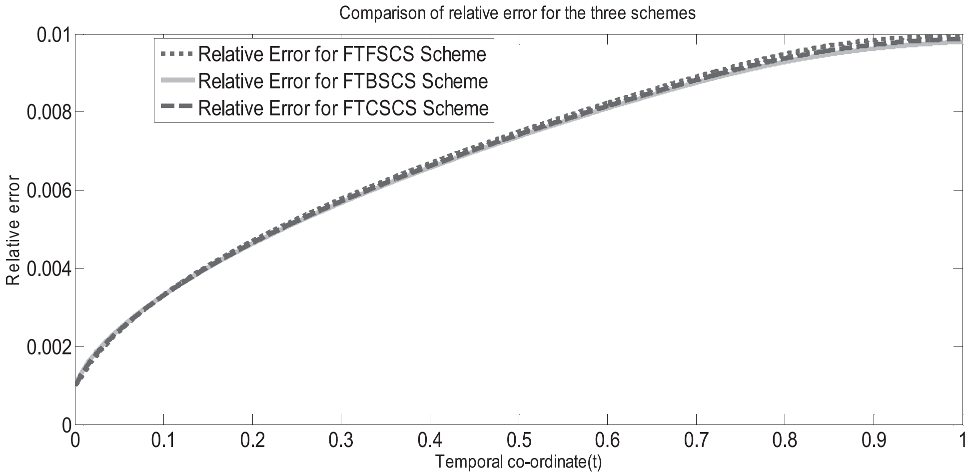

Figure 5: Comparison of relative error for the schemes.

Now, it demands for showing convergence of the solution due to the change of grid size variations. The convergence of relative error for the FTBSCS scheme is taken for time step $\Delta t = 0.0002\,s$, velocity u=6 cm/s at several positions, $\Delta x = 0.1,\ 0.3,\ 0.5$ as shown in Fig.6. It is clear that the variation of error is related to the value of Δx. If $\Delta x = 0.5$ then the relative error is maximum compared with other values of space increment which is shown by dot line (green). It is concluded that the larger value shows the larger error and vice versa within a certain time fractions for all schemes.

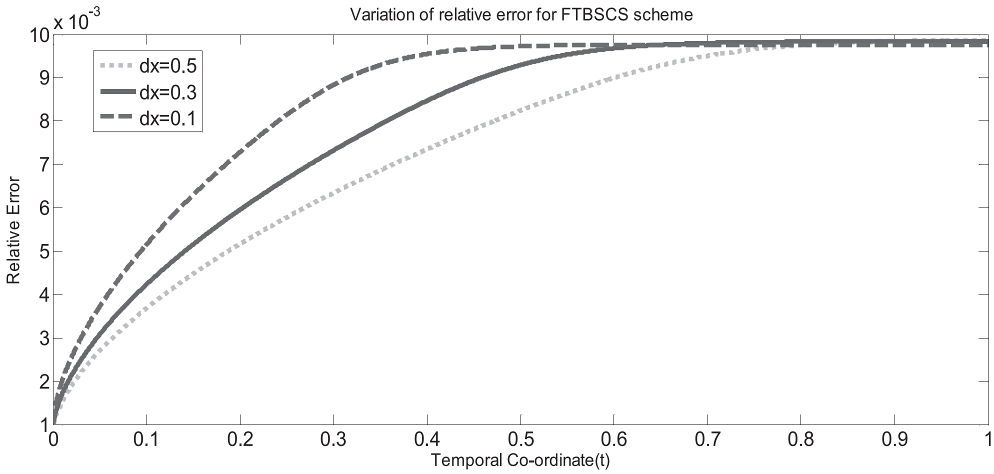

Figure 6: Variation of relative error for FTBSCS scheme.

5 Conclusion

In this work, we have presented numerical solution of 1D advection-diffusion transportation equation generated from lumped parameter model of human lung. Our model channel is very narrow and short in length. The AD effect is investigated for FTFSCS, FTBSCS and FTCSCS schemes numerically and presented graphically. The analytical result is used for code validation and for error comparison within the schemes. We found that the AD effect of the lung model equation (2) for the schemes are stable within the range of the inductive time constant, $t_L \in [0.01, 0.1]$. The inductive time constant introduced in this model plays a significant role in advection-diffusion effect. The FTBSCS scheme shows the maximum AD effect in comparison with FTCSCS and FTFSCS scheme in Fig.4. Also, FTBSCS scheme presents minimum relative error in comparison with FTCSCS and FTFSCS schemes as in Fig.5. Since FTBSCS scheme has minimum relative error, it is more suitable for our lung model problem. Moreover, we found that due to the increasing of the value of Δx for the schemes separately, the relative error is also increasing as in Fig. 6. This error reduction is due to a decrease in the influence of the initial data.

References

[1] C.G. Koutitas, 'Elements of computational hydraulics', Pentech Press, London, UK, 1983.

[2] B.J. Noye, 'Numerical solution of partial differential equations' Lecture notes, 1990.

[3] F.B. Agusto, O.M. Bamigbola, 'Numerical treatment of the mathematical models for water pollution', Research J. Appl. Sci. 2(5), 548-556, 2007.

[4] M.M. Aral and B. Liao, 'Analytic solutions for two-dimensional transport equation with time dependent dispersion coefficients', J. Hydrol. Eng., 1(1), 20-32, 1996.

[5] A. Kumar, D. Kumar and N. Kumar, 'Analytical solution of one dimensional advection diffusion equation with variable coefficients in a finite domain', J. Earth. Syst. Sci. 118(5), 539-549, 2009.

[6] R.B. Banks and J. Ali, 'Dispersion and absorption in porous media flow', J. Hydraulic Div., 90, 13-31, 1964.

[7] N. Kumar, 'Unsteady flow against dispersion in finite porous media', J. Hydrology, 63(3-4), 345-358, 1983.

[8] P.C. Chatwin and C.M. Allen, 'Mathematical models of dispersion in rivers and estuaries', Annual Review of Fluid Mechanics, 17, 119-149, 1985.

[9] M.H. Chaudhry, D.E. Cass and J.E. Edinger, 'Modeling of unsteady flow water temperatures', J. Hydraulic Eng. 109(5), 657-669, 1983.

[10] K.W. Morton, 'Stability of finite difference approximations to a diffusion-convection equation', Int. J. Numerical Methods in Eng., 15(5), 677-683, 1980.

[11] L.F. Leon, P.M., Austria, 'Stability criterion for explicit scheme on the solution of advection-diffusion equation', Maxican Institute of Water Technology.

[12] T.M.A.K. Azad and L.S. Andallah, 'Stability analysis of finite difference schemes for an advection diffusion equation', Bangladesh J. Sci. Res. 29(2), 143-151, 2016.

[13] H. Karahan, 'Unconditional stable explicit finite difference technique for the advection-diffusion equation using spread sheets', Advances in Eng. Software, 38(2), 80-86, 2007.

[14] D.M. Eckmann, J.B. Grotberg, 'Oscillatory flow and mass transport in a curved tube', *J. Fluid Mech.*, 188, 509– 527, 1988.

[15] H. Fujioka, K. Oka, and K. Tanishita, 'Oscillatory flow and gas transport through a symmetrical bifurcation', J. Biomechanical. Eng., 123, 145–153, 2001.

[16] H.K. Chang, 'Mechanisms of gas transport during ventilation by high-frequency oscillation', J. Appl. Physiology 56(3): 553-563.

[17] G. Tanaka, T. Ogata, K. Oka, and K. Tanishita, 'Spatial and temporal variation of secondary flow during oscillatory flow in model human central airways'J. Biomechanical. Eng., 121, 565–573, 1999.

[18] D. Elad, A. Shochat and R.J. Shiner, 'Computational model of oscillatory airflow in a bronchial bifurcation' Respiration Physiology, 112, 95-111, 1998.

[19] H. Hirahara, K. Iwazaki, M.U. Ahmmed, M. Nakamura, 'Numerical analysis of air flow in dichotomous respiratory channel with asymmetric compliance under HFOV condition' Journal of Fluid Science and Technology, 6(6), 932-948, 2011.

[20] S.G. Ahmed, 'A numerical algorithm for solving advection-diffusion equation with constant and variable coefficients', Dept. Eng. Physics and Mathematics, Faculty of Engg., Zagazig University, Egypt.

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