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A Numerical Study of Dispersion in Laminar Flow in Non-circular Ducts

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Abstract

After extended times, longitudinal dispersion of solutes in closed conduits may be described in terms of a dispersion coefficient. These systems have been extensively studied and expressions for the dispersion coefficients have been derived. However, during the initial stages after the injection of a solute, say, convective effects are likely to dominate those of diffusion. As a result the longitudinal dispersion is no longer Fickian in nature, and this is likely to have a profound effect on not only the residence time distribution of the solute, but also any chemical reactions that might take place. Despite of the availability of well-established analytical solutions for laminar flows in circular pipes, information on the non-circular case it is scant. In order to study the effects of dispersion at the initial stages of spreading in a square duct a numerical method has been devised. A feature of the approach is that numerical dispersion is negligible, and as a result it is possible to study dispersion in great detail. The method has been validated against experimental data obtained in the case of flow in circular pipes. It is observed that at short times the longitudinal distribution of the concentration of the solute exhibits a double peak indicating that convection dominates the dispersion. However, at lower Peclet numbers the effect of diffusion become more important and the scalar disperses in a manner that is analogous to Fick's law.

Introduction

Engineering transport phenomena involving convective dispersion in laminar flow through ducts has great theoretical interest as well as practical significance. The axial dispersion of a solute slug by a fluid being convected in laminar flow through tube is significantly affected by the non-uniform velocity profile across the cross section and lateral diffusion. These counter acting aspects of the phenomenon have been elucidated theoretically by Taylor [1] for the first time who solved the mean concentration in the asymptotic case of long tubes with circular cross section at high Peclet number.

Besides axis-symmetric case for pipes, the process is more interesting and complex for the three dimensional non-circular case, specially square and rectangular duct because of a wide range of applicability of these cross section in thermal and material pollution, chromatography, chemical flow reactors, physiological transport system and other applications (Fischer [2]). To investigate this issue, a simplified form of dispersion in laminar flow through closed rectangular duct was first studied by Aris [3] considering the duct with large aspect ratio as a two dimensional flow between parallel plates. It was found that the effective dispersion coefficient at large time neglecting the side wall effect in this case is given by

$$D_{eff} = \frac{8Pe^2 D_m}{945} \tag{1}$$

Where, Pe is Peclet number defined as, $Pe = au_0/D_m$, a is the width of the duct, u_0 is the centreline velocity and D_m is the molecular diffusion coefficient.

This result was confirmed by Sankarasubramanian and Gill [4], as a special case of the more broader analysis for laminar flow dispersion in diverging channel and annulus pipe, Prenosil [5] and Manton [6] . Further, Fischer [2] have reviewed turbulent flow dispersion in open channel flow which reveals that the effect of side walls or banks in case of rivers is so significant that the effect of vertical gradient can be entirely neglected. In absence of wall resistance, Doshi, et al. [7] and Chatwin and Sullivan [8] determined the D_{eff} for dispersion in laminar flow through a long straight duct with rectangular cross section. They discussed the effect of aspect ratio in the dispersion coefficient and compared with those of flow between parallel plates. This outcome was confirmed by Takahashi and Gill [9] who studied Field flow fractionation (FFF), a chromatographic process for three dimensional laminar dispersion in rectangular conduit in the presence of a transverse flow. The effect of secondary flow in the laminar dispersion in rectangular duct have been studied by McConalogue [10] and Johnson and Kamm [11] with a conclusion that the dispersion can be reduced by introducing a transverse flow with the main flow field. However it can be further reduced by introducing artificial secondary flow by an external means (Zhao and Bau [12]).

However most of the previous studies on three dimensional domains were restricted to certain assumptions and covered very particular range of time and length. The purpose of this work is to study numerically the three dimensional unsteady problems of laminar flow dispersion in rectangular ducts. It is expected that this work shall elucidate the dispersion phenomena in a closed rectangular in an unprecedented detail.

Mathematical Model

The concentration profile, $C(x,y,z,t)$ due to an instantaneous source at z=0 during solute transport in laminar flow in a three dimensional Cartesian domain can be described by the convection diffusion equation:

$$\frac{\partial C}{\partial t} + u(x,y)\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(D_m \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_m \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_m \frac{\partial C}{\partial z}\right) \tag{2}$$

Along with the following initial and boundary conditions

$$C(x,y,0,0) = C_0 \tag{3}$$

$$C(x,y,z,0) = 0 \tag{4}$$

$$\frac{\partial C}{\partial r}(0,y,z,t) = \frac{\partial C}{\partial r}(x,0,z,t) = \frac{\partial C}{\partial r}(x,b,z,t) = \frac{\partial C}{\partial r}(a,y,z,t) = 0 \quad (5)$$

Where, *u(x,y)* is fully developed laminar velocity profile in the longitudinal direction for a rectangular duct. It can be obtained by following the approximate analytical solution of Navier-Stokes equation

$$u(x,y) = (x^2 - a^2) + \sum_{n=0}^{\infty}\left(\frac{4}{a}\frac{(-1)^n}{\alpha_n^3}\frac{\cosh(\alpha_n y)}{\cosh(\alpha_n b)}\cos(\alpha_n y)\right) \quad (6)$$

Where, a and b are the breadth and width of the rectangular cross section and $\alpha_n = (n + 1/2)\,\pi/a\,,\ \ n = 0,1,2\ldots$

The above equations are subjected to following assumptions:
(i) the fluid is incompressible and Newtonian; (ii) there is no chemical reaction; (iii) no material transfer across the walls; (iv) fully developed, laminar flow persists for the infinitely long rectangular duct; (v) initial concentration of the solute is distributed uniformly along the cross section of tube.

Method of Solution

The governing convection diffusion equation is solved numerically to obtain the local and mean concentration. The solution domain is divided into a grid. The governing equation is then transformed into a set of algebraic equations using a discretization scheme that renders the numerical dispersion negligible. An iterative scheme is used to solve these set of algebraic equations.

The steep axial concentration gradient of the solute under the initial conditions gives rise to numerical dispersion at the start of the simulation (Roache [13]) and obfuscates the actual dispersion. This phenomenon is readily observed by convecting a slug numerically without any molecular diffusion. The sharp discontinuities at the leading and trailing edges of the slug are not preserved but a spreading appears which reflects the presence of numerical diffusion although no molecular diffusion was introduced. To compensate for this numerical diffusion, the governing equation is discretized using the QUICKEST scheme proposed by Leonard [14]. This scheme exhibits a high degree of stability and is third order accurate. It reduces false diffusion by interpolating the variable up to three preceding points. In order to solve the problem at hand, the scheme is reformulated by considering the nature of dispersion through square ducts. Fully developed convection with constant velocity in the axial direction is assumed. Non-uniformity of the velocity profile has been taken into account along lateral directions.

Selecting appropriate spatial grid spacing for the domain and realistic time step is crucial for any numerical solution. Failure to do so may lead to an unstable and inaccurate solution. Keeping this in mind, a wide range of mesh sizes was tested in both the transverse and axial directions to find the optimum grid size. An optimum grid size is the finest size of the mesh that does not cause significant variation in the numerical solution upon further refinement. For a grid convergence test of the model, the solute was introduced at z = 1 up to z = 3 cm. The length of the pipe was taken 10 cm. The breadth and width of the duct was taken *a* = *b* = 0.02 cm.

Figure 1 and Figure 2 reveals that a significant amount of change in the breakthrough curve observed while changing number of grid points from 10 up to 70 for lateral direction and from 25 up to 400 for axial direction. Further mesh refinement after 40 and 150 in the corresponding directions results in a negligible difference in the solution. Hence, grid sizes were chosen as 5×10^{-4}cm in radial direction and 0.1 cm in axial direction. In order to account for the temporal grid independence test, the simulations were carried out with different time steps ranging from Δt = 0.0075 and decreasing to Δt = 0.0001 s. A time step greater than 0.0075 causes instability of the scheme in the situation considered. It is clear from Figure 3 that further decreasing in time step beyond 0.0075 s makes negligible difference to the solution.

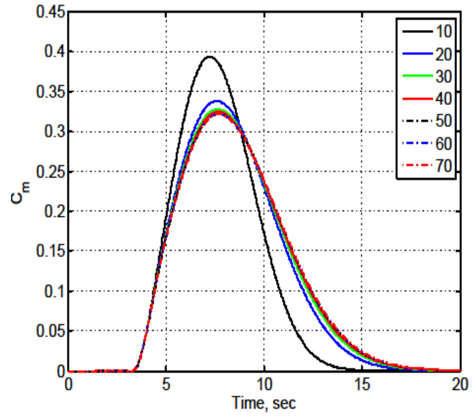

Figure 1. Axial grid independence test

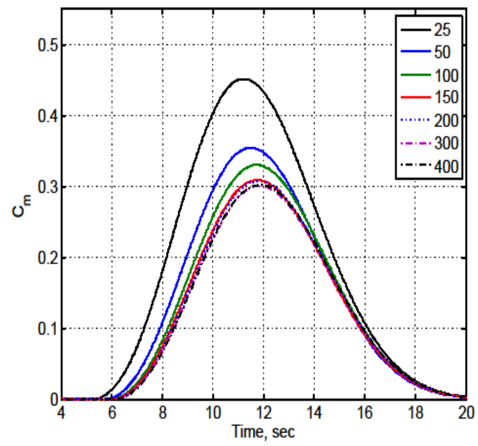

Figure 2. Transverse grid independence test

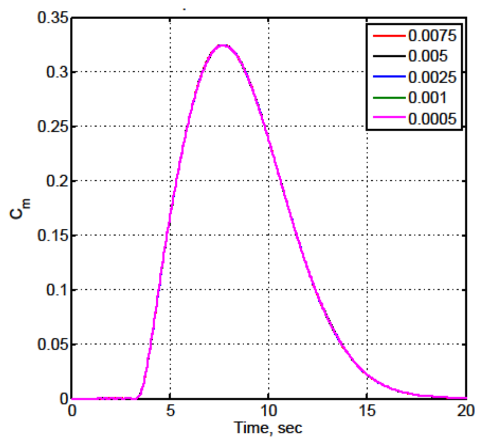

Figure 3. Time-step independence test

Results and Discussion

In a recent work of Rahman, et al. [15], the model was validated for the circular case and they compared the dispersion in circular and square ducts. It was found that the dispersion in square ducts is higher than in circular ducts.

The evolution of concentration across the cross section at a short dimensionless distance Z $(= z/(a * Pe))$= 0.01 and long distance Z= 0.1 has been presented in Figure 4 and Figure 5 to compare the result with the analytical result obtained by Doshi, et al. [7]. From the figure it is clear that the model is consonant with the analytical solution.

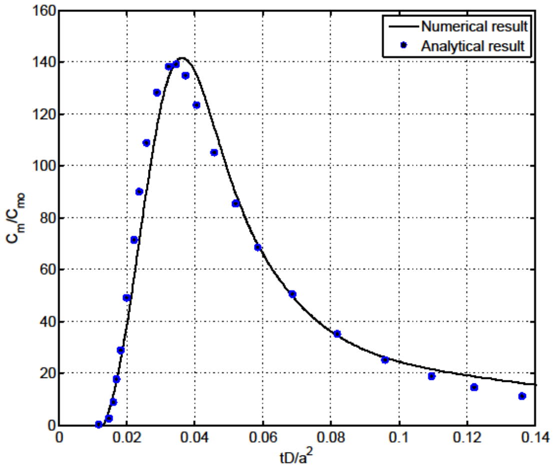

Figure 4. Comparison of the numerical model at short distance

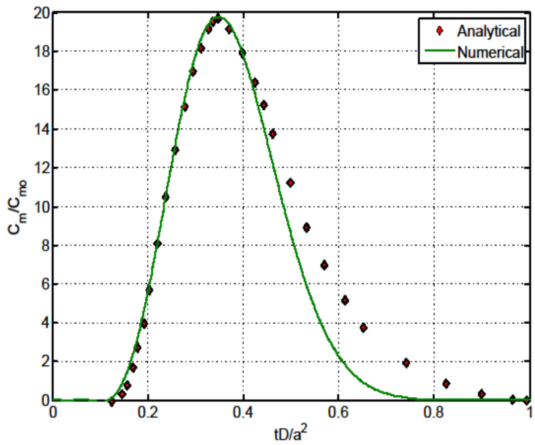

Figure 5. Comparison of the numerical model al long distance

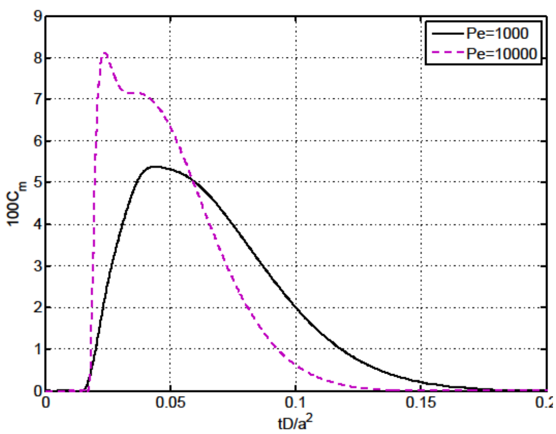

Figure 6. Mean breakthrough curve at *Z*=0.01

The analytical solution does not demonstrate any significant change due to variation of Peclet number of the system. We used the numerical model to study the effect of changing Peclet number at the same lateral positions.

At a higher Peclet number (Pe =10000) the breakthrough curve (which is the mean concentration curve over the cross section during entire time interval at a axial particular position) at Z=0.01 is distinguished by a surprising double peak (Figure 6). The sharp peak at the beginning demonstrates the domination of convection in the core region of the duct. The smooth second peak is an artefact of the increasing domination of diffusion as the flow proceeds down the pipe as can be also inferred from Figure 7. As can be seen from Figure 6 and Figure 7, at a lower Peclet number the effect of convection domination is neutralized even before *Z*=0.01. After a long time (at *Z*=0.07) the mean elution curve represents single peak without any shoulder (Figure 8) and it is reasonably well approximated by the analytical solution of Doshi, et al. [7] for both cases, high and low Peclet number.

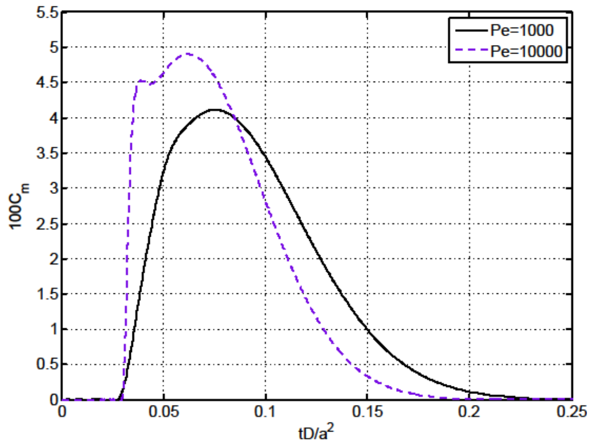

Figure 7. Mean breakthrough curve at *Z*=0.017

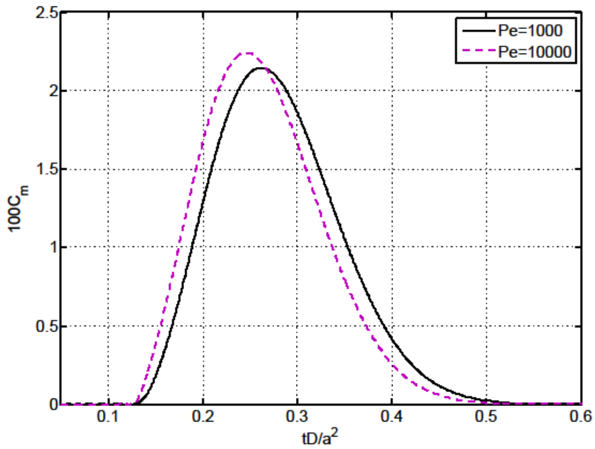

Figure 8. Mean breakthrough curve at *Z*=0.07

Conclusions

A numerically accurate method has been developed to study the dispersion of a solute in a laminar flow through a noncircular duct. The salient feature of this method is that it renders numerical dispersion negligible which makes the solution accurate and reliable. Available analytical solutions for this case can describe the spreading after a long duration from the initial developed which has been confirmed by the model. In addition to that, at initial development of the spreading, it was observed that the breakthrough curve at short distance manifest the domination of convection over diffusion. This effect is not observed in the case of comparatively lower Peclet numbers; instead, the solute spreads in a similar manner to Fickian diffusion, and it can be characterised with an effective dispersion coefficient.

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