International Journal of Mathematics and Systems Science (2022) Volume 5 Issue 1
doi:10.24294/ijmss.v1i4.815

A Lattice Boltzmann Scheme for Diffusion Equation in Spherical Coordinate

Debabrata Datta[1], **T K Pal**[2]

[1] Radiological Physics & Advisory Division, BARC, Mumbai, India

[2] Technology Development Division, BARC, Mumbai, India

ABSTRACT

Lattice Boltzmann models for diffusion equation are generally in Cartesian coordinate system. Very few researchers have attempted to solve diffusion equation in spherical coordinate system. In the lattice Boltzmann based diffusion model in spherical coordinate system extra term, which is due to variation of surface area along radial direction, is modeled as source term. In this study diffusion equation in spherical coordinate system is first converted to diffusion equation which is similar to that in Cartesian coordinate system by using proper variable. The diffusion equation is then solved using standard lattice Boltzmann method. The results obtained for the new variable are again converted to the actual variable. The numerical scheme is verified by comparing the results of the simulation study with analytical solution. A good agreement between the two results is established.

Keywords: Radial Diffusion; Lattice Boltzmann Method; Spherical Coordinate

1. Introduction

Nowadays the Lattice Boltzmann (LB) method[1-3] has emerged as a prominent numerical technique for solving partial differential equations that model various scientific and engineering problems[2,4]. LB method, which was initially introduced to solve Navier Stokes equation[5], has been successfully applied to solve flow, heat and mass transport problems[1,6,7]. Diffusion equation is a second order parabolic equation which is generally appears in the field of heat and mass transport. Diffusion equation in spherical and cylindrical coordinate systems has important practical applications because most of engineering problem are associated with spherical or cylindrical geometry. Standard LB method solves diffusion equation in Cartesian coordinate system. To solve diffusion equation in spherical coordinate system, researchers have modeled the extra term that arises due to increase in surface area along radial direction as source term in the LB equation[8–10].

In this work, the diffusion equation in spherical coordinate system is first converted to diffusion equation which is similar to that in Cartesian coordinate system. This conversion is done by making a proper substitution of the actual variable. The diffusion equation in the new variable is then solved using standard LB method. The solutions of the LB equation are then converted back to its original variable. The LB solutions are tested by solving bench mark problems.

The paper is organized in the following way. In Section 2, one dimensional diffusion equation in spherical coordinate system is converted to the form which is similar to diffusion equation in Cartesian coordinate system. The LB diffusion model for Cartesian coordinate system is described in Section 3. The LB scheme is verified and tested by solving benchmark problem in Section 4. Finally, conclusions are drawn in Section 5.

2. Diffusion Equation in Spherical Coordinate System

The diffusion equation in spherical coordinate system for a uniform and isotropic material is written as

$$\frac{\partial y}{\partial t}=\frac{k}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial y}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial y}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 y}{\partial\phi^2} \quad (2.1)$$

where y is the diffusive variable (it may be temperature, solute concentration etc.), k is called diffusion coefficient, (r, θ, ϕ) is a point in spherical coordinate. One dimension form of Eq. (2.1) in radial direction can be written as

$$\frac{\partial y(r,t)}{\partial t}=k\frac{\partial^2 y(r,t)}{\partial r^2}+\frac{2k}{r}\frac{\partial y(r,t)}{\partial r} \quad (2.2)$$

The second term of the right hand side of the above equation is due to increase in surface area along radial direction. Because of this term standard LB method cannot be used to solve the Eq. (2.2). In the rest of this Section, Eq. (2.2) is modified to the form of diffusion equation which is similar to that in Cartesian coordinate system by substituting the actual diffusive variable (y) by a new variable of the form

$$u(r,t)=ry(r,t) \quad (2.3)$$

The derivatives terms in the above equation can also written in term of the new variable as

$$\frac{\partial y(r,t)}{\partial t}=\frac{1}{r}\frac{\partial u(r,t)}{\partial t} \quad (2.4)$$

$$\frac{\partial y(r,t)}{\partial r}=\frac{1}{r}\frac{\partial u(r,t)}{\partial r}-\frac{u(r,t)}{r^2} \quad (2.5)$$

$$\frac{\partial^2 y(r,t)}{\partial r^2}=\frac{1}{r}\frac{\partial^2 u(r,t)}{\partial r^2}-\frac{2}{r^2}\frac{\partial u(r,t)}{\partial r}+\frac{2u(r,t)}{r^3} \quad (2.6)$$

Using the above equations Eq. (2.1) can be written as

$$\frac{1}{r}\frac{\partial u(r,t)}{\partial t}=\frac{k}{r}\frac{\partial^2 u(r,t)}{\partial r^2}-\frac{2k}{r^2}\frac{\partial u(r,t)}{\partial r}+\frac{2ku(r,t)}{r^3}+\frac{2k}{r^2}\frac{\partial u(r,t)}{\partial r}-\frac{2ku(r,t)}{r^3} \quad (2.7)$$

Since the last 4 terms of the above equation cancel out each other, we get the modified equation as

$$\frac{\partial u(r,t)}{\partial t}=k\frac{\partial^2 u(r,t)}{\partial r^2} \quad (2.8)$$

The above equation is similar to diffusion equation in Cartesian coordinate system and therefore can easily be solved using standard LB diffusion model. The LB solution of Eq. (2.8) is in terms of $u(r,t)$, which can be written in terms of $y(r,t)$ using Eq. (2.3).

3. Lattice Boltzmann Diffusion Model

LB equation which governs the evolution of particle distribution function is a discrete velocity Boltzmann equation. The discrete velocity Boltzmann equation is solved in a uniform domain of lattice nodes. The LB equation with Bhatnagar-Gross-Crook (BGK) collision operator can be written as

$$f_i(\vec{r}+\vec{e_i}\Delta t,\ t+\Delta t)=f_i(\vec{r},t)+\Omega_i^{BGK}(\vec{r},t) \quad (3.1)$$

$$\Omega_i^{BGK}(\vec{r},t)=\frac{1}{\tau}\left[f_i^{eq}(\vec{r},t)-f_i(\vec{r},t)\right] \quad (3.2)$$

where $f_i(\vec{r},t)$ is particle distribution function at spatiotemporal coordinate $(\vec{r},t)$ along i^{th} direction, $\vec{e_i}$ represents particle velocity along i^{th} direction, $\Omega_i^{BGK}(\vec{r},t)$ is BGK collision operator along i^{th} direction at same spatiotemporal coordinate, Δt is time step, τ is relaxation coefficient, and $f_i^{eq}(\vec{r},t)$ is particle equilibrium distribution function (EDF) along i^{th} direction. The EDF for diffusion process is written as

$$f_i^{eq}(\vec{r},t)=w_i C(\vec{r},t) \quad (3.3)$$

where w_i are the weights for particle's distribution function along i^{th} direction. For 1-D most commonly used lattices are D1Q2, D1Q3, for 2-D most commonly used lattices are D2Q4, D2Q5 and for 3-D, D3Q15, D3Q19 etc. Here for DnQm lattice n represent the dimension of the problem and m represent the number of discrete velocity vectors. Schematic of D1Q3 and D2Q5 lattices are shown in **Figure (3.1)** and **(3.2),** respectively. The values of w_i for a D1Q3 lattice are 4/6 for i=0 and 1/6 for i=1 and 2.

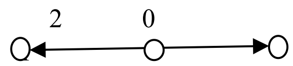

Figure 3.1; D1Q3 Lattice.

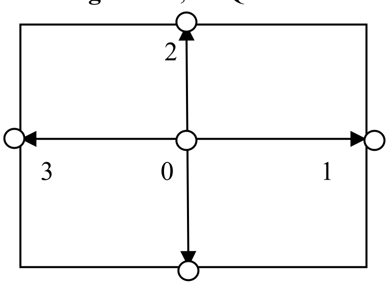

Figure 3.2; D2Q5 Lattice.

The EDF defined in Eq. (3.3) follows following constraints.

$$\sum_i f_i^{eq}(\vec{r},t) = C(\vec{r},t) \qquad (3.4)$$

$$\sum_i e_{ij} f_i^{eq}(\vec{r},t) = 0 \qquad (3.5)$$

$$\sum_i e_{ij} e_{ik} f_i^{eq}(\vec{r},t) = e_s^2 \left(\tau - \frac{1}{2}\right) \delta_{jk} \qquad (3.6)$$

where e_s is called pseudo sound speed[3]. Particle velocity directions are connected to the neighboring lattice points such that there is a free streaming in between two lattice points. Velocity components for D1Q3 and D2Q5 lattices are as given in Eq. (3.7) and (3.8), respectively.

$$e_i = \begin{cases} 0, & i = 0 \\ (cos\,(i-1)\,\pi)e, & i = 1, 2 \end{cases} \qquad (3.7)$$

$$e_i = \begin{cases} 0, & i = 0 \\ \left(cos\frac{(i-1)\pi}{2}, sin\frac{(i-1)\pi}{2}\right) e, & i = 1, 2,3,4 \end{cases} \qquad (3.8)$$

During the recovery of macroscopic diffusion equation (2.8) from LB equation (3.1 and 3.2) using Chapmann-Enskog multiscale expansion technique, following relationship between lattice diffusion coefficient and relaxation parameter (τ) is established[8]

$$D = e_s^2 \left(\tau - \frac{\Delta t}{2}\right) \qquad (3.9)$$

Macroscopic particle density is calculated by summing over distribution functions as

$$C(\vec{r},t) = \sum_i f_i(\vec{r},t) \qquad (3.10)$$

The LB equation (3.1 and 3.2) can be solved numerically by LB algorithm which consists of following two processes.

Collision process:

In collision process particles distribution function relaxes towards local equilibrium distribution function and it can be described by the following equation

$$f_i^*(\vec{r},t+\Delta t) = f_i(\vec{r},t) + \Omega_i^{BGK}(\vec{r},t) \qquad (3.11)$$

where $f_i^*(\vec{r},\ t+\Delta t)$ is the post collision particle's distribution function, the values of collision operators as same as given in Eq. (3.2).

Streaming process:

In this process, particles move from one lattice point to nearest lattice point along the direction of the lattice velocity. Computationally this process is just memory swapping. Algorithm of this process can be written as

$$f_i(\vec{r} + \vec{e_i}\Delta t,\ t+\Delta t) = f_i^*(\vec{r},\ t+\Delta t) \qquad (3.12)$$

Additional bounce-back boundary conditions are imposed at obstacle sites and along boundary walls at which particles reverse its direction after collision with obstacles or boundary walls.

4. Numerical Examples

The developed LB scheme is verified and validated by solving following benchmark problems.

4.1 Diffusion of solute from the surface to the center of a sphere

This test problem models the diffusion of solute from the surrounding environment to a cementitious facility of spherical shape. Since the surrounding media is very large, constant supply of solute at the surface of the facility is a reasonable assumption. This process can be mathematically modeled as a radial diffusion equation (2.2) with following initial and boundary conditions.

$$\begin{cases} y(r,t=0) = 0 \\ y(r=0,t) = 0 \\ y(r=a,t) = C_0 \end{cases} \qquad (4.1)$$

In terms of the new variable, $u(r,t)$ as given in Eq. (2.2), the above initial and boundary conditions can be written as

$$\begin{cases} u(r,t=0) = 0 \\ u(r=0,t) = 0 \\ u(r=a,t) = aC_0 \end{cases} \qquad (4.2)$$

Closed form solution of the problem can be written as

$$C(r,t) = C_0 + \frac{2a}{\pi r}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\sin\frac{n\pi r}{a}\exp\left[-\frac{Dn^2\pi^2 t}{a^2}\right]C_0 \qquad (4.3)$$

The LB simulation is carried out in lattice unit with 101 lattice points. The physical lattice length is 0.1 m. Following input parameters are used in the simulation. The concentration profile of solute inside the spherical object is calculated and the results are compared with analytical solution. Graphical plots of spatial profile of solute concentration after 365, 1000 and 3000 days are shown in the **Table 1**.

Parameter	**Value**
Radius (a) of the sphere	10 m
Inlet concentration (C_0)	1.0 mg/l
Diffusion coefficient (D)	1.0×10^{-8} m²/s
Simulation time	365, 1000 and 3000 days
Relaxation parameter (τ)	1.0
Physical lattice length (dr)	0.1 m

Table 1. Various parameters used in the simulation

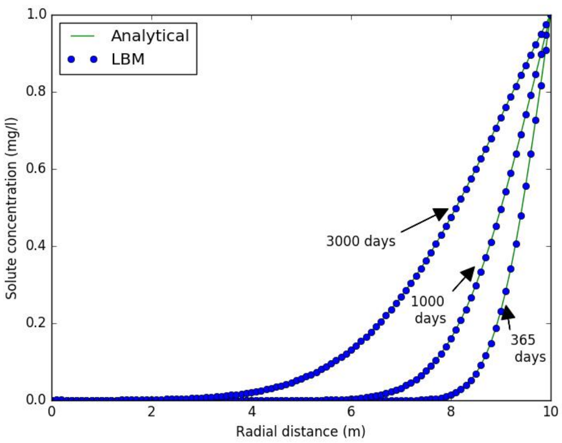

Figure 4.1; Spatial profile of solute concentration after 365, 1000 and 3000 days**.**

5. Conclusions

One dimensional radial diffusion equation in spherical coordinate system is solved using standard LB equation. The extra term in the governing radial diffusion equation is not modeled as source term, rather the diffusion equation is modified using a proper variable and the resultant equation is exactly similar to that in Cartesian coordinate system. The results show that the scheme is capable to simulate the radial diffusion equation very accurately.

References

1. Chen S, Doolen GD. Lattice Boltzmann method for fluid flows. Annu. Rev Fluid Mech. 1998; 30: 329-364.
2. Succi, S. The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Oxford, U. K.: Oxford Univ. Press 2001.
3. Wolf-Gladrow, D.A. Lattice-Gas Cellular Automata and Lattice Boltzmann Models: An Introduction. New York: Springer 2000.
4. Benzi R, Succi S, Vergassola M. The lattice Boltzmann equation: theory and applications, Phys. Rep. 1992; 222: 145-197.
5. Frisch U, Hasslacher B, Pomeau Y. Lattice-gas automata for the Navier-Stokes equation, Phys. Rev. Lett. 1986; 56 (14): 1505-1508.
6. Guo ZL, Shu C. Lattice Boltzmann method and its application in engineering, World Scientific press 2013.
7. Zhao CY, Dai LN, Tang GH, et al. Numerical study of natural convection in porous media (metals) using Lattice Boltzmann Method (LBM), International Journal of Heat and Fluid Flow 2010; 31 (5): 925-934.
8. Mohamad A. Lattice Boltzmann Method Fundamentals and Engineering Applications with Computer Codes, Springer, London 2011.
9. Zhou JG. Axisymmetric lattice Boltzmann method, Phys. Rev. E 2008; 78: 036701.
10. Mohamad AA. Lattice Boltzmann method for heat diffusion in axis-symmetric geometries, Prog. Comput. Fluid Dyn. 2009; 9 (8): 490-494.