The Soret effect with the D1Q2 and D2Q4 lattice Boltzmann model

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The paper analysis the incorporation of the source term in the advection-diffusion equation for the BGK Lattice Boltzmann Method (LBM). The problem is the coupled energy and species conservation equations with the Soret term. The problem is extremely important for people using LBM in simulating multi-physics, because multi-physics effect added as a source term to LB. A Few BGK LBM models were used, namely D1Q2, D1Q3, D2Q4 and D2Q5 to solve advection-diffusion-reaction problems. The aim of this work is to demonstrate that the lattice Boltzmann method is able to simulate Soret effect, where the source term is the curvature of the temperature field. Theoretical analysis of the force inclusion is also presented in the paper. To insure that the predictions are correct and consistent with the traditional methods, comparison of LBM predictions with the finite difference method (FVM) predictions were illustrated. Also, the results show that prediction of D1Q2 may suffer from oscillation.

Nomenclature

ϕ	Nondimensional species concentration
Θ	Nondimensional temperature
^{eq}	Superscript for the equilibrium function
^{m}	Superscript for the macroscopic quantities
g_i	Species population in direction $\boldsymbol{c_i}$
Pe	Peclet number, advection rate over diffusion rate
Sc	Schmidt number, viscous rate over diffusion rate

I. INTRODUCTION

Lattice Boltzmann Method (LBM) is a relatively new technique for solving transport equations, being developed for the last 20 years. The method is successfully applied for simulating hydrodynamics, heat and mass transfer, and multiphysics [1]. The method is applied for a wide range of problems [2–4]. However, there are many issues need to be resolved for efficient applications of the method for problems with complicated physics. Simulating multi-physics by adding appropriate source to the LBE (Lattice Boltzmann Equation) is an elegant and simple. Though a lot of attention was given to the incorporation of the force term to the Navier-Stokes equation [5–7], the problem need to clarified and tested for more complex cases. The existing publications [8] which give the general idea of the mass term implementation do not provide the examples for the mass incorporation validation. Still the validation of the mass terms in the advection-diffusion equation is subtle. We chose one interesting problem, the Soret effect, which couples energy and species conservation equations, due to its coupled complexity and non-uniformity of the source terms, i.e. the term depends on the second derivative of the temperature with respect to coordinates (curvature). The coupled nature of equations for the Soret effect is the interesting example to assess accuracy and efficiency of the lattice Boltzmann solutions. Therefore, the main focus of the paper is to validate the complex coupled system with a benchmark solution obtained using the explicit finite volume method (FVM). The authors used D1Q2, D1Q3, D2Q4 and D2Q5 with source (mass) terms to simulate heat and mass dispersion with the Soret effect (coupled problem), for one and two dimensional problems, respectively. Hence, energy and species conservation equations are solved for a given velocity field.

The paper is organized as follows: First we introduced the advection-diffusion equation with the Soret effect. The incorporation of the Soret effect term, which is mass term in the nature, needs the proper incorporation to the lattice Boltzmann equation. Though the general mass term incorporation is presented in [8], there is no step-by-step derivations of the mass term incorporations using the Chapman-Enskog expansion. As a tutorial example we present incorporation of the mass term through the Chapman-Enskog expansion for D2Q4 model. Then the numerical results for the double-dispersion problem are presented. In conclusion, we summarize the main findings.

II. ADVECTION DIFFUSION EQUATION WITH THE SORET EFFECT

Consider the advection-diffusion equation with the source term as,
Energy equation:

$$\partial_t\Theta + \partial_\alpha \Theta u_\alpha = \frac{1}{Pe}\,\partial_{\beta\beta}\Theta \tag{1}$$

Species conservation equation:

$$\partial_t\phi + \partial_\alpha \phi u_\alpha = \frac{1}{ScRe}\,\partial_{\beta\beta}\phi + S, \tag{2}$$

where Pe, Re and Sc are Peclet, Reynolds and Schmidt numbers, respectively. The source term $S = -\frac{1}{ScRe}\,\partial_{\beta\beta}\Theta$ is the Soret effect source term with Θ representing the temperature field. For simplicity let us replace $Sc\,Re$ by Sp. The above equation is nondimensionalizes by using H (length for 1-D and height for 2-D problems), u (inlet velocity) and L/u for length, velocity and time scales. θ and ϕ are nondimensional temperature and species concentration, respectively.

III. CHAPMAN-ENSKOG EXPANSION FOR THE SPECIES FIELD

We start with the LBE formulation of the advection-diffusion equation with the mass term S_i:

$$\begin{aligned} &g(\boldsymbol{x}+\boldsymbol{c_i}\epsilon, t+\epsilon) = \\ &-\frac{g_i(\boldsymbol{x},t)-g_i^{eq}(\boldsymbol{x},t)}{\tilde{\tau}} + \epsilon S_i, \end{aligned} \tag{3}$$

where ϵ is the Knudsen number. We perform the standard Chapman-Enskog procedure represented as:

$$\begin{aligned} g &= \sum_{n=0} \epsilon^n f^{(n)} \\ \partial_t &= \sum_{n=0} \epsilon^n \partial_{t_n} \end{aligned} \tag{4}$$

Notice that the formulation is equivalent to the most common in the literature formulation of the Chapman-Enskog expansion with $\partial_t = \epsilon\partial_{t_1} + \epsilon^2\partial_{t_2}$ and $\partial_x = \epsilon\partial_{x\prime}$. By collecting all terms with different powers of ϵ one can obtain the following:

$$\begin{aligned} \epsilon^0 :\quad & g_i^{(0)} = g_i^{eq} \\ \epsilon^1 :\quad & (\partial_{t_0} + c_{i\alpha}\partial_\alpha) g_i^{(0)} = -\frac{g^{(1)}}{\tau} + S_i \\ \epsilon^2 :\quad & \partial_{t_1} g_i^{(0)} + (\partial_{t_0} + c_{i\alpha}\partial_\alpha) g_i^{(1)} + \\ & \frac{1}{2}(\partial_{t_0} + c_{i\alpha}\partial_\alpha)^2 g_i^{(0)} = -\frac{g_i^{(2)}}{\tau} \quad , \end{aligned} \tag{5}$$

where the form of S_i will be determined through Chapman-Enskog analysis. By substituting the $f_i^{(1)}$ from the second equation of the system (5) to the third equation, one can obtain:

$$\begin{aligned} &\partial_{t_1} g_i^{(0)} + \left(1 - \frac{1}{2\tau}\right)(\partial_{t_0} + c_{i\alpha}\partial_\alpha) g_i^{(1)} + \\ &\frac{1}{2}(\partial_{t_0} + c_{i\alpha}\partial_\alpha) S_i = -\frac{g_i^{(2)}}{\tau} \end{aligned} \tag{6}$$

Note that the mass term inclusion to Eq. 6 forces to redefine macroscopic and equilibrium quantities. Hereafter, the superscript ^{m} is related to the macroscopic quantities obtained after the Chapman-Enskog expansion. Superscript ^{eq} outlines the equilibrium quantities. There are many different possibilities as to reformulate the equilibrium and macroscopic species concentrations [8]. We adapt the most popular one as:

$$\phi^m = \phi^{eq} = \phi + S/2. \tag{7}$$

Thus, $\sum_i g_i^{(0)} = \phi^{eq}$, $\sum_{n>0,i} g_i^{(n)} \neq 0$, but $\sum_{n>0,i} c_{i\alpha} g_i^{(n)} \neq \phi u_\alpha$.

The macroscopic species concentration ϕ^{eq} is defined above, thus we can obtain the condition for $g_i^{(1)}$ as follows:

$$\begin{aligned} &\phi^{eq} = \phi + \frac{S}{2} \\ &\sum_i g_i^{(0)} = \sum_i g_i^{(0)} + \epsilon \sum_i g_i^{(1)} + \ldots + \frac{S}{2} \end{aligned} \tag{8}$$

Therefore,

$$\sum_i g_i^{(1)} = -\frac{S}{2} \quad , \tag{9}$$

Performing the summation by i of the system (5) one can obtain

$$\begin{aligned} &\partial_{t_0}\phi^m + \partial_\alpha\Big(\sum_i g_i^{(0)} c_{i\alpha}\Big) = \frac{S}{2\tau} + \sum_i S_i \\ &\partial_{t_1}\phi^m + \left(1 - \frac{1}{2\tau}\right)\left(\partial_{t_0}\sum_i g_i^{(1)} + \partial_\alpha \sum_i c_{i\alpha} g_i^{(1)}\right) + \\ &\frac{1}{2}(\partial_{t_0} + c_{i\alpha}\partial_\alpha) S_i = 0 \end{aligned} \tag{10}$$

The right-hand side of the first equation of system (10) should be equal to S. It apparently follows if the original advection-diffusion equation with the mass term is need to be restored. This fixes the first order summation for mass populations:

$$\begin{aligned} &\frac{S}{2\tau} + \sum_i S_i = S \\ &\sum_i S_i = \left(1 - \frac{1}{2\tau}\right) S \end{aligned} \tag{11}$$

In the second equation of the system (10), there is the nonzero term $\sum_i c_{i\alpha} f_i^{(1)}$, which we can obtain by summation with $c_{i\alpha}$ the second equation of the system (5) as:

$$\begin{aligned} c_{i\alpha} g_i^{(1)} = \tau\Bigg(&\sum_i S_i c_{i\alpha} - \partial_{t_0}\sum_i g_i^{(0)} c_{i\alpha} - \\ &\partial_\beta \sum_i g_i^{(0)} c_{i\alpha} c_{i\beta}\Bigg) \end{aligned} \tag{12}$$

By defining the equilibrium distribution function the closure for relations (10) can be obtained.

IV. EQUILIBRIUM DISTRIBUTION FUNCTION

We model the advection-diffusion equation with the D2Q4 model. In general, it can be presented in the following form:

$$g_i^{eq} = w_i \phi^m (1 + 2c_{i\alpha} u_{i\alpha}). \tag{13}$$

By defining equilibrium distribution function we obtain the closure relationship. Note that this formulation introduces the numerical diffusion which shifts the effective diffusion $D \to D + u_x^2$ In this work we concentrate on the simplest form of the equilibrium distribution functions using the BGK scheme. Also we can rewrite the first moment of $f_i^{(1)} c_{i\alpha}$, Equation (12), as:

$$\begin{aligned} c_{i\alpha} g_i^{(1)} =& \tau \big(\sum_i S_i c_{i\alpha} - \partial_{t_0} \phi^m u_\alpha - \\ & \frac{1}{2} \partial_\alpha \phi^m \big) \end{aligned} \tag{14}$$

In case of external constant velocity, the term $\partial_{t_0} \phi^m u_\alpha$ is rewritten through the first equation of system (10) as:

$$\begin{aligned} &\partial_{t_0} \phi^m + \partial_\alpha (\phi^m u_\alpha) = S \\ &\partial_{t_0} \phi^m u_\alpha = u_\alpha \partial_{t_0} \phi^m \\ &u_\alpha \partial_{t_0} \phi^m = u_\alpha (S - \partial_\beta \phi^m u_\beta) \end{aligned} \tag{15}$$

Equation (14) can be rewritten as:

$$\begin{aligned} c_{i\alpha} g_i^{(1)} &= \tau \big(\sum_i S_i c_{i\alpha} - u_\alpha (S - \partial_\beta \phi^m u_\beta) - \\ & \quad \frac{1}{2} \partial_\alpha S \big) \\ c_{i\alpha} g_i^{(1)} &= \tau \big(\sum_i S_i c_{i\alpha} - u_\alpha S - \frac{1}{2} \partial_\alpha \phi^m \big), \end{aligned} \tag{16}$$

where for the last equation the term $u_\alpha \partial_\beta \phi^m u_\beta$ is neglected due to higher order. After substitution of first moment of $f_i^{(1)}$ the system (10) can be expressed as

$$\begin{aligned} &\partial_{t_0} \phi^m + \partial_\alpha (\phi^m u_\alpha) = S \\ &\partial_{t_1} \phi^m + \left(1 - \frac{1}{2\tau}\right) \partial_{t_0} \frac{(-S)}{2} + \frac{1}{2} \partial_{t_0} \sum_i S_i + \\ &\left(1 - \frac{1}{2\tau}\right) \tau \partial_\alpha \big(\sum_i S_i c_{i\alpha} - u_\alpha S - \frac{1}{2} \partial_\alpha \phi^m \big) + \\ &\partial_\alpha \frac{\sum_i S_i c_{i\alpha}}{2} = 0 \end{aligned} \tag{17}$$

Taking into the account that

$$\left(1 - \frac{1}{2\tau}\right) \partial_{t_0} \frac{(-S)}{2} + \frac{1}{2} \partial_{t_0} \sum_i S_i = 0 \quad , \tag{18}$$

the system (17) is reformulated:

$$\begin{aligned} &\partial_{t_0} \phi^m + \partial_\alpha (\phi^m u_\alpha) = S \\ &\partial_{t_1} \phi^m + \tau \partial_\alpha \sum_i S_i c_{i\alpha} - \left(\tau - \frac{1}{2}\right) \partial_\alpha u_\alpha S - \\ &\frac{1}{2} \left(\tau - \frac{1}{2}\right) \partial_\alpha^2 \phi^m = 0 \end{aligned} \tag{19}$$

Let us imply the following condition:

$$\tau \partial_\alpha \sum_i S_i c_{i\alpha} = \left(\tau - \frac{1}{2}\right) \partial_\alpha u_\alpha S \tag{20}$$

That defines our source populations as follows:

$$S_i = w_i \left(1 - \frac{1}{2\tau}\right) S \left(1 + 2c_{i\alpha} u_\alpha\right) \tag{21}$$

Eventually after algebraic manipulations one can obtain the following:

$$\begin{aligned} &\partial_{t_0} \phi^m + \partial_\alpha (\phi^m u_\alpha) = S \\ &\partial_{t_1} \phi^m - \frac{1}{2} \left(\tau - \frac{1}{2}\right) \partial_\alpha^2 \phi^m = 0 \end{aligned} \tag{22}$$

By multiplying the second equation of the system (22) on ϵ and summing it with the first equation, one can obtain the following equation:

$$\partial_t \phi^m + \partial_\alpha (\phi^m u_\alpha) = S + \epsilon \frac{1}{2} \left(\tau - \frac{1}{2}\right) \partial_{\beta\beta} \phi^m \tag{23}$$

In the case of the equation of double diffusion the system is the following:

$$\partial_t \phi^m + \partial_\alpha (\phi^m u_\alpha) = -\frac{\Delta\Theta}{Sp} + \frac{1}{Sp} \Delta \phi^m, \tag{24}$$

where $Sp = \dfrac{2}{\tau - \frac{1}{2}}$. For the D2Q4 $Sp = \dfrac{4}{2\tau - 1}$.

V. SOURCE TERM

In the work two schemes were used to add source term to the LBM. Scheme I, using exactly what the theory suggested as in equation (21). Scheme II, just simply add the source term as [6]:

$$S_i = w_i S \Delta t \tag{25}$$

VI. TEST PROBLEMS

In the following paragraph, the results of comparison of LBM predictions with finite volume methods are illustrated. Note that in both cases the temperature and species equations were resolved both either with the LBM

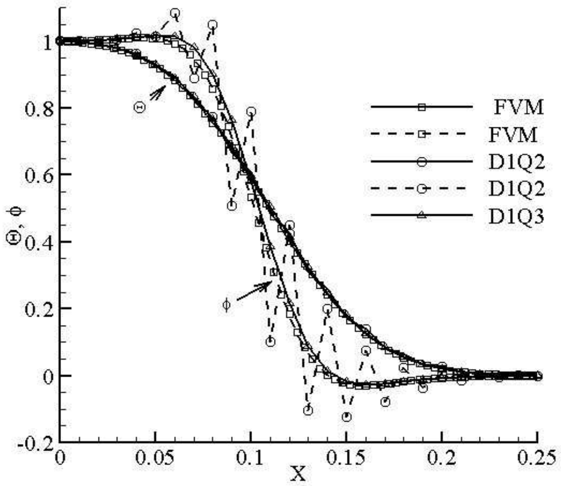

FIG. 1: Temperature and species concentration profiles predicted by different schemes, 1-D.

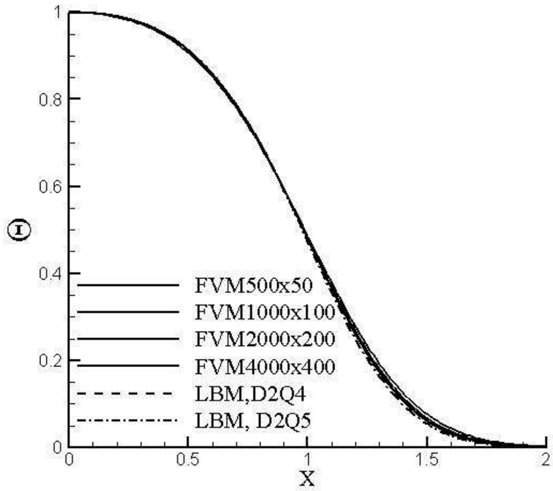

FIG. 2: Temperature profiles predicted by different schemes, 2-D.

or with the FVM (no mixed schemes were used). Figure 1 compares the predictions of D1Q2 and D1Q3 compared with predictions of explicit finite difference. One dimensional problem is a domain initially (at time equal to zero) at zero nondimensional temperature and zero nondimensional species concentration; then suddenly a flow with uniform velocity is forced to the domain with unit temperature and species concentration. It should mentioned that the results of finite volume presented in the Fig 1. is for a very fine grides. The results were tested for many incremental grid size until the results insured grid independency (number of grids were used equal to 1000, with interval between two nodes of 0.001 and time step of 0.00001, thermal diffusivity=0.01 and species diffusivity of 0.0025). Such a small time step is necessary to insure stable solution for explicit scheme. The results are presented for at dimensionless time of 0.1 in macroscale. As the grid size decreases the time step drastically reduced to insure stable solution. The difference between predictions of all models are consistent. It is noticed that model D1Q2 results oscillate locally (Fig. 1) but it is bounded. Different tests done by changing relaxation parameters, all the results show such local oscillation with D1Q2, which was not the case with D1Q3. Also, should mention that finite volume solution suffers from numerically diffusion (artificial diffusion) due to truncated nature of Taylor series in approximating the derivatives. It should mention that both schemes (I and II) of adding force term yield similar results. There was no noticeable difference between the predictions of the both schemes. Furthermore, two dimensional problem is tested. The domain of a solution is rectangular with aspect ratio of 10, i.e., one unit in vertical direction and 10 units in the stream wise direction. A uniform flow is imposed in the domain. Initially, the fluid in the channel was at cold

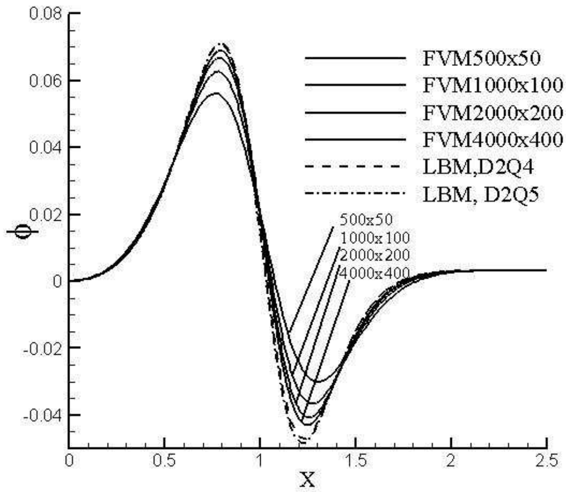

FIG. 3: Species concentration profiles predicted by different schemes, 2-D.

temperature (zero dimensionless temperature) and with zero dimensionless species concentration. At time greater than zero, a uniform flow with a constant velocity is induced into the domain. The upper and lower boundaries are kept at cold temperature (equated to zero) with unity of species concentrations. The results are produced for thermal diffusivity of 0.05 and mass diffusivity of 0.0125. The results of all models (D2Q4, D2Q5 and FVM) are consistent, Fig. 2 and Fig. 3. The results are presented at macroscopic time equal to 1.0. However, FVM needs fine grids in order to reduce numerical diffusion, especially in high gradient region. The FVM as well has the same form of the numerical diffusion which shifts the effective diffusion tensor $D \to D + u_x^2$. Also, the results tested by adding source term in simple way and as the theory suggested, both schemes yield the same results. It should mention that the results of D2Q4 predictions were consistent with D2Q5 and no oscillations were observed.

Furthermore, a test done to simulate double dispersion in a square differentially heated cavity. The flow is driven by buoyancy forces induced by temperature and species gradient. The results revealed that both schemes (eq. 21 and eq. 25) of adding force term yield same results.

VII. CONCLUSION

The present work derives and validates the incorporation of the mass term to the advection-diffusion equation. The Soret effect is the complicated coupled problem. It was shown that the lattice Boltzmann method is able to simulate the Soret effect and results were consistent with FVM predictions. Predictions of D1Q2 suffered from bounded oscillations. While D2Q4 predictions was consistent with D2Q5 and to insure that further simulations were performed to verify the conclusion. It is important to mention that we did not noticed a difference between adding source terms by using two different schemes (eq. 21 and eq. 25), which is consistent with our previous work.

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