

Simulation of Advection-Diffusion Problems with a Unified Lattice Boltzmann Equation

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ABSTRACT

A more general advection-diffusion equation, which can describe the mass transport in both single- and two-phase fluid flow is proposed. A field distribution parameter was coupled in a modified governing differential equation, which can be used not only to account for the change of diffusivity in single-phase flow, but also to account for the sharp concentration jump at the interface of two-phase fluid flow. A unified multiple-relaxation-time (MRT) lattice Boltzmann equation (LBE) for simulating the advection-diffusion problems is also proposed. Two test cases with transient and steady conjugate mass transfer problems with straight or curved interfaces were calculated to validate the present method. The results show that the proposed MRT LBE is simple and accurate, and has good numerical stability against large difference in mass diffusivity.

1. Introduction

Advection-diffusion phenomena can be widely observed in nature and many industry applications, for examples, the spreading of contaminants in heterogeneous porous media (Masciopinto, 2018) (Amaziane, 2008), bioreactors (Dumont et al., 2006), proton exchange membrane (PEM) fuel cell (Molaeimanesh and Akbari, 2015), and geothermal modelling in fractures (Chiba, et al., 2008) etc. An accurate model for the mass transport by advection and diffusion is very important. The key feature of this problem is that the concentration may evolve

with a sharp jump distribution at the phase interface of two-phase flow. The diffusivities of one solute in different solvents are in general different. Even in a same solvent, the diffusivity may vary with temperature, such as the salty water, the salt concentration may vary with temperature even at a mass equilibrium state (Lemos, 2019).

The mass transfer phenomenon in a homogeneous solvent is generally described by Fick's Law in a form of $q_m = -D \nabla C$, the corresponding governing equation describing an advection-diffusion problem can be written as

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - \nabla \cdot (u C) \quad (1)$$

where D is the mass diffusivity of a solute, C is the solute concentration, u is the velocity vector of fluid flow. It is noticed that while the solute in different solvents or in a solvent with a temperature (or some other parameters) dependent diffusivity, i.e. double diffusion problem, the numerical procedure for solving equation (1) will become difficult. The solute concentration at equilibrium state may have a jump from one phase (solvent) to the other phase (another solvent). As pointed out by Lu et al. (2019) that the governing equation of mass transfer in a single solvent, Eq. (1), cannot be extended to conjugate mass transfer directly, and Henry's Law must be taken into account for modification.

The unified scheme that simulates the entire concentration field in different solvents with a unified equation has been widely used to simulate conjugate mass transfer. Davidson and Rudman (2002) developed a volume of fluid (VOF) method for the conjugate heat and mass transfer. However, they did not consider the concentration jump between different phases. Onea et al. (2009) also proposed a method based on VOF and Henry's law to simulate conjugate mass transfer by adding an additional source term to the governing equation. Yang and Mao (2005) simulated the conjugate mass transfer of a droplet moving in a continuous immiscible liquid with level set method. The concentration field is calculated by introducing a new scalar that corresponds to $C^L He^{1/2}$ in the liquid phase and $C^G / He^{1/2}$ in the gas phase. The transformation can make the transformed concentration continuous at the interface. However, several parameters such as local velocity and diffusivity have to be transformed as well to satisfy the mass flux continuity at the interface. This leads to additional computation cost.

2. A General Governing Equation for Advection-Diffusion Problems

It is worthy to point out that the key problem of Fick's law is taking concentration as the driving potential in conjugate mass transfer. Take a gas-liquid two-phase diffusion problem as an example, there is no mass flux across the interface, however, there exists a concentration difference determined by Henry's law. While a diluted solution reaches a chemical equilibrium with the gas mixture, a dynamic mass balance for the solute exists at the gas-liquid interface even there is a concentration difference for the solute in different phases respectively. It certainly proves that it is unreasonable to take concentration as the driving potential in conjugate mass transfer. In fact, the diffusion velocities for the solute in different phases are different even the two phases are at chemical equilibrium. In order to overcome the drawback of Fick's law, a

modified advection-diffusion equation was proposed recently by Lu et al. (2019), which is written as follows,

$$\frac{\partial C}{\partial t} = \nabla \cdot \left(\frac{D}{\phi} \nabla (C\phi) \right) - \nabla \cdot (\mathbf{u}C) \quad (2)$$

The interface conditions of the governing equation for a two phase problem are

$$(C\phi)_L = (C\phi)_G \quad (3)$$

$$\left[\frac{D}{\phi} \nabla (C\phi) \right]_G = \left[\frac{D}{\phi} \nabla (C\phi) \right]_L \quad (4)$$

The parameter ϕ in Eqs. (2)-(4) is called the field distribution parameter. In a two phase advection-diffusion problem, it can be given by

$$\phi = \begin{cases} 1/\max(1, He) & \text{in gas} \\ He/\max(1, He) & \text{in liquid} \end{cases} \quad (5)$$

where He is the Henry's number, reflecting the chemical potential ratio of such a solute in the gas phase and liquid phase.

The modified governing equation (2) can be certainly used for describing the advection-diffusion problem in a single-phase, however, in this case the field parameter ϕ can be regarded as the ratio of local diffusivity to the reference diffusivity.

3. Numerical Method

As an alternative numerical method to solve the Navier-Stokes equation and advection-diffusion equation, the lattice Boltzmann method based on the Boltzmann equation in statistical mechanics has been developed rapidly in recent years. As proved by some previous researchers, LBM is an effective and very simple method in simulating multiphase liquid flow (Shan and Chen, 1992; Yan and Zu, 2007). A unified MRT LBE is proposed to simulate the advection-diffusion problem with a concentration jump at the interface.

To achieve better numerical accuracy and stability, the MRT LBE with multiple relaxation times (Huang and Wu, 2015) was used in the simulation. The MRT LBE is given as

$$g_i(\mathbf{x} + \mathbf{e}_i \Delta x, t + \Delta t) - g_i(\mathbf{x}, t) = - \sum_j (M^{-1} S M)_{ij} [g_j(\mathbf{x}, t) - g_j^{eq}(\mathbf{x}, t)] \quad (6)$$

where g_i is the discrete concentration distribution function, g_i^{eq} is the equilibrium concentration distribution function, Δx and Δt are the unit space step and the time step, respectively. Here, D3Q7 model (three dimensional with seven discrete velocities) is adopted for simulation, the

discrete velocities \mathbf{e}_i and the equilibrium energy distribution functions are given as Eqs. (4) and (5), respectively.

$$\mathbf{e}_i = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} \quad (7)$$

$$g_i^{eq} = \begin{cases} (1-6w)C & i = 0 \\ wC[1 + e_{i\alpha}u_\alpha\Delta t / (2w\Delta x)] & i = 1,2,3,4,5,6 \end{cases} \quad (8)$$

where u_α is the velocity, w is the weight coefficient for directions $i=1$ to 6, within the range (0, 1/6). The relaxation time τ_g and the constant w are related to the diffusivity coefficient as follows:

$$D = 2w(\tau_g - 0.5)c^2\Delta t \quad (9)$$

where M is the matrix that projects a vector onto the moment space $|m\rangle$, which can be expressed as (Li and Tong et al., 2017):

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 6 & -1 & -1 & -1 & -1 & -1 & -1 \\ 0 & 2 & 2 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 1 & 1 & -1 & -1 \end{bmatrix} \quad (10)$$

The corresponding equilibrium moment $|m^{eq}\rangle$ is given as

$$|m^{eq}\rangle = |C, u_x/c, u_y/c, u_z/c, (6-40w)C, 0, 0\rangle \quad (11)$$

The relaxation matrix S , which is a diagonal matrix, can be expressed as

$$S = \text{diag}[s_0, s_1, s_2, s_3, s_4, s_5, s_6] \quad (12)$$

where c is the lattice speed defined as $c = \Delta x / \Delta t$. In the lattice Boltzmann equation, the bulk concentration is obtained by

$$C = \sum_i g_i \quad (13)$$

Among the relaxation parameters in the diagonal relaxation matrix, the values of s_0 , s_1 , s_2 and s_3 are set as $s_0 = 1$ and $s_{1,2,3} = 1/\tau_g$, respectively, and the rest relaxation parameters, which can be adjusted to achieve better performance in real application, are variable in a range of $0 < s_{4,5,6} < 2$. In the present paper, a parameter one fourth is kept in the MRT collision scheme, which is defined as

$$\Lambda = \left(\frac{1}{s_1} - \frac{1}{2} \right) \left(\frac{1}{s_4} - \frac{1}{2} \right) = \frac{1}{4} \quad (12)$$

By keeping the two parameters of s_1 and s_4 in such a relation, better numerical accuracy and stability can be achieved. And it has been proved by Li et al. (2017) that the parameter can significantly eliminate the numerical diffusion across the interface in a solid-liquid phase change problem with discontinuous heat flux across the interface.

4. Numerical Validation

To verify the proposed MRT LBE, a transient advection-diffusion problem between the liquid and gas with a moving interface was performed. At the initial time, the physical model is shown in Fig. 1.

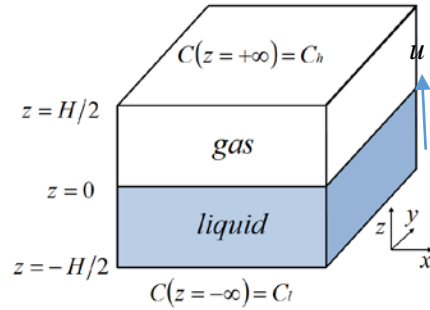


Figure 1: 1D conjugate mass transfer in an infinite system

The entire area will move toward z axis with a constant velocity $u = 20D_G/H$ when the time $t > 0$. For the moving interface, the volume of fluid (VOF) method is used, and its position is implicitly captured by the fluid fraction F . The distributions of F at different time is given in advance as follows:

$$F = \begin{cases} 1 & x < ut - d_m/2 \\ 1 - \frac{x - ut + R_m}{2R_m} & ut - d_m/2 \leq x \leq ut + d_m/2 \\ 0 & x > ut + d_m/2 \end{cases} \quad (14)$$

where d_m is width of the interface with a value of $d_m = \Delta x$. The parameters including D and w can be determined by following equations, respectively.

$$w = \left[F/w^L + (1-F)/w^G \right]^{-1} \quad (15)$$

$$\frac{D}{w} = \left[F \left(\frac{D^L}{w^L} \right)^{-1} + (1-F) \left(\frac{D^G}{w^G} \right)^{-1} \right]^{-1} \quad (16)$$

The problem is solved by the proposed MRT LBE, and the dimensionless concentration distribution at four different transient periods including $Fo = 0$, $Fo = 4 \times 10^{-4}$, $Fo = 1 \times 10^{-3}$, $Fo = 2 \times 10^{-3}$ are compared with the corresponding analytical solutions (Haroun, et al., 2010). The relaxation times in the liquid and gas are set as 0.516 and 0.54, respectively, while the mesh size is $\Delta x = H/100$. Figure 2 shows the comparisons between the MRT LBE results and the analytical solutions at different times. With the time step increasing, the concentration peak moves toward the velocity direction, and the concentration distribution near the peak varies sharply. It can also be seen that the MRT LBE results always show good agreement with the corresponding analytical solutions at different periods. It is noted that the concentration jump at the moving interface cannot be described precisely owing to using the diffusive interface to replace the real shape interface. The numerical error increases when the interface becomes wider. The numerical tests for trying different diffusive interface thickness d_m indicates that we should use thinner diffusive interface to decrease the numerical error. However, on the other hand, diffusive interface with enough width is needed to ensure the stability for simulating multiphase flow with lattice Boltzmann models. Therefore, choosing an approximate interface width is necessary for simulating conjugate mass transfer accompanying with multiphase flow.

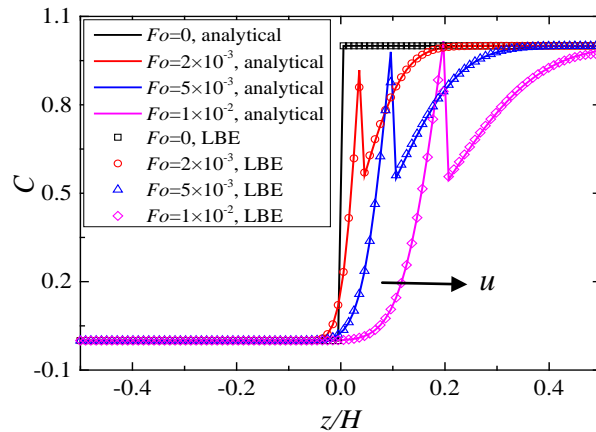


Figure 2: Comparisons of C between the MRT LBE results and the analytical solutions for transient mass transfer between the liquid and gas with a moving interface

5. Conclusion

A more general governing equation for describing the advection-diffusion problem was proposed, and this equation can be numerical simulated by using MRT LBE. It is found that Henry's Law, which relates to variable concentration distribution at the two sides of interface, can be expressed as a relation between two constant weight coefficients in LBE. The numerical test for a transient advection-diffusion problem between the liquid and gas with a moving interface shows that the MRT LBE has a better numerical stability than the SRT LBE against large distribution coefficients and diffusivity coefficient ratios.

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REFERENCES

- Amaziane, B., Ossmani, M. E., and Serres, C., "Numerical Modeling of the Flow and Transport of Radionuclides in Heterogeneous Porous Media," *Computat. Geosci.*, 12, (2008), 437-449.
- Chen, C.F, Turner, J.S. "Crystallization in a double-diffusive system." *J Geophys Res*, 85,(1980), 2573-2593.
- Chiba, R., Okaze, T., Fomin S., Chugunov V., Niibori Y., Fukunaga H., Hashida T. "Numerical simulations of the anomalous solute transport in a fractured porous aquifer", *Transactions - Geothermal Resources Council*, 32, (2008), 375-377.
- Couto, P. R. L., and Malta, S. M. C. "Interaction between Sorption and Biodegradation Processes in the Contaminant Transport." *Ecol. Modell.*, 214, (2008), 65-73.
- Davidson, M. R., and Rudman, M. "Volume-of-fluid calculation of heat or mass transfer across deforming interfaces in two-fluid flow." *Numerical Heat Transfer: Part B: Fundamentals*, 41(3-4), (2002), 291-308b
- Dumont, E., Andres, Y., and Le Cloirec, P. "Effect of organic solvents on oxygen mass transfer in multiphase systems: application to bioreactors in environmental protection. " *Biochemical Engineering Journal*. 30(3), (2006), 245-252.
- Haroun, Y., Legendre. D., Raynal. L. "Volume of fluid method for interfacial reactive mass transfer: application to stable liquid film", *Chemical Engineering Science*, 65 (10), (2010) 2896-2909.
- Huang, R., and Wu, H. "Phase interface effects in the total enthalpy-based lattice Boltzmann model for solid-liquid phase change". *Journal of Computational Physics*, 294, (2015), 346-362.
- Lemos, Marcelo J. S., De, Carvalho, and Paulo, H. "Modified Lewis Number and Buoyancy Ratio Effects on Turbulent Double-Diffusive Convection in Porous Media Using the Thermal Nonequilibrium Model." *ASME Journal of Heat Transfer*, 141(1), (2019), 1-18.

- Li, D., Tong, Z.X., and Ren, Q., et al. "Three-dimensional lattice Boltzmann models for solid-liquid phase change." *International Journal of Heat and Mass Transfer*, 115, (2017), 1334-1347.
- Lu, J.H, Lei, H.Y, and Dai, C.S. "Analysis of Henry's law and a unified lattice Boltzmann equation for conjugate mass transfer problem." *Chemical Engineering Science*, 18, (2019), 319-331.
- Masciopinto, C., Passarella, G. "Mass-transfer impact on solute mobility in porous media: a new mobile-immobile model." *Journal of Contaminant Hydrology*, 215, (2018), 21-28.
- Molaeimanesh, G. R., and Akbari, M. H. "Agglomerate modeling of cathode catalyst layer of a PEM fuel cell by the lattice Boltzmann method." *International Journal of Hydrogen Energy*, 40(15), (2018), 5169-5185.
- Onea, A., Wörner, M., and Cacuci, D.G. "A qualitative computational study of mass transfer in upward bubble train flow through square and rectangular mini-channels." *Chemical Engineering Science*. 64(7), (2009), 1416-1435.
- Shan, X., and Chen, H. "Lattice Boltzmann model for simulating flows with multiple phases and components." *Physical Review E*. 47(3), (1993), 1815.
- Yan, Y.Y., Zu, Y.Q. "A lattice Boltzmann method for incompressible two-phase flows on partial wetting surface with large density ratio." *Journal of Computational Physics*, 227(1), 2007.763-775.
- Yang, C., and Mao, Z.S. "Numerical simulation of interphase mass transfer with the level set approach." *Chemical Engineering Science*, 60(10), (2005), 2643-266.