

Tong, Zi-Xiang; He, Ya-Ling; Chen, Li; Xie, Tao

A multi-component lattice Boltzmann method in consistent with Stefan-Maxwell equations: derivation, validation and application in porous medium. (English) [Zbl 1391.76641](#)
[Comput. Fluids 105, 155-165 \(2014\)](#).

Summary: In this paper, a multi-component lattice Boltzmann method (LBM) with different lattice speeds and multiple linearized collision terms is improved. The molecular weights, viscosities of each component and the diffusivities can be tuned separately. An exact calculation for relaxation times of the cross-collision terms is derived, which makes the model to be consistent with the Stefan-Maxwell equations. The derivation also demonstrates that the tuning-molecular-weight strategy is only available for the ternary diffusion. The expressions of the fluxes and the boundary conditions are proposed. A simulation of the one-dimensional diffusion demonstrates that the second-order interpolation is better than the first-order one to deal with the different lattice speed. The simulation of Couette flow shows that the model behaves like a single fluid with high Schmidt number, and the components tend to flow independently with small Schmidt number. The model is validated by the simulation of one-dimensional diffusion and two-dimensional opposed jet flow, where the LBM results coincide well with the results of the Stefan-Maxwell equations. Finally, the diffusion in a porous media is simulated as an example of the application of the model. This lattice Boltzmann model is suitable for simulating multi-component convection-diffusion problems with complex boundary conditions.

MSC:

[76M28](#) Particle methods and lattice-gas methods
[76Txx](#) Multiphase and multicomponent flows

Cited in 1 Document

Keywords:

[lattice Boltzmann method](#); [multi-component simulation](#); [Stefan-Maxwell equation](#); [second-order interpolation](#); [tuning molecular weights](#); [porous medium](#)

Full Text: [DOI](#)

References:

- [1] Luo, L. S.; Girimaji, S. S., Theory of the lattice Boltzmann method: two-fluid model for binary mixtures, *Phys Rev E*, 67, 036302, (2003)
- [2] McCracken, M. E.; Abraham, J., Lattice Boltzmann methods for binary mixtures with different molecular weights, *Phys Rev E*, 71, 046704, (2005)
- [3] Chen, L.; Kang, Q.; He, Y. L.; Tao, W. Q., Pore-scale simulation of coupled multiple physicochemical thermal processes in micro reactor for hydrogen production using lattice Boltzmann method, *Int J Hydrogen Energy*, 37, 13943-13957, (2012)
- [4] He, Y. L.; Wang, Y.; Li, Q., Lattice Boltzmann method: theory and application, (2009), Science Press Beijing · [Zbl 1229.76090](#)
- [5] Chen, S.; Doolen, G. D., Lattice Boltzmann method for fluid flows, *Annu Rev Fluid Mech*, 30, 329-364, (1998)
- [6] Sofonea, V.; Sekerka, R. F., BGK models for diffusion in isothermal binary fluid systems, *Physica A*, 299, 494-520, (2001) · [Zbl 0972.82079](#)
- [7] Shan, X. W.; Doolen, G., Multicomponent lattice-Boltzmann model with interparticle interaction, *J Stat Phys*, 81, 379-393, (1995) · [Zbl 1106.82358](#)
- [8] Zheng, L.; Guo, Z. L.; Shi, B. C.; Zheng, C. G., Finite-difference-based multiple-relaxation-times lattice Boltzmann model for binary mixtures, *Phys Rev E*, 81, 016706, (2010)
- [9] Asinari, P., Viscous coupling based lattice Boltzmann model for binary mixtures, *Phys Fluids*, 17, 067102, (2005) · [Zbl 1187.76029](#)
- [10] Inamuro, T.; Yoshino, M.; Inoue, H.; Mizuno, R.; Ogino, F., A lattice Boltzmann method for a binary miscible fluid mixture and its application to a heat-transfer problem, *J Comput Phys*, 179, 201-215, (2002) · [Zbl 1065.76164](#)
- [11] Li, Q.; He, Y. L.; Wang, Y.; Tao, W. Q., Coupled double-distribution-function lattice Boltzmann method for the compressible Navier-Stokes equations, *Phys Rev E*, 76, 056705, (2007)
- [12] Flekkøy, E. G., Lattice Bhatnagar-Gross-Krook models for miscible fluids, *Phys Rev E*, 47, 4247-4257, (1993)

- [13] Asinari, P.; Luo, L. S., A consistent lattice Boltzmann equation with baroclinic coupling for mixtures, *J Comput Phys*, 227, 3878-3895, (2008) · [Zbl 1142.82017](#)
- [14] Sirovich, L., Kinetic modeling of gas mixtures, *Phys Fluids*, 5, 908-918, (1962) · [Zbl 0118.23602](#)
- [15] Luo, L. S.; Girimaji, S. S., Lattice Boltzmann model for binary mixtures, *Phys Rev E*, 66, 035301, (2002)
- [16] Facin, P. C.; Philippi, P. C.; dos Santos, L. O.E., A non-linear lattice-Boltzmann model for ideal miscible fluids, *Future Gener Comput Syst*, 20, 945-949, (2004)
- [17] Xu, A. G., Two-dimensional finite-difference lattice Boltzmann method for the complete Navier-Stokes equations of binary fluids, *Europhys Lett*, 69, 214-220, (2005)
- [18] Xu, A. G., Finite-difference lattice-Boltzmann methods for binary fluids, *Phys Rev E*, 71, 066706, (2005)
- [19] Hamel, B. B., Kinetic model for binary gas mixtures, *Phys Fluids*, 8, 418-425, (1965)
- [20] Asinari, P., Semi-implicit-linearized multiple-relaxation-time formulation of lattice Boltzmann schemes for mixture modeling, *Phys Rev E*, 73, 056705, (2006)
- [21] Arcidiacono, S.; Ansumali, S.; Karlin, I. V.; Mantzaras, J.; Boulouchos, K. B., Entropic lattice Boltzmann method for simulation of binary mixtures, *Math Comput Simulat*, 72, 79-83, (2006) · [Zbl 1116.76065](#)
- [22] Arcidiacono, S.; Mantzaras, J.; Ansumali, S.; Karlin, I. V.; Frouzakis, C.; Boulouchos, K. B., Simulation of binary mixtures with the lattice Boltzmann method, *Phys Rev E*, 74, 056707, (2006)
- [23] Kang, J.; Prasianakis, N. I.; Mantzaras, J., Lattice Boltzmann model for thermal binary-mixture gas flows, *Phys Rev E*, 87, 053304, (2013)
- [24] Arcidiacono, S.; Karlin, I. V.; Mantzaras, J.; Frouzakis, C. E., Lattice Boltzmann model for the simulation of multicomponent mixtures, *Phys Rev E*, 76, 046703, (2007)
- [25] Asinari, P., Lattice Boltzmann scheme for mixture modeling: analysis of the continuum diffusion regimes recovering Maxwell-Stefan model and incompressible Navier-Stokes equations, *Phys Rev E*, 80, 056701, (2009)
- [26] Asinari, P., Multiple-relaxation-time lattice Boltzmann scheme for homogeneous mixture flows with external force, *Phys Rev E*, 77, 056706, (2008)
- [27] Joshi, A. S.; Peracchio, A. A.; Grew, K. N.; Chiu, W. K.S., Lattice Boltzmann method for continuum, multi-component mass diffusion in complex 2D geometries, *J Phys D - Appl Phys*, 40, 2961-2971, (2007)
- [28] Merk, H. J., The macroscopic equations for simultaneous heat and mass transfer in isotropic, continuous and closed systems, *Appl Sci Res, Sect A*, 8, 73-99, (1959) · [Zbl 0089.19302](#)
- [29] Bird, R.; Stewart, W.; Lightfoot, E., *Transport phenomena*, (2002), John Wiley New York
- [30] Qian, Y. H.; Dhumieres, D.; Lallemand, P., Lattice BGK models for Navier-Stokes equation, *Europhys Lett*, 17, 479-484, (1992) · [Zbl 1116.76419](#)
- [31] Joshi, A. S.; Grew, K. N.; Peracchio, A. A.; Chiu, W. K.S., Lattice Boltzmann modeling of 2D gas transport in a solid oxide fuel cell anode, *J Power Sources*, 164, 631-638, (2007)
- [32] Taylor, R.; Krishna, R., *Multicomponent mass transfer*, (1993), John Wiley & Sons New York
- [33] Zou, Q. S.; He, X. Y., On pressure and velocity boundary conditions for the lattice Boltzmann BGK model, *Phys Fluids*, 9, 1591-1598, (1997) · [Zbl 1185.76873](#)
- [34] Joshi, A. S.; Grew, K. N.; Izzo, J. R.; Peracchio, A. A.; Chiu, W. K.S., Lattice Boltzmann modeling of three-dimensional, multicomponent mass diffusion in a solid oxide fuel cell anode, *J Fuel Cell Sci Technol*, 7, 011006, (2010)
- [35] O'Hayre, R. P.; Cha, S.-W.; Colella, W. G.; Prinz, F. B., *Fuel cell fundamentals*, (2006), John Wiley & Sons New York
- [36] Kundu, P. K.; Cohen, I. M., *Fluid mechanics*, (2008), Academic Press Burlington
- [37] Wesselingh, J. A.; Krishna, R., *Mass transfer in multicomponent mixtures*, (2000), Delft University Press Delft
- [38] Cussler, E. L., *Diffusion: mass transfer in fluid systems*, (2009), Cambridge University Press Cambridge
- [39] Grew, K. N.; Joshi, A. S.; Chiu, W. K.S., Direct internal reformation and mass transport in the solid oxide fuel cell anode: a pore-scale lattice Boltzmann study with detailed reaction kinetics, *Fuel Cells*, 10, 1143-1156, (2010)
- [40] Wang, M.; Wang, J.; Pan, N.; Chen, S., Mesoscopic predictions of the effective thermal conductivity for microscale random porous media, *Phys Rev E*, 75, 036702, (2007)
- [41] Lallemand, P.; Luo, L.-S., Theory of the lattice Boltzmann method: dispersion, dissipation, isotropy, Galilean invariance, and stability, *Phys Rev E*, 61, 6546-6562, (2000)

This reference list is based on information provided by the publisher or from digital mathematics libraries. Its items are heuristically matched to zbMATH identifiers and may contain data conversion errors. It attempts to reflect the references listed in the original paper as accurately as possible without claiming the completeness or perfect precision of the matching.