Lattice Boltzmann method for the simulations of miscible gases

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Abstract

The model proposed here is derived from an alternative theory of multicomponent fluid diffusion by Kerkhof [1] based on an expansion of the legacy theory of Hirschfelder, Curtiss and Bird [2]. In contrast with the previous lattice Boltzmann models, **the diffusion force is directly added to the momentum equation** through a Guo's forcing scheme [3]. In addition the corresponding **transport coefficients**, viscosity and diffusion coefficients for each species, **are computed according to the molecular proprieties of the components**. Then some numerical simulations are presented for validation purposes.

A new multicomponent lattice Boltzmann model

The σ superscript denotes different fluid components by specifying $\sigma = 1, 2, ..., N$ with N being the total number of the components. For simplicity, the components are supposed to have the **same molar weight**.

$$f_\alpha^\sigma\left(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t\right) = f_\alpha^\sigma\left(\mathbf{x},t\right) - \frac{1}{\tau^\sigma}\left[f_\alpha^\sigma\left(\mathbf{x},t\right) - f_\alpha^{\sigma(eq)}\left(\mathbf{x},t\right)\right] + S_\alpha^\sigma$$

Where $f_\alpha^{\sigma(eq)}$ is the equilibrium distribution functions of each fluid species:

$$f_\alpha^{\sigma(eq)} = \rho^\sigma\omega_\alpha\left[1 + \frac{\mathbf{u}^\sigma\cdot\mathbf{e}_\alpha}{c_s^2} + \frac{(\mathbf{u}^\sigma\cdot\mathbf{e}_\alpha)^2}{2c_s^4} - \frac{\mathbf{u}^\sigma\cdot\mathbf{u}^\sigma}{2c_s^2}\right]$$

And S_α^σ is the source term from Guo forcing scheme where $\mathcal{F}^\sigma$ is the total force acting on the σth component:

$$S_\alpha^\sigma = (1-\frac{\delta_t}{2\tau^\sigma})\omega_\alpha\left[\frac{\mathbf{e}_\alpha-\mathbf{u}^\sigma}{c_s^2} + \frac{(\mathbf{e}_\alpha\cdot\mathbf{u}^\sigma)\mathbf{e}_\alpha}{c_s^4}\right]\cdot\mathcal{F}^\sigma$$

As a **multi-fluid** approach of the mixture, the density and the momentum of each fluid components are defined as:

$$\rho^\sigma = \sum_\alpha f_\alpha^\sigma, \quad \rho^\sigma\mathbf{u}^\sigma = \sum_\alpha f_\alpha^\sigma\mathbf{e}_\alpha + \frac{\delta_t}{2}\mathcal{F}^\sigma$$

$\mathcal{F}^\sigma$ is the sum of **diffusion forces** and other external forces:

$$\mathcal{F}^\sigma = \mathcal{F}_D^\sigma + \mathcal{F}_{ext}^\sigma, \quad \text{with } \mathcal{F}_D^\sigma = -p\sum_{\varsigma=1}^{N}\frac{x_\sigma x_\varsigma}{\mathcal{D}_{\sigma\varsigma}}(\mathbf{u}^\sigma-\mathbf{u}^\varsigma)$$

A Chapman and Enskog expansion procedure gives the following macroscopic equations for low mach number and isothermal flow:

$$\partial_t\rho^\sigma + \nabla\cdot(\rho^\sigma\mathbf{u}^\sigma) = 0$$

$$\partial_t(\rho^\sigma\mathbf{u}^\sigma) + \nabla\cdot(\rho^\sigma\mathbf{u}^\sigma\otimes\mathbf{u}^\sigma) = -\nabla p^\sigma + \nabla\cdot\left[\mu^\sigma\left(\nabla\mathbf{u}^\sigma + (\nabla\mathbf{u}^\sigma)^T\right)\right] - p\sum_{\varsigma=1}^{N}\frac{x_\sigma x_\varsigma}{\mathcal{D}_{\sigma\varsigma}}(\mathbf{u}^\sigma-\mathbf{u}^\varsigma) + \mathcal{F}_{ext}^\sigma$$

Where $p^\sigma = \rho^\sigma c_s^2$, $p = \sum_{\sigma=1}^N p^\sigma$, $\mu^\sigma = \rho^\sigma c_s^2(\tau^\sigma - \frac{\delta_t}{2})$

Transport coefficients

$$(\mu^\sigma) = [P_{\sigma\varsigma}]^{-1}\begin{pmatrix}1\\ \vdots\\ 1\end{pmatrix}$$

$$P_{\sigma\sigma} = \frac{2}{k_BT}\left[\frac{4}{5}\Omega_\sigma^{(2,2)} + \sum_{\varsigma\neq\sigma}^{N}\frac{x_\varsigma}{x_\sigma}\frac{16}{15}\frac{m_\varsigma}{(m_\sigma+m_\varsigma)^2}\left(5m_\sigma\Omega_{\sigma\varsigma}^{(1,1)} + \frac{3}{2}m_\varsigma\Omega_{\sigma\varsigma}^{(2,2)}\right)\right]$$

$$P_{\sigma\varsigma} = -\frac{2}{k_BT}\left[\frac{16}{15}\frac{m_\sigma m_\varsigma}{(m_\sigma+m_\varsigma)^2}\left(5\Omega_{\sigma\varsigma}^{(1,1)} - \frac{3}{2}\Omega_{\sigma\varsigma}^{(2,2)}\right)\right]$$

$$\mu^{mixture} = \sum_\sigma^N\mu^\sigma, \quad \mathcal{D}_{\sigma\varsigma} = \frac{3(m_\sigma+m_\varsigma)}{16pm_\sigma m_\varsigma}\frac{(k_BT)^2}{\Omega_{\sigma\varsigma}^{(1,1)}}$$

Where k_B is the Boltzmann constant, T the temperature, m_σ the mass of the component σ, x_σ **the mole fraction** and Ω-integrals have the same definition as in [2] and depend on the temperature and the molecular proprieties based on the Lennard-Jones potential.

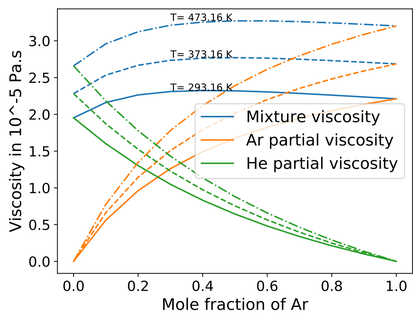

Figure 1: Viscosity of a *Ar* - *He* mixture

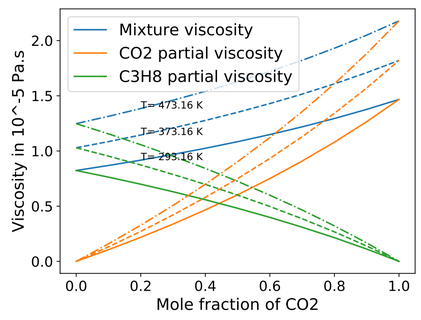

Figure 2: Viscosity of a CO_2 - C_3H_8 mixture

Limit expression: decay of a sinusoidal density wave

For binary equimolar mixture with negligible convection, the flow dynamics are essentially governed by diffusion and equivalent equations **reduce to a diffusion equation**. Measured diffusion coefficients is then compared to the theoretical values [4].

$$\rho^\sigma(x,t) = \rho^{mean} + \delta\sin(kx)\exp\left(-k^2\mathcal{D}t\right)$$

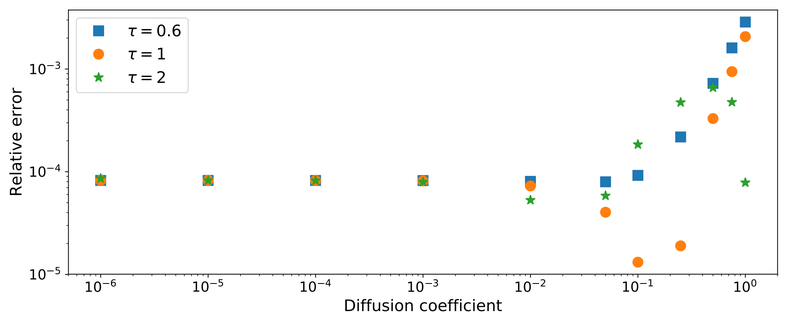

Figure 3: Relative error of the diffusion coefficient

Perspectives

- Different molar mass
- Three and more species
- More validation test-cases
- Chemical reactions: source/sink terms and temperature

Simulation of the viscous fingering instability

Viscous fingering instability occurs when a less viscous fluid displaces a more viscous one.

Macro-scale simulation:

$\Delta x \gg$ **pore length**

- Partial bounce-back [5] : $f_\alpha^{coll} = (1-n_s)\times\mathcal{C}oll + n_s\times f_{opp}$
- $n_s^\sigma[i,j] = \nu^\sigma/(2K+\nu^\sigma)$ where K is the permeability of the medium.

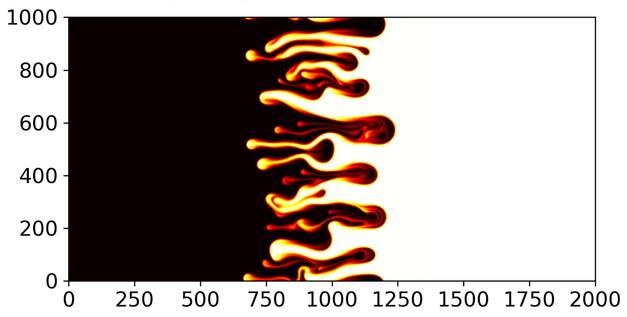

Figure 4: Macro-scale

Pore-scale simulation:

$\Delta x <$ **pore length**

- Diameter of the pores: 16 Lu
- Standard bounce-back with MRT formulation [6]
- Emergence of asymmetric patterns in the mixing zone

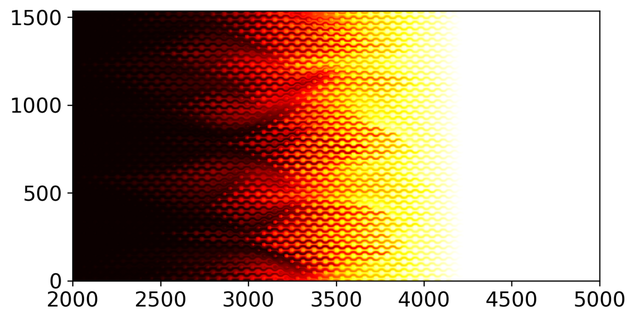

Figure 5: Pore-scale

References

[1] P. J. A. M. Kerkhof and M. A. M. Goeboers. "Toward a unified theory of isotropic molecular transport phenomena". In: *AIChE Journal* 51 (1 2005), pp. 79–121.

[2] Hirschfelder, Curtiss, and Bird. *Molecular theory of gases and liquids*. 1965.

[3] Z. Guo, C. Zheng, and B. Shi. "Discrete lattice effects on the forcing term in the lattice Boltzmann method". In: *Physical Review E* 65.046308 (2002).

[4] P. Asinari. "Multiple-relaxation-time lattice Boltzmann scheme for homogeneous mixture flows with external force". In: *Physical Review E* 77.056706 (2008).

[5] S. D.C. Walsh, H. Burwinkle, and M. O. Saar. "A new partial-bounceback lattice-Boltzmann method for fluid flow through heterogeneous media". In: *Computers & Geosciences* (2009).

[6] C. Pan, L. Luo, and C. T. Miller. "An evaluation of lattice Boltzmann schemes for porous medium flow simulation". In: *Computers & Fluids* (2006).

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