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A novel numerical strategy for mesoscale species transport with the lattice Boltzmann method

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Abstract
Addressing the global challenge of climate change necessitates reducing greenhouse gas emissions, with CO_2 transportation and sequestration playing pivotal roles in mitigating economic and environmental impacts. The integration of these processes within the oil and gas industry, particularly in enhanced oil recovery techniques, underscores the importance of minimizing CO_2 leakage and optimizing recycling rates. However, effective implementation encounters hurdles in mass transport over long distances and secure underground storage. The lattice Boltzmann method (LBM) emerges as a promising solution, offering efficient modeling of CO_2 transport and sequestration at the mesoscale. Leveraging Kinetic Theory, LBM provides a versatile approach to simulate fluid flow, accounting for complex interactions and thermodynamic principles. This study proposes a forcing term correction in LBM to ensure accurate representation of mass transport phenomena, validated through simulations of Couette flow with suction-injection. The inclusion of this term enables precise recovery of both the Navier-Stokes and Maxwell-Stefan equations, enhancing the reliability of LBM simulations for diverse engineering applications.

Keywords
Miscible mixtures; mass transport; Maxwell-Stefan.

Introduction
As the world grapples with the impacts of climate change, reducing greenhouse gas emissions has become a global priority. Specifically, CO_2 transportation and sequestration play vital roles in addressing both economic and environmental challenges associated with carbon emissions [1]. In the context of the oil and gas industry, this process is closely linked to enhanced oil recovery techniques, where CO_2 is injected into oil reservoirs to extract additional oil [2], in which the minimization of CO_2 leakage into the reservoir and optimization of CO_2 recycling rates are desired [1,2]. However, the effective implementation of CO_2 transportation and sequestration faces significant challenges, particularly in mass transport over long distances and the safe and secure storage of large volumes of CO_2 underground. The lattice Boltzmann method (LBM) emerges as a potential strategy to address these challenges. By simulating fluid flow and transport processes at the mesoscale, LBM offers a versatile and efficient approach to modeling CO_2 transport and sequestration, enabling researchers and engineers to optimize transport networks and storage strategies for maximum efficiency and environmental benefit [3].
Based on Kinetic Theory, LBM represents a mesoscopic approach to model transport phenomena, where the fluid is modeled as a collection of fictitious particles moving and interacting on a discrete lattice [4]. This approach offers simplicity and ability to incorporate thermodynamics modeling to fluid flow. By simulating the streaming and collision processes of these particles, LBM can accurately capture the macroscopic behavior of the fluid, making it widely applicable in engineering. Its versatility and computational efficiency have made the LBM a popular choice for studying fluid flow phenomena ranging from simple flow patterns to highly complex multiphase and multiscale systems [5].
Implementing models in LBM for mass transport of multicomponent miscible mixtures requires ensuring physical consistency. Specifically, multicomponent effects must be taken into account to accurately capture the behavior of the mixture. Merely relying on passive scalar or interaction forces strategies alone is insufficient, as they may lack consistency. Passive scalar models are suitable only for modeling mass transport in diluted mixtures, while interaction forces are primarily used for segregation and agglomeration of species [6]. In contrast, this study adopts rigorous kinetic-based models for particle collisions, enabling consistent mesoscale mass transfer simulations. Incorporating these models allows LBM to accurately represent complex interactions, offering

reliable insights for scientific and engineering applications.

In this work, we propose a forcing term correction in LBM to accurately recover the Navier-Stokes equation without spurious terms and enable the incorporation of species forcing contributions for mass transport modeling. This forcing term was validated by implementing the Couette flow with suction-injection.

Methodology

The lattice Boltzmann equation (LBE) describes the evolution of the density distribution function f_α^i in the discrete space $\mathbf{x}$, time t, and velocity $\mathbf{e}_\alpha^i$,

$$f_\alpha^i(\mathbf{x}+\mathbf{e}_\alpha^i\delta t, t+\delta t) = f_\alpha^i(\mathbf{x},t) + \left[\Omega_\alpha^i(\mathbf{x},t) + \left(1 - \frac{1}{2\tau_i}\right) S_\alpha^i(\mathbf{x},t)\right]\delta t \ , \quad (1)$$

where i represents the species, α the orientation in the discrete domain, and Ω_α^i and S_α^i the collision and forcing terms, which are responsible for inserting the relaxation dynamics to the equilibrium.

Here, we adopt the explicit velocity-difference model, which, based on the Sirovich original collisional model [7], assumes $\Omega_\alpha^i = \Omega_\alpha^{ii} + \sum_{j\neq i}^N \Omega_\alpha^{ij}$, where the self- and cross-collision terms accounting for collisions between identical (i-i) and different particles (i-j) are

$$\Omega_\alpha^{ii}(\mathbf{x},t) = -\frac{1}{\tau_i}\left(f_\alpha^i - f_\alpha^{i(0)}\right) \ , \quad (2)$$

$$\Omega_\alpha^{ij}(\mathbf{x},t) = -\frac{1}{\tau_{ij}}\left(\frac{\rho_j}{\rho}\right)\frac{f_\alpha^{i(eq)}}{c_{s,i}^2}(\mathbf{e}_\alpha^i - \mathbf{u})\cdot\left(\mathbf{u}_i^{eq} - \mathbf{u}_j^{eq}\right). \quad (3)$$

The parameters τ_i and τ_{ij} are the relaxation times related to the viscosity and mass transfer coefficient.

Due to the discretization following a second-order Hermite expansion, the achieved equilibrium distribution functions based on the Maxwell-Boltzmann distributions are

$$f_\alpha^{i(0)}(\mathbf{x},t) = \left[1 + \frac{1}{c_{s,i}^2}(\mathbf{e}_\alpha^i - \mathbf{u})\cdot\left(\mathbf{u}_i^{eq} - \mathbf{u}\right)\right] f_\alpha^{i(eq)} \ , \quad (4)$$

$$f_\alpha^{i(eq)}(\mathbf{x},t) = \omega_\alpha \rho_i \left[1 + \frac{\mathbf{e}_\alpha^i\cdot\mathbf{u}}{c_{s,i}^2} + \frac{(\mathbf{e}_\alpha^i\cdot\mathbf{u})^2}{2c_{s,i}^4} - \frac{\mathbf{u}^2}{2c_{s,i}^2}\right] , \quad (5)$$

where $c_{s,i}^2$ is the sound speed related to species i and ω_α are lattice weights.

At the end of each time step, the species density ρ_i and the species equilibrium velocity $\mathbf{u}_i^{eq}$ are computed through the zeroth- and first-order moments of f_α^i,

$$\rho_i(\mathbf{x},t) = \sum_\alpha f_\alpha^i(\mathbf{x},t) \ , \quad (6)$$

$$\mathbf{u}_i^{eq}(\mathbf{x},t) = \frac{1}{\rho_i(\mathbf{x},t)}\sum_\alpha \mathbf{e}_\alpha^i f_\alpha^i(\mathbf{x},t) + \frac{\delta t}{2}\mathbf{F}_i \ , \quad (7)$$

which allows to further compute the mixture density $\rho = \sum_i \rho_i$ and the mixture velocity $\mathbf{u} = \sum_i \mathrm{w}_i \mathbf{u}_i^{eq}$, where w_i is the mass fraction of species i.

After performing a perturbation analysis of the LBE through the Chapman-Enskog expansion, we found out that the forcing term S_α^i must be given by

$$S_\alpha^i = \omega_\alpha \frac{\mathbf{e}_\alpha^i}{c_{s,i}^2}\cdot\mathbf{F}_\mathrm{i} + \omega_\alpha\left[\frac{(\mathbf{e}_\alpha^i\mathbf{e}_\alpha^i - c_{s,i}^2\mathbf{I})}{\left(1-\frac{\delta t}{2\tau_i}\right)c_{s,i}^4}\cdot\mathbf{u}\right]\cdot\sum_{j\neq i}^N \frac{\rho_i\rho_j}{\rho\tau_{ij}}\left(\mathbf{u}_i^{eq} - \mathbf{u}_j^{eq}\right) \quad (8)$$

to fully recover both the Navier-Stokes equation, devoid of any spurious terms, and the Maxwell-Stefan equation with species forcing contributions $\mathbf{F}_\mathrm{i}$. Specifically, the term responsible for eliminating the spurious term is the final term in Eq. (8). In this work, this term is validated by implementing the Couette flow problem with suction-injection, represented in Fig. (1).

In this benchmark, a fluid is compelled to flow with a velocity u_0 towards impermeable walls separated by a distance H. The top wall is moving to the right with velocity U_x. The mass fractions of species 1 (binary mixture) are fixed as w_{1_b} and w_{1_t} in the bottom and top walls. Here, we set $\mathrm{w}_{1_b} = 0.1$ and $\mathrm{w}_{1_t} = 0.9$. u_0 is adjusted to accommodate different conditions of Reynolds number ($Re = u_0H/\nu$) and Péclet number ($Pe = u_0H/D_{12}$), where ν is the kinematic viscosity and D_{12} is the binary diffusion coefficient. The analytical solutions of the velocity and concentration profiles read

$$\frac{u_x(y)}{U_x} = \frac{exp\left(\frac{Re\, y}{H}\right)-1}{exp(Re)-1} \ , \quad (9)$$

$$\frac{\mathrm{w}_1(y)-\mathrm{w}_{1_b}}{\mathrm{w}_{1_t}-\mathrm{w}_{1_b}} = \frac{exp\left(\frac{Pe\, y}{H}\right)-1}{exp(Pe)-1}. \quad (10)$$

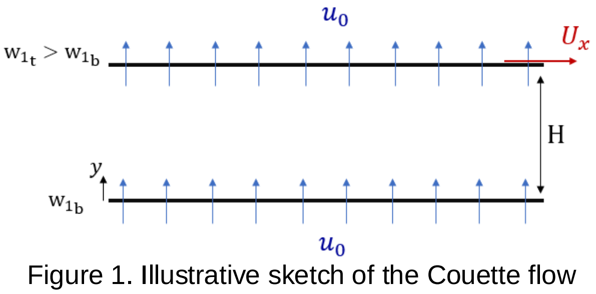

Figure 1. Illustrative sketch of the Couette flow with suction-injection.

Results and Discussion

The LBM simulations were evaluated with and without the forcing term, and both sets of simulations exhibited close agreement with the steady-state concentration and velocity profiles for the Couette flow with suction-injection, as illustrated in Fig. (2) for Re = 100 and Pe = 20. No significant differences were observed between the cases with and without the forcing term. However, this result was anticipated, as in the steady-state (equilibrium), the species velocities align ($\mathbf{u}_i^{eq} \rightarrow$

$\mathbf{u}_j^{eq}$ and $\Omega_\alpha^{ij} \to 0$), setting the last term of Eq. (8) to zero. Hence, the transient profiles should be compared to comprehensively assess the impact of the forcing term.

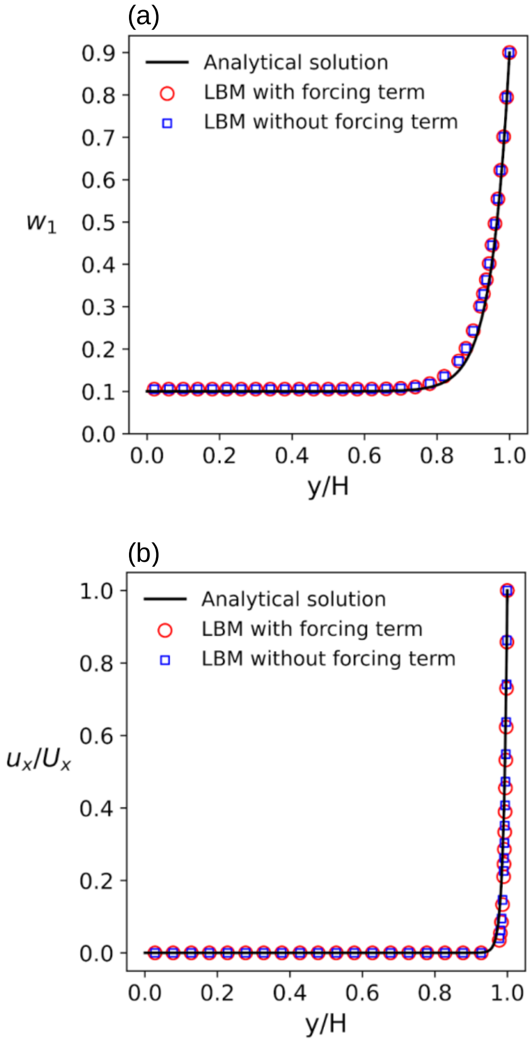

Figure 2. Steady-state (a) concentration and (b) velocity profiles of the Couette flow with suction-injection for Re = 100 and Pe = 20.

Concentration and velocity profiles for simulations with and without forcing terms were compared for Re = 50, Re = 100, and Re = 200, maintaining a fixed Pe = 20. Figs. (3) and (4) depict the concentration and velocity profiles, respectively, over time. The concentration profiles remain identical regardless of the presence of forcing terms at all evaluated time points. This suggests that the forcing term The forcing term maintains mass conservation and preserves the dynamic behavior of mass transfer.

Fig. (4) reveals there are no significant differences observed in the velocity profiles during the transient regime either. Only slight deviations were noted upon reaching steady-state ($t^* = 1$), as also depicted in Fig (2)b. As the Re increases, the velocity profiles become steeper, making it numerically challenging to verify and compare between simulated cases. However, within the evaluated range of Re, no significant differences were observed. Despite the lack of noticeable discrepancies between simulations with and without the forcing term during the transient regime, its inclusion remains crucial for algebraically eliminating spurious terms.

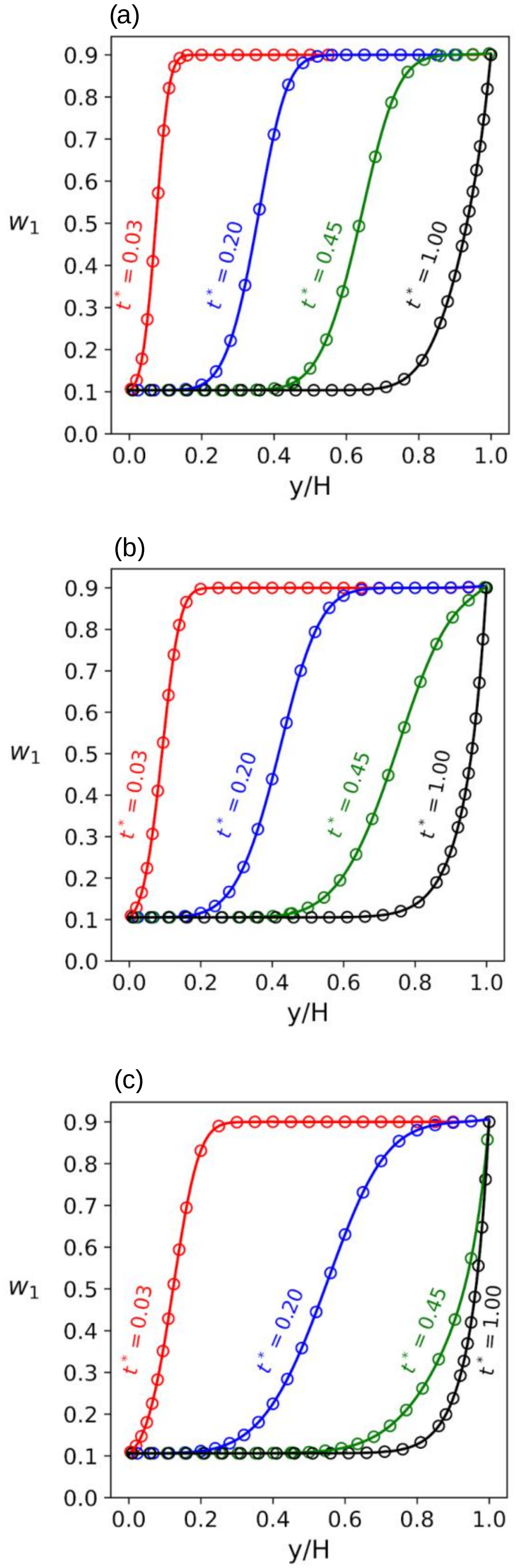

Figure 3. Transient concentration profiles of the Couette flow with suction-injection for Pe = 20 and (a) Re = 50, (b) Re = 100, and (c) Re = 200. t^* represents a normalized time relative to the duration required to attain steady state.

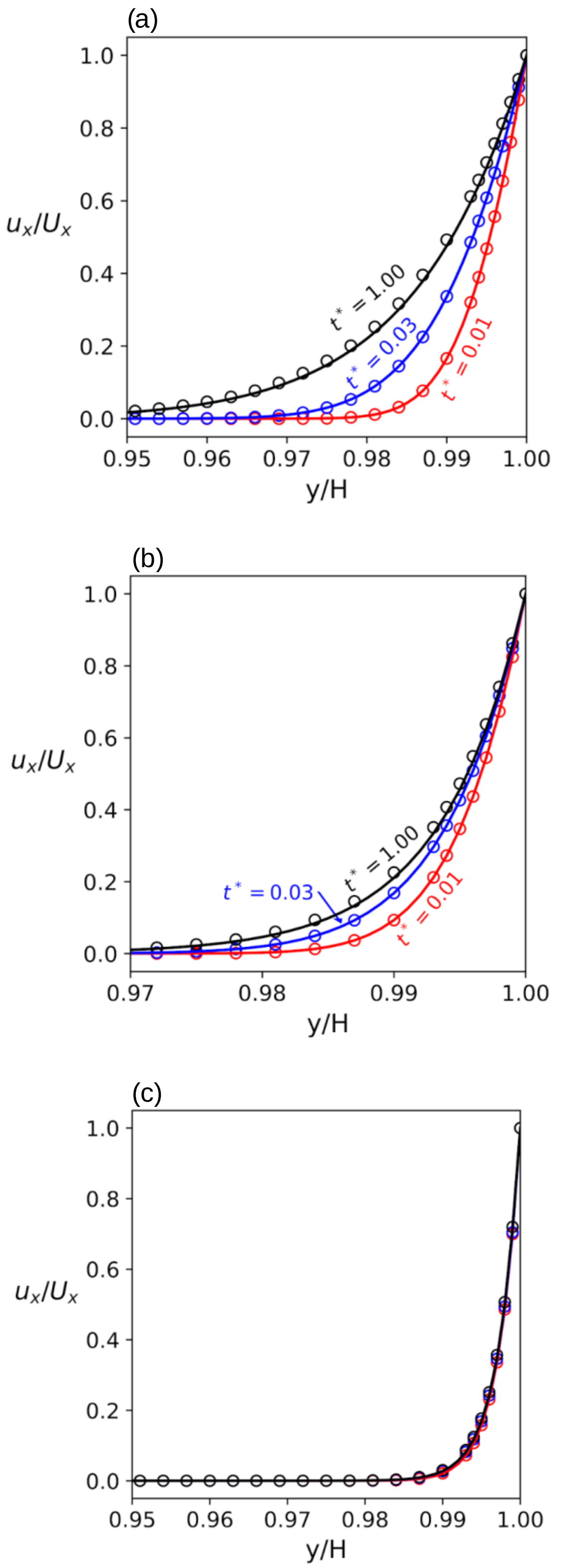

Figure 4. Transient velocity profiles of the Couette flow with suction-injection for Pe = 20 and (a) Re = 50, (b) Re = 100, and (c) Re = 200. t^* represents a normalized time relative to the duration required to attain steady state.

Conclusions

In this study, a forcing term is introduced to accurately recover both the Navier-Stokes equation, devoid of spurious terms, and the Maxwell-Stefan equation with additional forcing contributions. The term in the proposed model responsible for eliminating spurious contributions was validated through the Couette flow problem with suction-injection, resulting in precise outcomes for the steady-state. Although no significant differences were observed between the simulations with and without this term in the transient regime for the considered Re range, its inclusion remains essential for algebraically eliminating the spurious terms.

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Responsibility Notice

The authors are the only responsible for the paper content.

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