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Research highlight

Lattice Boltzmann pseudopotential multiphase modeling of transcritical CO_2 flow using a crossover formulation

Assetbek Ashirbekov[1], Bagdagul Kabdenova[1], Alibek Kuljabekov[1], Ernesto Monaco[2], Lei Wang[3], Luis Rojas-Solórzano[1]*

[1]Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan

[2]Engineering Software Steyr, Steyr 4400, Austria

[3]State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, College of Energy, Chengdu University of Technology, Chengdu 610059, P. R. China

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Abstract:
This report summarizes our recent implementation of a crossover formulation in the lattice Boltzmann method and its application in modeling transcritical CO_2 sequestration in water-saturated porous media. A crossover enhancement of the Peng-Robinson equation of state increases the accuracy in predicting fluid properties in transcritical conditions, which is relevant in modeling CO_2 sequestration. The crossover formulation leads to the prediction of liquid-vapor coexistence curves closer to experimental data. The formulation was validated with several tests and applied to model the displacement of H_2O with CO_2 in a homogeneous porous medium in multiple conditions. This investigation provides a promising strategy for improving the accuracy of the lattice Boltzmann method in modeling transcritical CO_2 sequestration in aquifers using realistic transcritical conditions.

Carbon dioxide (CO_2) emission is one of the top contributors to global warming. Greenhouse gas emissions from burning fossil fuels for energy and cement production reached over 34 gigaton of CO_2 annually (Ritchie et al., 2020). Thus, capture and sequestration of CO_2 in deep aquifers under transcritical conditions can help to attenuate climate change.

Accurately modeling the transcritical CO_2 injection in a saturated porous medium will facilitate this technology. However, one of the complications of CO_2 sequestration is the low critical temperature of CO_2, around 31 °C, meaning that the process goes in supercritical or near-critical conditions, with fluid properties changing drastically from standard conditions. Previous works in the field applied classical equation of states (EoS) using the lattice Boltzmann method (LBM), which works well for fluid properties in subcritical conditions but deviates considerably near critical conditions due to the large fluctuations in density (Nikolai et al., 2019). A crossover formulation, which uses non-analytical scaling, initially proposed by Kiselev and Ely (2004), can be utilized to increase LBM's accuracy when modeling CO_2 in transcritical conditions.

The present work summarizes the outcomes obtained after incorporating a crossover formulation into Peng-Robinson (P-R) EoS (Kabdenova et al., 2021) for a two-dimensional (2D) LBM model. The introduced EoS is a hybrid formulation, including analytical and non-analytical solutions for transcritical conditions. It uses non-analytical scaling laws asymptotically closer to the critical point and transforms into the regular classical EoS in regions far below the critical point. When applied to model a 2D static droplet (Fig. 1(a)), it yielded more accurate results, compared to regular P-R EoS, with better

*Corresponding author.
E-mail address: assetbek.ashirbekov@nu.edu.kz (A. Ashirbekov); bagdagul.dauyeshova@alumni.nu.edu.kz (B. Kabdenova); alibek.kuljabekov@nu.edu.kz (A. Kuljabekov); ernesto.monaco@essteyr.com (E. Monaco); wanglei@cdut.edu.cn (L. Wang).
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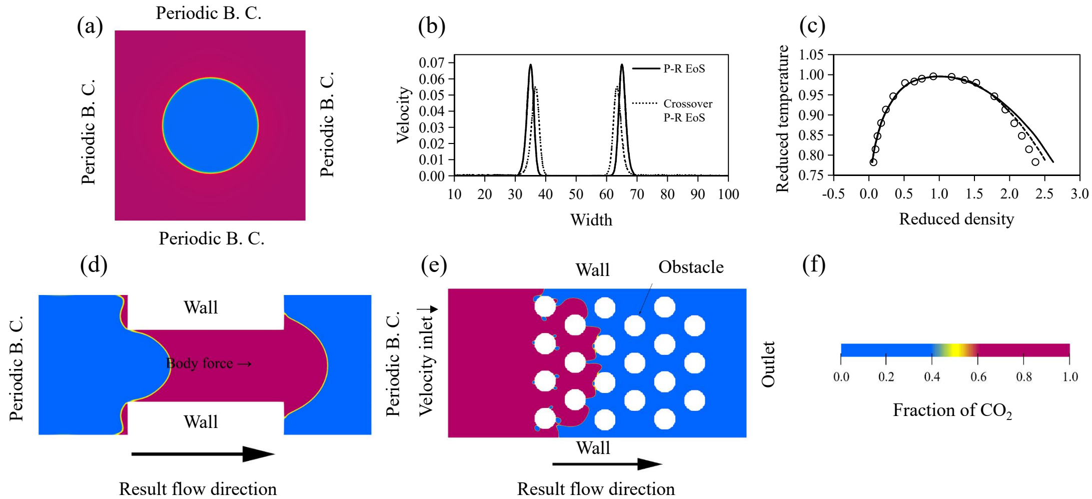

Fig. 1. (a) CO_2 in red surrounding a H_2O droplet in blue, (b) the magnitude of spurious currents at the phase interface, (c) comparison of coexistence curves for CO_2 obtained from P-R EoS (solid curve) and crossover P-R EoS (dashed curve) with experimental data (circles), (d) CO_2 penetration into a narrow channel initially filled with H_2O after the capillary pressure is overcome, (e) CO_2 displacing H_2O in an artificial porous medium. (Lattice units are used)

evaluation of surface tension due to reduced magnitude of spurious, unphysical currents around the boundary, at least in the explored conditions (Fig. 1(b)). The crossover model predicts vapor-liquid coexistence curves for CO_2 and H_2O more accurately than regular P-R EoS (Fig. 1(c)), with consistently lower root mean square errors compared to experimental data by Harris and Yung (1995).

The model was validated by reproducing a suspended droplet to verify the immiscibility of the two fluids (Fig. 1(a)) (Ashirbekov et al., 2021). The contact angle was controlled through the coefficient of wall interaction force and verified using a sessile droplet setup. The capillary pressure was validated by forcing the CO_2 flow through a narrow channel, as shown in Fig. 1(d). The validated model was used to simulate the CO_2 injection into a 2D homogeneous water-saturated porous medium driven by a pressure gradient, as shown in Fig. 1(e). The effect of the inlet velocity profile is studied, revealing the water displacement sensitivity to boundary conditions. Future work on crossover formulation can focus on the effect of contact angle, viscosity, and density ratios on the flow.

In summary, modeling transcritical CO_2 and water interactions using LBM gives significant insight into mesoscale CO_2 sequestration. Key novelties introduced here include:

- EoS crossover formulation for accurate, transcritical regime modeling.
- Procedure for validation using stationary suspended droplet and flow through a capillary channel.
- Combination of these studies in model of porous medium.

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Additional information: Author's email

luis.rojas@nu.edu.kz (L. Rojas-Solórzano).

Conflict of interest

The authors declare no competing interest.

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