An improved multicomponent pseudopotential lattice Boltzmann method
for immiscible fluid displacement in porous media

M. Sedahmed†(1), R. C. V. Coelho (2,3), H. A. Warda (1)

(1) Mechanical Engineering Department, Alexandria University, Alexandria 21544, Egypt.
(2) Centro de Física Teórica e Computacional, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal.
(3) Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal.

*Corresponding author email: mahmoud.sedahmed@alexu.edu.eg

Abstract

In this work, we introduce an improved multicomponent (MC) pseudopotential lattice Boltzmann method (LBM) for the simulation of immiscible fluids displacement in porous media. The model is based on a set of recent developments from the literature in addition to a newly introduced treatments of the pressure boundary conditions at the inlet and outlet. It is shown that the model provides several favorable features such as realistic viscosity ratio and independent tuning of surface tension from the viscosity ratio. Additionally, the model is shown to suppress a non-physical behavior of the original MC pseudopotential model in which changes of entrapped fluids volumes are observed during displacement processes. The model is characterized using the Laplace and contact angle tests. Then we show that the model provides stable and satisfactory results for immiscible fluids displacement. Moreover, primary drainage and imbibition displacement processes were simulated in a heterogeneous porous medium. The simulation results showed that the introduced model was able to correctly capture many physical phenomena of oil-water displacements in porous media. Irreducible water and residual oil saturations resulted from the simulations are comparable to
realistic values. The displacement processes were simulated at different wetting conditions and the results were in good agreement with experimental results.

**Keywords**

Lattice Boltzmann Method,
Multicomponent pseudopotential,
Wetting,
Primary drainage,
Imbibition,
Capillary pressure bump.
1. INTRODUCTION

Multicomponent fluid flows are abundant in many natural and industrial systems. Major challenges of the twenty-first century are providing clean water and sufficient energy supplies for the world population, which both have a common scientific underpinning: multicomponent fluid flows in porous media [1], which consist of different immiscible chemical species such as oil and water. These types of flows have been studied extensively due to their economic importance. A practical example of multicomponent fluid flow is the recovery and enhanced recovery of petroleum from underground reservoirs [2]. Petroleum recovery has a major impact on the world energy demand and on the current energy crisis making it a critical application with global impact. Understanding of petroleum recovery relies on the study of fluids flow through porous rocks, which is confronted with many challenges such as the sophisticated underlying physics of multicomponent flows in such complicated geometries. A branch of science named Petroleum engineering was dedicated for dealing with such challenges relying on fundamentals of Fluid mechanics and focusing on tackling the challenges on the petroleum reservoir scale (meters to kilometers) [2]. However, many of these challenges and physical phenomena are originated in the pore scale (micrometers) where the different fluid components interact with each other and still could be described using fundaments of Fluid mechanics but from a different perspective [1].

For years, understanding of multicomponent fluid flow in petroleum reservoirs relied on laboratory experiments that mimic the different displacement processes of immiscible fluids. For example, Special Core Analysis (SCAL) is a group of experiments that quantify vital fluid and rock properties that are used for describing petroleum flow in reservoirs [3]. Many relationships are established using SCAL such as capillary pressure-saturation curves and relatively permeability curves. Such relationships are essential for quantifying petroleum behavior in reservoirs on its scale. However, they are originated from flow behaviors on the
pore scale. Despite being the standard method of quantifying such relationships, SCAL experiments are expensive and time consuming, which adds an additional challenge in petroleum reservoir management and decision-making hierarchy. With recent advances in image processing, computational power, and numerical models, such experiments could be replicated numerically [1]. In this work, we focus on a numerical model to describe multicomponent fluid flows in porous media, and we introduce a treatment for inlet and outlet boundary conditions that would be shown to be resulting in stable and satisfactory results for multicomponent fluids flow simulations. In the literature, different models have been used for such task with the most used approach being the Lattice Boltzmann Method (LBM) [4]. LBM originated in molecular dynamics (lattice gas automata), was enhanced by statistical mechanics, and is currently being used in Computational Fluid Dynamics (CFD) [5] [6] [7] [8]. LBM is based on a mesoscopic scale approach, which allows the method to capture physical phenomena on the microscale and translate them into macroscale parameters, within manageable and efficient use of computer resources. Several reviews of the LBM and its application were published in recent years that provide an insight into the capabilities of the LBM in multicomponent and multiphase flow applications [9] [10] [11]. Also, several textbooks were published that provide comprehensive explanation for LBM bases and algorithms [8] [12].

In the past three decades several LBM models were developed for simulating multicomponent fluid flow problems, with the following three being the most popular: color gradient model [13], free energy model [14] and pseudopotential model [15]. In this work, we use the pseudopotential model, which is also known in the literature as the Shan Chen model. There are mainly two versions of it: the single component multiphase (SCMP) pseudopotential and the multicomponent multiphase (MCMP) pseudopotential model [12], with the multicomponent (MC) pseudopotential model as a special case of the MCMP model.
Several authors in the literature used the multicomponent pseudopotential model to simulate immiscible fluids displacement for different applications. Since the early days of the LBM and the introduction of the MCMP pseudopotential model, it was used drainage and imbibition processes in 3D porous medium which was reconstructed from a microtomography image of a Fontainebleau sandstone [16]. Pan et al. [17] simulated two-phase flow in a porous medium comprised of a synthetic packing with a relatively uniform distribution of spheres and they achieved good agreement between the measured hysteretic capillary pressure-saturation relations and the LBM simulations when comparing entry pressure, displacement slopes, irreducible saturation, and residual entrapment. Schaap et al. [18] used the MCMP pseudopotential model to simulate displacement processes in a glass bead porous medium obtained from computed tomography and compared the numerical results with experimental results in a quantitate manner. Porter et al. [19] investigated the hysteresis in the relationship between capillary pressure $P_c$ and wetting phase saturation $S_w$ between the drainage and imbibition processes in a similar porous medium and showed that the MCMP pseudopotential model captured important physical processes in the experimental system. Zhao et al. [20] simulated two immiscible fluids flow in 2D porous media and analyzed the effects of capillary number (Ca), viscosity ratio (M) and wettability on the relative permeability curves. Dou et al. [21] investigated the effects of capillary number and viscosity ratio on non-uniqueness of the relative permeability – wetting saturation relationships of steady-state immiscible two-phase flow in generated porous media.

Warda et al. [22] simulated the primary drainage and imbibition displacement processes in a 2D generated heterogeneous porous medium and showed that the MCMP pseudopotential was able to capture the capillary pressure bump phenomenon which occurred due to the heterogeneity of the porous medium. Fager et al. [23] presented a digital SCAL workflow based on multiphase LBM simulations to directly simulate an Enhanced Oil Recover (EOR)
technique named Water Alternating Gas (WAG) on a digitized rock geometry and produced relative permeability curves as the result of the displacement simulations. The curves resulted from the simulations on the pore scale using the LBM were used as input data for reservoir simulator to illustrate the impact relative permeability hysteresis has on injectivity at the reservoir scale. M. Nemer et al. [24] investigated the relative importance of the wettability-altered fraction, the degree of wettability alteration, and the accurate contact angle assignment, and their effects on relative permeability and fluid configurations using the MCMP pseudopotential model and they found that the fraction altered, the degree of alteration, and the accurate contact angle assignment are all correlated, and play a role to varying extents in influencing the flow behavior and the resulting relative permeability curves. André Matias et al. [25] extended the lattice Boltzmann model to consider the changes in porous medium due to swelling and erosion, and they analyzed the competition between swelling and erosion and identify a transition between regimes where either swelling or erosion dominate.

The original versions of the pseudopotential suffered from several drawbacks such as limited density ratio (that is critical for multiphase flow problems), limited viscosity ratio (that is critical for multicomponent flow problems), high spurious currents and independent tuning of surface tension (that is harmful to many multicomponent and multiphase flow problems) [10]. Moreover, the original pseudopotential model suffered from non-physical changes in the fluids volume as shown in Ref. [26], such changes in entrapped volumes was shown to be contaminating the results of fluids displacement in porous media [27]. Several studies and advancements were proposed for the SCMP pseudopotential model that greatly enhanced its performance via achieving higher density ratios, approximate thermodynamic consistency, and lower spurious currents [10]. Such enhancements made it one of the best candidates in the literature.
The MCMP pseudopotential model did not receive the same attention as the SCMP despite its importance in many industries, particularly the petroleum one. However, major developments and enhancements were presented in the literature for the MCMP pseudopotential model. Porter et al. [28] introduced a more advanced version of the MCMP model named the Explicit Forcing (EF) model, where external forces were incorporated into the discrete Boltzmann equation via forcing term rather than through an equilibrium velocity shift as in the original pseudopotential model. The EF model was also combined with more advanced schemes such as higher order isotropy interactions [29] and Multiple Relaxation Time (MRT) [30] [31] formulation of the collision operator for better performance. The model resulted in viscosity independent equilibrium densities and could simulate a wide range of kinematic viscosity ratios (1000 when combined with higher order isotropy and MRT formulations). Recently, Zhao et al. [32] provided a modified version of the EF model that correctly recovers the Navier-Stokes equations with the Single Relaxation Time (SRT) approximation when the viscosity ratio is not the unity. Such a model is favorable due to the simplicity of the SRT approximation and its lower computational cost. The model was reported to achieve a stable viscosity ratio of 250 using the SRT approximation and 4th order isotropy [32].

Although the collision model is the workhorse of the LBM algorithm boundary conditions, as in most numerical models, play a vital role the stability and accuracy of the model. In LBM, macroscopic boundary conditions (e.g., Dirichlet boundary conditions) are not directly implemented as in conventional computational fluid dynamics (CFD) models where the boundary condition value (e.g., fixed velocity or pressure) is directly implemented in the equations. A conversion technique is needed to construct a relationship between the macroscopic boundary condition value to be implemented and the basic unit of the LBM which is the particle distribution function. A widely used technique for such conversion is the scheme proposed in Ref. [33] and known as the Zou-He technique. However,
multicomponent flow problems would need additional treatments to accommodate the flow of different components and achieve stable results, which is a challenging task. To overcome this difficulty, many studies in the literature follow alternate techniques to drive the flow other than with inlet and outlet boundary conditions, as, for example, using an external body force on the flow domain to drive the flow with periodic conditions (e.g., [20]). Moreover, very few studies included stable treatments for open boundary conditions for multicomponent flow problems. An example is the work of Hou et al. [34] where a new multiphase open boundary condition was proposed to enable fluid droplets to pass the outlet boundary naturally and without deformations.

Since we are concerned with the immiscible fluids flow displacement in porous media, the wetting boundary condition is expected to have a major role and greatly affect the results. A recent wetting boundary condition for the MCMP pseudopotential model known as the Improved Virtual Density (IVSD) model was developed [35] and it was shown to be more accurate than the original technique used in the pseudopotential model to consider fluid-solid interfaces, especially in complex geometries such as porous media.

To conclude this section, it could be observed from the previous literature review that the pseudopotential model could be a good candidate for simulating immiscible fluids displacement in porous media, however its original version suffered from several drawbacks that need special treatments to provide reliable results.

In this work, we present an improved pseudopotential model based on a set of enhancements and special treatments that would be shown to alleviate many of the drawbacks of the previous pseudopotential models in the literature. The presented model is based on the modified EF model with SRT approximation [32] (section 2.1), combined with the IVSD scheme for wetting boundary conditions [35] (section 2.2) and newly introduced inlet and outlet boundary condition treatments (section 2.3). The presented model alleviates many
drawbacks of the original pseudopotential model, suppresses several negative behaviors, and
provides several favorable features such as wide range of viscosity ratio, independent tuning
of surface tension, stable volume of fluids and a reasonable computational cost, making it a
good tool for immiscible fluids flow simulations in porous media.

The remainder of this manuscript is organized as follows. In section 2, we present the
numerical model and boundary conditions. In section 3, we provide extensive numerical tests
for the model using widely used benchmarks from the literature. In section 4, we provide
numerical results and interpretations for simulations of immiscible fluids displacement
processes over an obstacle and in a heterogeneous porous medium. Moreover, we provide
qualitative comparisons with well-known physical phenomena that occur in oil-water systems
in petroleum reservoirs. Finally, we provide a concise summary in section 5.
2. METHODOLOGY

2.1. Multicomponent lattice Boltzmann method

In this work, we employ the multicomponent pseudopotential LBM with modified explicit forcing (EF) term and the SRT approximation of the collision operator [32].

The discretized Lattice Boltzmann Equation (LBE) for this model is written as follows,

\[
\begin{align*}
    f_i^{(\sigma)}(x + e_i \Delta t, t + \Delta t) - f_i^{(\sigma)}(x, t) &= -\frac{1}{\tau_s} \left( f_i^{(\sigma)}(x, t) - f_i^{(\sigma)eq}(x, t) \right) \\
    &\quad + \Delta t \left( 1 - \frac{1}{2\tau_s} \right) S_i^{(\sigma)F}(x, t),
\end{align*}
\]

(1)

where, \( f_i^{(\sigma)} \) is the particle distribution function at position \((x)\) and time \( (t) \), \( \sigma \) is the fluid component number \((\sigma = 1, \ldots n)\). We study only two fluid components, i.e. \( n = 2 \). \( i \) is the lattice direction which belongs to the selected lattice arrangement; Here we use the \( D_2Q_9 \) lattice arrangement for 2D simulations \((i = 0, 1, \ldots 8)\). \( f_i^{(\sigma)eq} \) is the equilibrium distribution function and it is given by,

\[
\begin{align*}
    f_i^{(\sigma)eq}(x) &= w_i \rho^{(\sigma)} \left[ 1 + \frac{e_i \cdot u^{eq}(x)}{c_s^2} + \frac{(e_i \cdot u^{eq}(x))^2}{2c_s^4} - \frac{u^{eq}(x) \cdot u^{eq}(x)}{2c_s^2} \right],
\end{align*}
\]

(2)

where, \( c_s \) is the lattice sound speed and it is defined as \( c_s = \frac{\Delta x}{\sqrt{3} \Delta t} \). \( \Delta x \) and \( \Delta t \) are commonly chosen as unity in the LBM, \( w_i \) and \( e_i \) are the lattice weights and the discrete velocity vector in the \( i^{th} \) direction of the selected lattice arrangement, which are defined for \( D_2Q_9 \) by,

\[
\begin{align*}
    e_i &= \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \ \end{bmatrix}, \\
    w_i &= \begin{bmatrix} 4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 36 \ 9 & 9 & 9 & 9 & 9 & 36 & 36 & 36 & 36 \ \end{bmatrix}.
\end{align*}
\]

The macroscopic fluid component density, velocity, and mixture (total) density are defined by,

\[
\begin{align*}
    \rho^{(\sigma)}(x) &= \sum_i f_i^{(\sigma)}(x), \\
    u^{(\sigma)}(x) &= \frac{1}{\rho^{(\sigma)}(x)} \sum_i e_i f_i^{(\sigma)}(x),
\end{align*}
\]

(3)
\[\rho(x) = \sum_{\sigma} \rho^{(\sigma)}(x).\]  
(5)

The system relaxation time \(\tau_s\) is defined as:

\[\tau_s(x) = \frac{\sum_{\sigma} \rho^{(\sigma)}(x) v^{(\sigma)}}{\rho(x) c_s^2 \Delta t} + \frac{1}{2},\]  
(6)

where, \(v^{(\sigma)}\) is the kinematic viscosity of the \(\sigma^{th}\) fluid component,

\[v^{(\sigma)} = c_s^2 \left( \tau^{(\sigma)} + \frac{1}{2} \right) \Delta t,\]  
(7)

where, \(\tau^{(\sigma)}\) is the relaxation time of the \(\sigma^{th}\) fluid component.

The system relaxation time \(\tau_s\) is used to reduce the instability in the collision model due to the abrupt change of the viscosity across the interface in case the viscosity ratio is not unity, since the value of \(\tau_s\) will change smoothly between the regions of different fluid components across the interface.

The equilibrium velocity \(u^{eq}\) reads:

\[u^{eq}(x) = \frac{\sum_{\sigma} \rho^{(\sigma)}(x) u^{(\sigma)}(x)}{\sum_{\sigma} \rho^{(\sigma)}(x) \tau_s(x)}.\]  
(8)

Also, the common velocity of the two fluids is defined as:

\[u(x) = u^{eq}(x).\]  
(9)

The forcing term in the LBE equation \(S_{i}^{(\sigma),F}\) is defined as follows,

\[S_{i}^{(\sigma),F}(x) = W_i \left( \frac{e_i \cdot P^{(\sigma),tot}(x)}{c_s^2} \right) \]  

\[+ \frac{(e_i e_i - c_s^2 I) : \left( u^{eq}(x) P^{(\sigma),tot}(x) + P^{(\sigma),tot}(x) u^{eq}(x) \right)}{2 c_s^4},\]  
(10)

which can be rewritten as:
\[ S_i^{(\sigma),F}(x) = w_i \left( \frac{e_i - u_i^e(x)}{c_s^2} + \frac{e_i \cdot u_i^e(x)}{c_s^4} e_i \right) F^{(\sigma),\text{tot}}(x). \] (11)

\[ F^{(\sigma),\text{tot}} \] is the total force exerted on the \( \sigma^{th} \) fluid component and it is defined for the pseudopotential model by,

\[ F^{(\sigma),\text{tot}} = F^{(\sigma),f-f} + F^{(\sigma),f-s} + F^{(\sigma),b}, \] (12)

where, \( F^{(\sigma),f-f} \) is the fluid-fluid interaction force of the \( \sigma^{th} \) fluid component and it is defined by,

\[ F^{(\sigma),f-f}(x) = -G^{(\sigma,\bar{\sigma})}_\text{coh} \psi^{(\sigma)}(x) \sum_i w_i \psi^{(\bar{\sigma})}(x + e_i) e_i, \] (13)

where, \( \psi^{(\sigma)} \) is the pseudopotential of the \( \sigma^{th} \) fluid component. Here we define it as \( \psi^{(\sigma)} = \rho^{(\sigma)} \), \( G^{(\sigma,\bar{\sigma})}_\text{coh} \) is the fluid-fluid cohesion strength and it is used to tune the fluid-fluid interaction force. This parameter is used for tuning the surface tension in the pseudopotential model. It should be noted that only the inter-component interaction force is considered in this work \((\sigma \neq \bar{\sigma})\) while the intra-component interaction force is neglected \((G^{(\sigma,\sigma)}_\text{coh} = 0)\). We set \( G^{(\sigma,\bar{\sigma})}_\text{coh} = 3.5 \) for all cases in this paper.

We point out that at boundary points where non-periodic boundary conditions are applied (e.g., Dirichlet boundary condition), there will be an imbalance in the force summation term of Eq. (13) as the neighbor points located at \((x + e_i)\) will be located outside the domain boundary. In these cases, the missing terms are replaced with duplicates of the terms in the opposite direction \((\bar{i})\) (towards the interior of the domain instead of across the boundary of the domain) [36],

\[ \sum_i w_i \psi^{(\bar{\sigma})}(x + e_i) e_i = \sum_i w_i \psi^{(\bar{\sigma})}(x + e_{\bar{i}}) e_{\bar{i}}. \] (14)
Such a special treatment for interaction forces is essential with application of boundary conditions mentioned in section 2.3.

The external body forces exerted on the \( \sigma^{th} \) fluid component (e.g., gravity) is added using the term \( F^{(\sigma)} \). Several methods in the literature were introduced to incorporate these forces, one is referred to Ref. [10] for different techniques.

In the present pseudopotential model, the pressure is determined as follows

\[
P = c_s^2 \sum_{\sigma} \rho^{(\sigma)} + \frac{c_s^2}{2} \Delta t \sum_{\sigma, \overline{\sigma}} \rho^{(\sigma)} \rho^{(\overline{\sigma})}.
\]

(15)

We express our results in lattice units (l.u.) in which length is represented in lattice length unit \( (\Delta x = 1) \), time is represented lattice time unit in \( (\Delta t = 1) \) and density is also the unit \( (\rho = 1) \).

2.2. Improved virtual solid density scheme: wetting boundary condition

The fluid solid interaction force \( F^{(\sigma)f-s} \) is defined as follows

\[
F^{(\sigma)f-s}(x) = -G^{(\sigma)}_{ads} \psi^{(\sigma)}(x) \sum_i w_i s^{(\overline{\sigma})}(x + e_i)e_i,
\]

(16)

where, \( G^{(\sigma)}_{ads} \) is the fluid-solid adhesion strength and it is used to tune the fluid-solid interaction force (consequently contact angle \( \theta \)) in the original pseudopotential model. In this section, an alternative approach will be shown to tune the contact angle. \( s^{(\overline{\sigma})} \) is the solid pseudopotential of the \( \overline{\sigma} \) fluid component. In this work, the Improved Virtual Solid Density (IVSD) [35] is used to define the solid pseudopotential as:

\[
s^{(\sigma)}(x) = \phi(x) \tilde{\rho}^{(\sigma)}(x),
\]

(17)

where, \( \phi \) is a binary switch function which equals 0 for a fluid node and 1 for a solid node, \( \tilde{\rho}^{(\sigma)} \) is the virtual solid density and it is defined using the averaged density of the fluid:

\[
\tilde{\rho}^{(\sigma)}(x) = \chi^{(\sigma)} \frac{\sum_i w_i \rho^{(\sigma)}(x + e_i)(1 - \phi(x + e_i))}{\sum_i w_i (1 - \phi(x + e_i))}.
\]

(18)
\( \chi^{(\sigma)} \) is a factor that controls the wettability of the \( \bar{\sigma} \) fluid component. If the parameter \( \chi^{(\sigma)} \) is unity, the fluid component is naturally wetting \( (\theta = 90^\circ) \). To control the wettability of the fluid components, the parameter \( \chi^{(\sigma)} \) is selected as follows (only two components are considered in this work, i.e., \( \sigma = 1, 2 \))

\[
\chi^{(1)} = 1 + \xi \\
\chi^{(2)} = 1 - \xi
\]

where, fluid component-1 is forming the droplets and fluid component-2 is the surrounding fluid. Fluid component-1 becomes non-wetting if \( \xi < 0 \) and wetting if \( \xi > 0 \).

Practically, \( G_{ads}^{(\sigma)} \) and \( G_{ads}^{(\bar{\sigma})} \) are set equal to \( G_{coh}^{(\sigma\bar{\sigma})} \) and the wettability is controlled by \( \xi \). Hence, the same equation (Eq. 13) could be used for calculating the interaction forces using the neighboring pseudopotential values for fluid or solid.

It is beneficial to have grouping of fluid wettability based on contact angle. In this work, the grouping shown in Table 1 is used [37] and the contact angle is defined as in section (3.3).

### Table 1. Definitions of wettability based on contact angle measurements.

| Wettability state      | Contact angle (degrees) |
|------------------------|-------------------------|
| Complete water wet     | 0                       |
| Strongly water wet     | 0 – 50                  |
| Weakly water wet       | 50 – 70                 |
| Neutrally wet          | 70 – 110                |
| Weakly oil wet         | 110 – 130               |
| Strongly oil wet       | 130 – 180               |
| Complete oil wet       | 180                     |

**2.3. Inlet and outlet boundary conditions**
The definition and implementation of boundary conditions is critical to most fluid mechanics problems. It greatly affects the simulation results and – if ill defined – could ruin the full simulation [8]. Several boundary conditions were used in this work such as the periodic boundary conditions [8] and half-way bounce back boundary conditions [8]. Simulations of realistic fluid problems would require the definition of other types of boundary conditions such as Dirichlet boundary conditions, i.e., fixed pressure or velocity value. One technique to define a Dirichlet boundary condition is the well-known Zou-He method [33] – also known as non-equilibrium bounce-back (NEBB) method [8] – which provides equations to determine the missing distribution functions at the boundary. The Zou-He method is used here to define pressure boundary conditions where needed. A complete set of equations used in the inlet and outlet boundaries could be found in [33].

In multicomponent problems, it may not be sufficient to define a Dirichlet boundary condition for one of the fluid components at inlet and outlet sides as the density and velocity of the other fluid component would also need to be updated, where such information would be missing from the defined boundary condition. In this section we introduce a boundary condition treatment that resulted in favorable and stable results using the pseudopotential model.

For simulation cases such as in section 4 where it is needed to specify pressure boundary conditions at inlet and outlet sides, the known and missing distribution functions at boundaries for each component could be identified from Figure 1.

Starting with the outlet side, there are two sets of 6 known distribution functions

\[
\left(f_0^{(\sigma)}, f_1^{(\sigma)}, f_2^{(\sigma)}, f_4^{(\sigma)}, f_5^{(\sigma)}, f_8^{(\sigma)} \right)
\]

that their values are updated during the streaming step, and there are two sets of 3 missing distribution functions

\[
\left(f_3^{(\sigma)}, f_6^{(\sigma)}, f_7^{(\sigma)} \right)
\]

that their values are not updated during the streaming step as they would need information from outside the domain boundaries. To apply pressure boundary conditions for the MC model using Zou-He
technique, assuming the main fluid component at outlet is fluid component-2 and assuming zero normal velocity at outlet, the following equations would define the first set of missing distribution functions at outlet [33],

\[
    u_x^{(2)} = -1 + \frac{f_0^{(2)} + f_2^{(2)} + f_4^{(2)} + 2 \left( f_1^{(2)} + f_5^{(2)} + f_7^{(2)} \right)}{\rho_{\text{out}}^{(2)}}, \tag{19}
\]

\[
    f_3^{(2)} = f_1^{(2)} - \frac{2}{3} \rho_{\text{out}}^{(2)} u_x^{(2)}, \tag{20}
\]

\[
    f_6^{(2)} = f_8^{(2)} - \frac{1}{2} \left( f_2^{(2)} - f_4^{(2)} \right) - \frac{1}{6} \left( \rho_{\text{out}}^{(2)} u_x^{(2)} \right), \tag{21}
\]

\[
    f_7^{(2)} = f_5^{(2)} + \frac{1}{2} \left( f_2^{(2)} - f_4^{(2)} \right) - \frac{1}{6} \left( \rho_{\text{out}}^{(2)} u_x^{(2)} \right), \tag{22}
\]

where, \(\rho_{\text{out}}^{(2)}\) is the specified density of fluid component-2 at the outlet boundary and it is used to impose an outlet pressure boundary condition.

For completeness, we write down the set of equations that define the first set of missing distribution functions at the inlet side for a pressure boundary condition, assuming the main fluid component at inlet is fluid component-1 and assuming zero normal velocity at inlet

\[
    u_x^{(1)} = 1 - \frac{f_0^{(1)} + f_2^{(1)} + f_4^{(1)} + 2 \left( f_3^{(1)} + f_5^{(1)} + f_7^{(1)} \right)}{\rho_{\text{in}}^{(1)}}, \tag{23}
\]

\[
    f_1^{(1)} = f_3^{(1)} + \frac{2}{3} \rho_{\text{in}}^{(1)} u_x^{(1)}, \tag{24}
\]

\[
    f_5^{(1)} = f_7^{(1)} - \frac{1}{2} \left( f_2^{(1)} - f_4^{(1)} \right) + \frac{1}{6} \left( \rho_{\text{in}}^{(1)} u_x^{(1)} \right), \tag{25}
\]

\[
    f_8^{(1)} = f_6^{(1)} + \frac{1}{2} \left( f_2^{(1)} - f_4^{(1)} \right) + \frac{1}{6} \left( \rho_{\text{in}}^{(1)} u_x^{(1)} \right). \tag{26}
\]
where, $\rho^{(1)}_{in}$ is the specified density of fluid component-1 at the inlet boundary and it is used to impose an inlet pressure boundary condition.

Until this stage, the second set of missing distribution functions at outlet $(f_3^{(1)}, f_6^{(1)}, f_7^{(1)})$ and inlet $(f_1^{(2)}, f_5^{(2)}, f_8^{(2)})$ would still be missing.

We identify two techniques to define these sets of distribution functions. The first technique would be to define the missing values using Zou-He technique by assigning a fixed density value for the other fluid component as well (e.g. fluid component-1 at outlet side). Hence Equations (19-22) and (23-26) would be applied to fluid component-2 and fluid component-1, respectively, after altering the subscripts representing the fluid component. We call this treatment of boundary conditions, **Set-1**. The second technique would be to define the missing values using the method described in Ref. [34] where the unknown distribution functions maintain themselves in the update process,

\[
\begin{align*}
  f_{3,6,7}^{(1)} & \xrightarrow{\text{collision}} f_{3,6,7}^{(1)}_{out,t_1} & f_{3,6,7}^{(1)} & \xrightarrow{\text{streaming}} f_{3,6,7}^{(1)}_{out,t_2}, \\
  f_{1,5,8}^{(2)} & \xrightarrow{\text{collision}} f_{1,5,8}^{(2)}_{in,t_1} & f_{1,5,8}^{(2)} & \xrightarrow{\text{streaming}} f_{1,5,8}^{(2)}_{in,t_2},
\end{align*}
\]

(27) \hspace{1cm} (28)

where, $t_1$ is the current time step and $t_2$ is the new time step.

We call this treatment of boundary conditions, **Set-2**.

It will be shown in section 4.1 that applying pressure boundary conditions using either **Set-1** or **Set-2** resulted in a considerable change in the volume of the trapped fluid component within the simulation domain, which is an unphysical feature that would affect the simulation of displacement processes in porous media where entrapment of fluid components is expected to be encountered. Hence a new treatment of boundary conditions was developed, and it is presented in the following paragraphs.
We call the newly introduced pressure boundary condition treatment, **Set-3** and it is applied as follows:

1- Apply Zou-He technique for only one fluid component at each side as shown in Equations (19-22) and (23-26).

2- Apply Eq. (27) as an open boundary condition for fluid component-1 at outlet.

3- The set of missing distribution functions of fluid component-2 at inlet will be updated during the collision step by applying Eq. (1) and will not updated during the streaming step, hence they will keep their post-collision values as follows,

\[
    f_{1,5,8 \mid \text{in}, t_1}^{(2)} \xrightarrow{\text{collision}} f_{1,5,8 \mid \text{in}, t_2}^{(2)} \xrightarrow{\text{streaming}} f_{1,5,8 \mid \text{in}, t_2}^{(2)}.
\]

The above shown steps represent **Set-3** of boundary conditions treatment. This set combined with the modified EF model Eq. (1), special treatment for interaction forces at boundaries Eq. (14), and the IVSD model Eq.’s (17,18), represents an improved MC pseudopotential model that will be shown in section 4 to be providing superior and satisfactory results in simulating multicomponent immiscible fluids flow in porous media.

It should be noted that in **Set-3** the pressure value at boundaries will not be altered only by the input density at boundaries since the other density component is freely updated and will be calculated using Eq. (3). Hence, according to the model EOS (Eq. 15), the pressure value will not be fixed at both boundaries, and it shall be evaluated using the EOS to determine the exact value. In this work we report the pressure values at boundaries averaged over the boundary sides, with the values near the solid walls ignored. Moreover, step-2 is applied to the fluid component with higher kinematic viscosity, which is assumed to be fluid component-1 in this work, while step-3 is applied to the fluid component with lower kinematic viscosity which is assumed to be fluid component-2 in this work. Velocity artifacts near the boundaries were observed in case of reversing the component to which the relevant step was applied.
3. NUMERICAL TESTS

In this section, several benchmarks are used to characterize the developed model. Since the pseudopotential model is used, some of these benchmarks are also used to calibrate the model parameters which are needed for other simulation cases, such as surface tension and contact angle.

3.1. Miscibility test

This numerical test in one of the standard benchmarks for the MC pseudopotential LBM model that could be used to determine the effect of $G_{coh}^{(σ)}$ on the densities of the fluid components. It also shows the dependence of the density and surface tension values on the viscosity ratio of the two components. In this section, we carry out the test at three values of viscosity ratio ($M = 1, M = 25, M = \frac{1}{25}$) to show the effect of viscosity on the results. The relaxation times to achieve these viscosity ratios were set as follows

$$
τ^{(σ)} = \begin{cases}
τ^{(1)} = τ^{(2)} = 1, & M = 1 \\
τ^{(1)} = 3.5, τ^{(2)} = 0.62, & M = 25 \\
τ^{(1)} = 0.62, τ^{(2)} = 3.5, & M = \frac{1}{25}
\end{cases}
$$

Series of 2D simulations were carried out where a droplet of fluid component-1 was placed in a fully periodic domain of fluid component-2. The domain size was 192 x 192, and the initial droplet size was 40. The density field was initialized using the following hyperbolic formula

$$
ρ^{(σ)}(x) = \frac{ρ^{(σ)}_{in} + ρ^{(σ)}_{out}}{2} - \frac{ρ^{(σ)}_{in} - ρ^{(σ)}_{out}}{2} \times \tanh \left[ \frac{2\left(\sqrt{(x - x_{center})^2 + (y - y_{center})^2} - r_0\right)}{W} \right],
$$

(30)
where, $\rho_{in}^{(\sigma)} = 1$, $\rho_{out}^{(\sigma)} = 0.02$, $r_0 = 40$, $W = 5$. This initialization method reduces the numerical instability in the first few iterations of the simulation as it represents an initial density field with a diffusive interface between the fluid components. It should also be noted that starting the simulation with an initial density $\rho_{out}^{(\sigma)}$ far from the expected equilibrium value results in longer convergence time and a dramatic change in the droplet size as the simulation converges at a different droplet size. Hence, the initial dissolved density was set to 0.02 which is a value obtained from several trials and expected to be close to the equilibrium dissolved density value. After the simulation reached steady state, the density values of the fluid component-1 and fluid component-2 at the center droplet were measured and shown in Figure 2. Also, the pressure value at the center of the droplet and the domain corner away from the droplet were measured and used to calculate the surface tension using Laplace law (section 3.2).

It could be observed from Figure 2 that as the value of $G_{coh}^{(\sigma\bar{\sigma})}$ was increased, the density difference between the suspended fluid (fluid component-1 inside the droplet) and the suspending fluid (fluid component-2 inside the droplet) was increased which indicates lower miscibility between the two fluid components. Also, it could be observed from Figure 3 that the surface tension increased as $G_{coh}^{(\sigma\bar{\sigma})}$ was increased. Moreover, there was a critical value of $G_{coh}^{(\sigma\bar{\sigma})}$ below which the cohesion interaction strength was not strong enough to maintain a defined interface between the two fluid components and they became completely miscible. This critical value could be identified from Figure 3 as $G_{coh}^{(\sigma\bar{\sigma})} < 2.5$ below which the density of fluid component-1 at the center is greatly reduced and the density of the fluid component-2 is greatly increased, that indicates miscibility of the first fluid component in the second fluid component. Finally, it could be observed that changing the viscosity ratio did not result in major changes in the density and surface tension values, which will be elaborated more in the
Laplace test. Comparing the present results of the miscibility test with results shown in [38] shows that the present model exhibits independent tuning surface tension from the viscosity ratio.

3.2. Laplace test

This test is carried out to validate that the model obeys the Laplace law \( \Delta P = \frac{\gamma}{R} \), where \( \Delta P \) is the difference between the pressure inside the droplet and the pressure outside the droplet, \( \gamma \) is the surface tension and \( R \) is the droplet radius. Laplace law states that there is a linear relationship between the pressure difference and the inverse of the droplet radius, and the constant of this linear relationship is the surface tension. Series of 2D simulations were carried out where a droplet of fluid component-1 was placed in a fully periodic domain of fluid component-2. The domain size was 192 x 192, and the initial droplet size was 40. The density field was initialized using Eq. 30. The initial density values were selected as follows (from miscibility test at \( G_{coh}^{(\sigma\sigma)} = 3.5 \)): \( \rho_{in}^{(1)} = \rho_{out}^{(2)} = 1, \rho_{out}^{(1)} = \rho_{in}^{(2)} = 0.027 \), such values are selected to reduce the change in the droplet radius from the initial radius as the simulation converges to steady state due to the deviation of initial densities from the equilibrium densities. Three different viscosity ratios were simulated \( M = 1, M = 25, M = \frac{1}{25} \) by setting the relaxation times as shown in the miscibility test (section 3.1).

After the simulations reached steady state, the pressure inside and outside the droplet was measured and plotted against the inverse of the measured droplet radius as shown in Figure 4. The relationship between \( \Delta P \) and \( R \) was indeed linear and satisfied Laplace law. The surface tension could be determined as the slope of the line. It was shown in [39] that the relation between pressure difference \( \Delta P \) and the curvature \( \left(\frac{1}{R}\right) \) depends on the selected viscosity ratio, in other words the surface tension value of the original pseudopotential model – at a selected \( G_{coh}^{(\sigma\sigma)} \) – is dependent on the viscosity ratio, which is one of the original pseudopotential
model limitations. However, the present model does not have such a limitation as it could be observed from Figure 4 that the surface tension hardly depends on the selected viscosity ratio. This again confirms that the present model exhibits independent tuning surface tension from the viscosity ratio.

3.3. Contact angle measurement

This simulation is conducted to validate and calibrate the wetting boundary condition using the (IVSD) scheme introduced earlier and determine the relationship between $\xi$ and contact angle $\theta$ for the currently implemented model. It is one of the limitations of the pseudopotential model that the contact angle can not be set directly into the model like in the free energy model for instance [8]. Hence, this characterization is essential in the pseudopotential model to calibrate the model at a specific surface tension $G_{coh}^{(\sigma\bar{\sigma})}$ and properly set the desired contact angle in other simulations.

Series of 2D simulations were carried out where a semi-circular droplet of fluid component-1 with initial droplet radius 30 was initially placed on the surface of a solid wall. The domain size was 192 x 96 and periodic in the x-direction, while solid walls were located at the top and the bottom of the domain. The initial density values and $G_{coh}^{(\sigma\bar{\sigma})}$ were set like in section 3.2 using Eq. 30. Three different viscosity ratios were simulated ($M = 1, M = 25, M = \frac{1}{25}$) by setting the relaxation times as shown in section 3.1.

We specify the criteria of measuring the contact angle ($\theta$) by following the convention: the contact angle is measured through the denser fluid phase [1]. Since this work would focus on an oil-water system, then water is considered the denser fluid and contact angle will be measured through water as shown in Figure 5 [1]. The initial density field was initialized with the assumption that fluid component-1 (forming the droplet) is oil while fluid component-2 (surrounding fluid) is water. The contact angle of the droplet was measured in the steady
state. The contact angle was measured using the technique and geometrical relationships shown in [40], and the base width was measured five lattice units above the surface to avoid the influence of the surface on the measured interface. Additionally, a linear interpolation was used to determine an approximate location of the interface. Also, the half-way location of solid walls was considered [8].

The simulation results are plotted in Figure 6 where the desired relationship between $\xi$ and contact angle $\theta$ is well established. It could be observed that model produced the expected behavior in setting the wettability using the parameter $\xi$, where oil was non-wetting ($\theta < 90^\circ$) for $\xi < 1$ and vice versa. Also, a wide range of contact angles was successfully simulated which covers most of practical applications. Additionally, the contact angle value for the selected $\xi$ did not considerably change with viscosity ratio, except at the very high or very low contact angles, so the set contact angle is considered independent from the viscosity ratio with an attention to the extreme cases (e.g., superhydrophobic surfaces). Moreover, an empirical equation could be deduced from the curves to represent the $\xi$-$\theta$ relationship, a third order polynomial provided the best fit for our simulation results ($\theta = 47.5487 \xi^3 - 13.9067 \xi^2 + 92.0987 \xi + 90.8074$). Snapshots of the simulation results at different contact angles are shown in Figure 7.

4. Numerical Results

In this section we carry out several numerical simulations using the present model to show its features and evaluate its performance. Also, immiscible fluid displacement processes were simulated in a heterogeneous porous medium to relate the qualitative results of the present model against known physical behaviors and phenomenon encountered in media.

4.1. Fluid flow over an obstacle with entrapped fluid volume

Before carrying out simulations of displacement of immiscible fluids in porous medium, it is beneficial to evaluate the performance and show its advantages over the original
pseudopotential model. Critical items to displacement of immiscible fluids should be checked such as changes in entrapped fluid volumes, contact angle alteration with boundary conditions, and capturing physical phenomena. This is essential as the original pseudopotential model was shown to experience changes in trapped fluid volumes for similar simulations [27]. A simple case was simulated for that purpose, where a semi-circular droplet of fluid component-1 was placed on the vertical side of a u-shaped solid wall, which was placed inside a fluid channel mostly saturated with fluid component-2. Moreover, fluid component-1 was pushed inside the fluid channel using pressure boundary conditions. Such conditions were set to test behaviors of trapped volumes of the different fluid components under pressure boundary conditions and to evaluate if there were changes in the set contact angle under such conditions.

A 2D simulation was carried out using a setup as shown in Figure 8 where an 800 x 200. flow channel with upper and lower solid walls was partially filled with fluid component-2. The channel contained a u-shaped wall that served as an obstacle to the flow and would result in forcing the flow of fluid component-1 to the narrower upper and lower fluid passages, and it would also result in entrapment of fluid component-2 by these upper and lower flow streams. The initial droplet radius was 30. Fluid component-1 (invading fluid) was set to be more viscous and non-wetting, hence the simulation parameters were set as follows: \( \tau^{(1)} = 3.5 \) \( (\nu^{(1)} = 1) \), \( \tau^{(2)} = 0.62 \) \( (\nu^{(2)} = 0.04) \), \( M = 25 \), \( \xi = -0.4(\theta \approx 50^\circ) \) and the fluid-fluid cohesion strength was set as \( G_{coh}^{(\sigma \bar{\sigma})} = 3.5 \).

The set of boundary conditions described in section 2.3 were used, where the inlet density (pressure) of fluid component-1 was set to 1.025 and the outlet density (pressure) of fluid component-2 was set to 1. The results of the three boundary condition treatments were compared as shown in Figure 8. It could be observed that in all three sets of boundary conditions there was no reduction in the volume of the non-wetting fluid droplet on the
vertical side of the u-shaped wall, where the different sets of boundary conditions were combined with the IVSD wetting boundary conditions. Moreover, it could be observed that set-1 and set-2 resulted in a considerable change in the volume of the trapped fluid component due to the passage of the invading fluid (red) through the original fluid (blue) which is non-physical. However, set-3 greatly suppressed that unfavorable behavior and the entrapped fluid component survived until the end of the simulation. Preservation of such entrapped fluid volumes is essential for the immiscible displacement of fluids in porous media.

The dynamic evolution of the fluid invasion using set-3 of boundary condition treatments is shown in Figure 9 via snapshots at several time steps. Since the invading fluid is non-wetting, it could be observed at $t=10000$ that it started invading the regions away from the upper and solid walls firstly, however it was resisted by the existence of fluid component-2 in the central region where the u-shaped wall was located. Also, by comparing snapshots at $t = 0$ and $t = 10000$, it could be seen that the droplet of fluid component-1 initially set as neutrally wet changed to a non-wetting droplet. The contact angle was measured and found to be $\theta \approx 50^\circ$ as initially set using $\xi = -0.4$. Another interesting phenomenon could be observed in the upper and lower flow passages, where one side of the invading fluid is preceding the other. Since the invading fluid is non-wetting, it started invading regions away from the solid walls firstly, and by the time it approached the flow passages, the side of the fluid next to the channel solid wall was already succeeding other fluid regions. This matches the expected physical behavior of the non-wetting fluid in such cases. The invading fluid was forced to flow through the upper and lower flow passages where it was sandwiched by two solid walls as shown in snapshot at $t = 30000$. The entrapped volume of fluid component-2 could be observed throughout the remaining snapshots until the simulation ended to be preserved and keeping its shape without considerable changes.
The coalescing process of the upper and lower portions of the invading fluid with the form of a single interface of the invading fluid could be observed in the snapshots at \( t = 205000 \) and \( t = 210000 \). The non-wetting fluid kept invading the channel until it reached the end of the channel successfully as shown in last snapshot at \( t = 700000 \). It could also be observed that a film of fluid-component-2 remained in the channel since a fixed density (pressure) boundary condition is specified at the outlet. The entrapped volumes of both fluid components kept their shape and size till the end of the simulation. It should be mentioned that there was a small reduction in the entrapped volume of fluid component-2 inside the U-shaped wall that occurred as the invading fluid reached the end of the fluid channel. It is believed that such behavior occurred as the pressure inside the channel was increased due to the blockage at the end of the channel, also the LBM model used in this work is considered weakly compressible and that would allow small changes in the fluid volumes.

This simulation case shows that the used LBM model with the presented set of boundary conditions can properly simulate immiscible displacement of fluids, captures the wetting boundary conditions properly, it has stable fluid flow by the domain boundaries, and it preserves the volume of the entrapped fluids. Such features are essential for simulating fluid flow in porous medium and capturing the underlying physical phenomena.

4.2. Flow in heterogeneous porous medium

4.2.1. Primary Drainage

In this section, we simulate fluid displacements when one fluid replaces another in a porous medium. The initial state of the of the porous medium is assumed to be a clean and saturated porous medium where the solid walls are water wet. This matches the initial state of laboratory experiments carried out on porous samples for oil reservoirs where the extracted samples (core plugs) are cleaned and fully saturated with formation water. Starting with the pore space entirely saturated with water (wetting fluid) and pushing oil (non-wetting fluid)
into the pore space is known as the Primary Drainage process [1]. The word primary 
(meaning first) indicates that this is the first time the non-wetting phase enters the pore space: 
we start with a wetting phase saturation of $S_w = 1$. Drainage, in general, refers to the 
displacement of a wetting phase by a nonwetting phase or decreasing the wetting phase 
saturation. A common example of primary drainage process is the migration of oil from 
source rock to an oil reservoir where oil invades the pores that were initially saturated with 
water.

In laboratory experiments, the non-wetting phase does not penetrate the medium until the 
capillary pressure exceeds a threshold pressure $P_{c,t}$, which depends on the size and shape of 
the pores and wettability of the sample [2]. As capillary pressure increases beyond this value, 
the saturation of the water continues to decrease with water saturation approaching an 
irreducible level $S_{w,i}$ at very high capillary pressures. Irreducible water saturation $S_{w,i}$ is the 
lowest water saturation that could achieved by a displacement process [2].

A series of 2D simulations were carried out to simulate the primary drainage process in a 
heterogenous randomly generated porous medium. The geometry was adopted from a 
previous work [22]. We briefly describe the geometry in the following sentences. The 
generated geometry is bounded by upper and lower solid walls and filled with solid blocks 
creating the porous medium. The size of each solid block is $10 \times 10$, while the size of the 
whole domain is $400 \times 200$ lattices. The generated porous medium is shown in Figure 10 and 
the domain porosity is 81.17%. Internal solid blocks were removed from the first/last 10 
layers of the inlet/outlet sides to represent reservoirs for both fluids. The initial state of the 
primary drainage simulation is shown in Figure 10, where 5 layers of oil is assumed in the 
assigned inlet fluid reservoir. The initial density values are as assumed in section 3.2, i.e., 
$\rho_i^{(1)} = 1.0$, $\rho_i^{(2)} = 0.027$ where the layers of the non-wetting fluid are located. Other domain 
regions are assumed to have similar, but reversed, initial density values. The virtual solid
density values were computed at initial state using the technique mentioned in section 2.2 and their values are dedicated by the required wettability condition.

In these simulations, the non-wetting fluid (oil) is set to be more viscous than wetting fluid (water). A realistic viscosity ratio was chosen as $M = \frac{\rho_{nw} \nu_{nw}}{\rho_w \nu_w} = 25$, where the density of both fluids was set as unity. In this length scale (pore scale – μm), the density difference is not expected to have major impact on the displacement process, and in realistic experiments the sample is mostly placed horizontally, hence the gravity effects could be neglected. The relaxation times are set as in section 3.1. The contact angle was varied to represent different cases and inspect the effect of the contact angle ranging from strongly water wet to oil wet mediums. In this section the contact angle was set as $\theta \cong 50^\circ$ ($\xi = -0.4$) to represent a weakly water wet medium.

The capillary pressure $P_c$ is considered the difference between the inlet and outlet pressures $P_c = P_{in} - P_{out}$. Inlet and outlet pressures are specified using Dirichlet boundary conditions via Zou-He technique as explained in section 2.2 and set-3 was used in these simulations. Inlet and outlet density values of the relevant fluid component was altered to employ the pressure boundary condition. Despite the Zou-He method being a common technique to apply pressure boundary condition in the LBM, it should be expected to have a negative impact on multicomponent simulations due to the inherent compressibility effects. For the primary drainage simulation, the outlet density was kept fixed at $\rho^{(2)} = 1$ while the inlet density increased gradually and stabilized after some time.

The primary drainage simulation results are plotted in Figure 11. It could be observed that the current LBM model successfully captures the primary drainage curve in a qualitative manner. The oil started invading the medium after exceeding a critical threshold pressure ($P_{c,t} \cong 0.00511$) at a critical oil saturation $S_{o,t} \cong 0.053$ and kept invading the medium gradually with the increase of capillary pressure. An interesting phenomenon occurred at $S_w \cong 0.7$
where the capillary pressure was considerably increased but the water saturation was not decreased. This is known as the capillary pressure bump phenomenon, and it is known to occur due to the heterogeneity of the porous medium [2]. The LBM was firstly shown to capture this phenomenon in Ref. [22] using the original pseudopotential model and it is reassured in this study to be captured using the present model. Another smaller bump in the capillary pressure curve was also captured using the present model – for the same geometry – at $S_w \approx 0.35$. Snapshots for the porous medium are shown in figures at different capillary pressures when the phenomenon occurred. The oil kept invading the medium with the gradual increase of the capillary pressure till $S_w \approx 0.2$ where the oil arrived at the wetting fluid reservoir at outlet $P_c \approx 0.01136$. Moreover, any additional increase in the capillary pressure did not result in any further decrease/increase in the water/oil saturation. This indicates that the irreducible water saturation is achieved $S_{w,i} \approx 0.2$, which is close to realistic values of $S_{w,i}$ [2].

It should be highlighted that such realistic values of $S_{w,i}$ is one of the main advantages of the present model, as the proposed treatments and boundary conditions greatly suppressed the shrinkage of the entrapped fluid volume which is a known drawback of the pseudopotential model [22] [27]. For instance, in Ref. [22] the exact same geometry was used as in the present study, however the entrapped volumes of water shrank and that resulted in non-realistically low irreducible water saturations. However, using the present improved model, the trapped water volumes survived until the end of the primary drainage process with the increase of the inlet pressure. Notice that relatively small volumes of water did not survive and collapsed, however this is inevitable for the pseudopotential model as it is a diffusive interface model, hence approaching an interface width that is close to the fluid volume will result in such collapses. Moreover, some trapped water volumes experience a moderate change in volume with the increase of capillary pressure, which is believed to be due to the
compressibility effects accompanied with this model. Snapshots of the density distribution (to represent fluids distribution) in the porous medium are show in Figure 12 for the weakly water wet system ($\theta \approx 50^\circ$).

In the next sections, the same simulation parameters were set as in the previous section, however the contact angle was changed to represent different mediums.

4.2.1.1. Strongly water wet medium

In this case, the contact angle was set as $\theta \approx 22^\circ$ ($\xi = -0.55$) to represent a strongly water wet system. This would represent a core plug after being cleaned in the laboratory and fully saturated with water where the sample becomes strongly water wet.

The primary drainage results of this case are shown in Figure 11. Several interesting changes could be observed when compared to the weakly water wet case in the previous section. The critical threshold pressure slightly increased in this case ($P_{ct} \approx 0.005301$) and despite the increase is relatively small, it matches the expected physical behavior as the oil is less wetting in this case, hence it would need a larger capillary pressure threshold to start invading the medium. Looking at the snapshots of the dynamic evolution of the displacement process in Figure 13, it could be observed that the displacement pattern changed, consequently the capillary pressure bump did not occur in the same region as in the previous case, however it occurred in a different region at $S_w \approx 0.388$. Wettability is known to alter the shape of the capillary pressure curves [2] and such a change in the simulation results shows that the current LBM model can capture such effects. Since the oil phase is less wetting in this case, it had less tendency to stick to solid walls and more tendency to occupy pores away from the solid walls, that resulted in the high increase in the oil saturation once the capillary pressure exceeded the critical threshold pressure. In this case, oil was able to invade more pore spaces at lower capillary pressures due to its preference to fill pores away from solid walls and the nature of the used geometry aided in such behavior as it had relatively large pores. Moreover,
it could be observed that the irreducible water saturation $S_{w,i}$ was increased in this case to $S_{w,i} \approx 0.3$ which matches the expected physical behavior. As the medium had a stronger tendency for water wetting, more water was trapped in pore spaces that had larger interfaces with solid walls.

### 4.2.1.2. Weakly oil wet medium

In this case, the contact angle was set as $\theta \approx 110^\circ$ ($\xi = 0.2$) to represent a weakly non-wetting to water system. This would represent a typical oil reservoir where the porous medium is oil wet rather than water wet [2]. In order to avoid contradiction with the definition of drainage, this case could be called water drainage.

The water drainage results of this case are shown in Figure 11. It could be observed that the critical threshold pressure decreased, and oil immediately started invading the medium. That matches the expected physical behavior since oil was the wetting phase in this case and had the tendency to stick to solid walls. Again, by looking at the displacement snapshots in Figure 14, it could be observed that the displacement pattern changed, and the wetting fluid is invading more pore spaces with less non-wetting trapped. Also, the capillary pressure bump phenomenon was suppressed as the wetting fluid less resistance to flow in the medium.

Moreover, it could be observed that the irreducible water saturation $S_{w,i}$ was decreased in this case to $S_{w,i} \approx 0.128$ which matches the expected physical behavior. As the medium had a stronger tendency for oil wetting, less water was trapped in pore spaces that had larger interfaces with solid walls.

It could be concluded from this section that the presented model could capture different physical behaviors and phenomena that occur during the primary drainage displacement process in a qualitative manner.

### 4.2.2. Imbibition

After completing simulations of capillary pressure for primary drainage, the direction of
saturation change can be reversed, and another capillary pressure relationship can be measured. It is usually called an imbibition relationship. Imbibition, in general, refers to the displacement of a non-wetting phase by a wetting phase or the increase of wetting phase saturation. A common example of imbibition is waterflooding process where water is injected into an oil reservoir to displace oil. The primary drainage and imbibition relationships differ considerably. This difference is called capillary pressure hysteresis.

A series of 2D simulations were carried out to simulate the imbibition process in the same medium used in the previous section, with the end points of the primary drainage curves used as the initial saturation of the imbibition simulations. The capillary pressure was changed by reducing the inlet density of fluid component-1 and increasing outlet density of fluid component-2 until $P_c = 0$ to capture the spontaneous imbibition phenomenon, then further increase in the density of fluid component-2 resulted in negative capillary pressures to simulate forced imbibition. Also, we use the same contact angle as in the primary drainage case $\theta \cong 50^\circ$ ($\xi = -0.4$).

The imbibition simulation results are plotted in Figure 15, where it could be observed that for the initial reductions of capillary pressure, the water saturation did not considerably increase. However, as the capillary pressure approached zero, there was an increase in the water saturation, which shows that the model could capture the spontaneous imbibition phenomenon. Also, it could be observed that the water saturation at zero capillary pressure is not very large, which matches the expected physical behavior that for a less strongly wetting phase, the capillary pressure reaches zero at a lower saturation [2].

Snapshots for the imbibition process are shown in Figure 16, where the oil started retracting from the medium gradually resulting in increase in the water saturation until the medium is mostly filled with water. The last snapshot shows trapped volumes of oil that is known as residual oil. The residual oil saturation in this case was $S_{o,r} = 0.145$, which is relatively
small for a weakly water wet medium [2]. However, this could be attributed to the nature of
the simulated geometry which have relatively large porosity and pore spaces.

In the next sections, the same simulation parameters were set as in the previous section of
primary drainage simulations, where the contact angles were altered to represent different
systems. As mentioned earlier, the end points of the different primary drainage curves were
used as initial saturation for the imbibition simulations

**4.2.2.1. Strongly water wet medium**

In this case, the medium was set as strongly water wet with a contact angle as \( \theta \cong 22^\circ \) \((\xi = -0.55)\) during the primary drainage process, where oil was observed to need a
higher capillary pressure to invade the medium and irreducible water saturation was also
relatively high. The imbibition process results are shown in Figure 15, where it could be
observed that any decrease in the capillary pressure resulted in a decrease in the oil
saturation. Moreover, as the capillary pressure approached zero, the water saturation was
relatively high \((S_w = 0.736)\), which matches the expected physical behavior as for the
imbibition of a strongly wetting phase, the capillary pressure generally does not reach zero
until the wetting-phase saturation is large [2]. In this case, the spontaneous imbibition was
responsible for a major increase in the water saturation. Moreover, as capillary pressure was
further decreased and became negative, a residual oil saturation was achieved at \(S_o, r = 0.095\)
which is lower than the weakly water wet case. That matches the expected physical behavior
as comparable to the expected residual oil saturation of strong water wet media [2].

Snapshots for this case are shown in Figure 17.

**4.2.2.2. Weakly oil wet medium**

In this case, the contact angle was set as \( \theta \cong 110^\circ \) \((\xi = 0.2)\) to represent a weakly non-
-wetting to water system. The imbibition simulation results are shown in Figure 15, where it
could be observed that the initial reductions of capillary pressure did not result in any
increase of the water saturation and there was no spontaneous imbibition. In this case, the water phase is the non-wetting phase, hence it was harder for water to start invading the domain. As forced imbibition started, the water saturation started to increase gradually till most of the domain was filled with water. The residual oil saturation $S_{o,r} = 0.293$ for this case is a realistic value [2]. Moreover, it could be noted that the residual oil saturation value is larger than the previous two cases of weakly and strongly water wetting medium, which matches the expected physical behavior as oil has higher tendency to stick to solid walls. Hence, larger volumes of oil were trapped in the domain during the imbibition process. Snapshots of this imbibition process are shown in Figure 18, where a gradual increase in the water saturation could be observed till reaching $S_{o,r}$. Such a displacement process is encountered during production from oil reservoirs using water flooding, where water would trap oil in the reservoir and block its flow to production wells.

It could be concluded from this section that the presented model could capture different physical behaviors and phenomena that occur during the imbibition displacement process in a qualitative manner.

5. Summary

In this work, we introduced an improved version of the MC pseudopotential model using several enhancements, including a modified version of the Explicit Forcing (EF) model, an improved virtual solid density (IVSD) scheme, and a newly introduced set of inlet and outlet boundary condition treatments. The introduced model was shown to alleviate many of the original MC pseudopotential model, suppresses several non-physical behaviors and provides favorable features such as, higher range of viscosity ratio between the fluid components, independent tuning of surface tension from the viscosity ratio, suppressed the changes in fluid volumes, especially trapped fluids, captured physical phenomena that accompanied flow of oil and water in porous medium such capillary pressure bump, and provided realistic values
of irreducible water and residual oil saturations for simulations of primary drainage and imbibition displacement processes. This improved MC model opens the way to investigate fluid displacements in porous media using the Shan-Shen MC model, which is simple to implement and widely used, but suffers from non-physical effects without the enhancements presented here.

Several points could be addressed in future work such as assessing the model performance in 3D, simulating fluids displacement processes in realistic geometries of porous media obtained from micro computed tomography (µCT) scans, and potentially carrying out direct comparisons between numerical and experimental results.

No conflicts of interest

The authors have no conflicts to disclose.

Acknowledgments

RCVC acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under the contracts: PTDC/FISMAC/5689/2020, UIDB/00618/2020 and UIDP/00618/2020.
Figure 1. Illustration of known and missing distribution functions at inlet and outlet boundaries. Solid blue lines represent known distribution functions, while dotted green line represent unknown distribution functions.
Figure 2. Miscibility test results. Left axis shows the component density measured at the center of the domain while of the bottom axis shows the selected value of $G_{coh}^{(\sigma \bar{\sigma})}$. Different symbols represent different viscosity ratio.
Figure 3. Miscibility test results. Left axis shows the surface tension while of the bottom axis shows the selected value of $G_{coh}^{(\sigma\overline{\sigma})}$. Different symbols represent different viscosity ratio.
Figure 4. Laplace test results. Left axis shows the pressure difference while of the bottom axis shows the inverse of the droplet radius. Different symbols represent different viscosity ratio (black circle: $M = 1$, red cross: $M = 25$, blue square: $M = 1/25$). Dotted line in magenta represents the linear regression of data which gives a surface tension (slope) value $\gamma = 0.0692 \left(\sigma_{\text{coh}}^\infty = 3.5\right)$. 
Figure 5. An illustration of different contact angles measured through water in an oil/water system [1]. Here a droplet of oil is placed on a solid mineral surface, surrounded by water. The contact angle is measured through the water.
Figure 6. Contact Angle test results. Left axis shows the contact angle while of the bottom axis shows the factor $\xi$. Different symbols represent different viscosity ratio. Dotted line in magenta shows a polynomial (3rd order) fit of data.
Figure 7. Snapshots of contact angle test at different values of $\xi$ with corresponding values of contact angle $\theta$. The contact angle is measured through the water phase (surrounding fluid).
Figure 8. Comparison between simulation results for displacement of immiscible fluids in a channel and over a u-shaped wall using different sets of boundary condition treatments. Snapshots are shown at different time steps and for the first half the channel length only for clarification purpose. The colors represent fluid component-1 density contour field where red represents higher density (fluid component-1) and blue represents lower density (fluid component-2) with the interface region represented with gradient of colors. Top, bottom, and u-shaped solid walls are shown in yellow.
Figure 9. Simulation results for displacement of immiscible fluids in a channel and over a u-shaped wall using set-3 of boundary condition treatments. Snapshots are shown at different time steps and for half the channel length only for clarification purpose, starting at initial conditions ($t = 0$) (top left snapshot) until the invading fluid reached the end of the channel (bottom right snapshot). All snapshots are taken for the first half of the channel where the u-shaped is located, except for the last snapshot at $t = 700000$ which is taken for the second half of the channel to show the arrival of the invading fluid at outlet boundary. The colors represent fluid component-1 density contour field where red represents higher density (fluid component-1) and blue represents lower density (fluid component-2) with the interface region represented with gradient of colors.
Figure 10. Initial state of the primary drainage simulation case. Solid walls are represented with the yellow square blocks in addition to the top and bottom solid walls. Additional fluid layers were added to the left and right sides of the domain to represent inlet and outlet fluid reservoirs. The red colored layers on the left represent a reservoir of oil and the blue color represent the saturation of medium with water.
Figure 11. Capillary pressure ($P_c$) – water saturation ($S_w$) relationships for the primary drainage simulation process at different contact angles and viscosity ratio $M = 25$. Black circles represent the results at $\theta \approx 50^\circ$ (weakly water wet), red crosses represent the results at $\theta \approx 22^\circ$ (strongly water wet), and blue squares represent the results at $\theta \approx 110^\circ$ (weakly oil wet).
Figure 12. Snapshots for the primary drainage displacement process of weakly water wet system ($\theta \approx 50^\circ$) at different capillary pressures and water saturations. Snapshot was taken after oil stopped invading the medium at the specified capillary pressure.
Figure 13. Snapshots for the primary drainage displacement process of strongly water wet system ($\theta \approx 22^\circ$) at different capillary pressures and water saturations. Snapshot was taken after oil stopped invading the medium at the specified capillary pressure.
Figure 14. Snapshots for the primary drainage displacement process of weakly oil wet system ($\theta \approx 110^\circ$) at different capillary pressures and water saturations. Snapshot was taken after oil stopped invading the medium at the specified capillary pressure.
Figure 15. Capillary pressure ($P_c$) – water saturation ($S_w$) relationships for the imbibition simulation process at different contact angles and viscosity ratio $M = 25$. Black circles represent the results at $\theta \cong 50^\circ$ (weakly water wet), red crosses represent the results at $\theta \cong 22^\circ$ (strongly water wet), and blue squares represent the results at $\theta \cong 110^\circ$ (weakly oil wet).
Figure 16. Snapshots for the imbibition displacement process of weakly water wet system ($\theta \approx 50^\circ$) at different capillary pressures and water saturations. Snapshot was taken after oil stopped invading the medium at the specified capillary pressure.
Figure 17. Snapshots for the imbibition displacement process of strongly water wet system ($\theta \approx 22^\circ$) at different capillary pressures and water saturations. Snapshot was taken after oil stopped invading the medium at the specified capillary pressure.
Figure 18. Snapshots for the imbibition displacement process of weakly oil wet system (θ ≅ 110°) at different capillary pressures and water saturations. Snapshot was taken after oil stopped invading the medium at the specified capillary pressure.
References

[1] M. J. Blunt, MULTIPHASE FLOW IN PERMEABLE MEDIA, A Pore-Scale Perspective, Cambridge University Press, 2017.

[2] L. W. Lake, Petroleum Engineering Handbook, Vol. I, Richardson TX - USA: Society of Petroleum Engineers, 2006.

[3] C. McPhee, J. Reed and I. Zubizarreta, Core Analysis, A Best Practice Guide, vol. 64, Elsevier, 2015.

[4] M. J. Blunt, B. Bijeljic, H. Dong, O. Gharbi, S. Iglauer and P. Mostaghimi, "Pore-scale imaging and modelling," Advances in Water Resources, vol. 51, p. 197–216, 2013.

[5] R. Benzi, S. Succi and M. Vergassola, "The Lattice Boltzmann Equation: Theory and Applications," Physics Reports, vol. 222, no. 3, pp. 145-197, 1992.

[6] S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Oxford university press, 2001.

[7] Y. H. Qian, D. D’Humieres and P. Lallemand, "Lattice BGK Models for Navier-Stokes Equation.," Europhysics Letters, vol. 17, no. 6, pp. 479-484, 1992.

[8] T. Krüger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva and E. M. Viggen, The Lattice Boltzmann, Principles and Practice, Switzerland: Springer International Publishing, 2017.

[9] H. Liu, Q. Kang, C. R. Leonardi, B. D. Jones, S. Schmieschek, A. Narvaez, J. R. Williams, A. J. Valocchi and J. Harting, "Multiphase lattice Boltzmann simulations for porous media applications, A review," Computational Geosciences, vol. 20, no. 4, p. 777–805, 2014.

[10] L. Chen, Q. Kang, Y. Mu, Y.-L. He and W.-Q. Tao, "A critical review of the pseudopotential multiphase lattice Boltzmann model: Methods and applications," International Journal of Heat and Mass Transfer, vol. 76, p. 210–236, 2014.

[11] Q. Li, K. Luo, Q. Kang, Y. He, Q. Chen and Q. Liu, "Lattice Boltzmann methods for multiphase flow and phase-change heat transfer," Progress in Energy and Combustion Science, vol. 52, p. 62–105, 2016.

[12] H. Huang, M. C. Sukop and X.-Y. Lu, Multiphase Lattice Boltzmann Methods: Theory and Application, John Wiley & Sons, Ltd, 2015.

[13] A. K. Gunstensen, D. H. Rothman, S. Zaleski and G. Zanetti, "Lattice Boltzmann model of immiscible fluids," Physical Review A, vol. 43, no. 8, p. 4320, 1991.

[14] M. R. Swift, W. R. Osborn and J. M. Yeomans, "Lattice Boltzmann Simulation of Nonideal Fluids," Physical review letters, vol. 75, no. 5, p. 830, 1995.

[15] X. Shan and H. Chen, "Lattice Boltzmann Model for simulating flows with multiple phases and components," Physical review E, vol. 47, no. 3, pp. 1815-1819, 1993.

[16] H. Chen and N. S. Martys, "Simulation of multicomponent fluids in complex three-dimensional geometries by the lattice boltzmann method," Physical review E, vol. 53, no. 1, pp. 743-750, 1996.

[17] C. Pan, M. Hilpert and C. T. Miller, "Lattice-Boltzmann simulation of two-phase flow in porous media," Water Resources Research, vol. 40, no. W01501, 2004.

[18] M. G. Schaap, M. L. Porter, B. S. B. Christensen and D. Wildenschild, "Comparison of pressure-saturation characteristics derived from computed tomography and lattice Boltzmann simulations," Water Resources Research, vol. 43, 2007.
[19] M. L. Porter, M. G. Schaap and D. Wildenschild, "Lattice-Boltzmann simulations of the capillary pressure–saturation–interfacial area relationship for porous media," *Advances in Water Resources*, vol. 32, no. 11, pp. 1632-1640, 2009.

[20] H. Zhao, Z. Ning, Q. Kang, L. Chen and T. Zhao, "Relative permeability of two immiscible fluids flowing through porous media determined by lattice Boltzmann method," *International Communications in Heat and Mass Transfer*, vol. 85, pp. 53-61, 2017.

[21] Z. Dou and Z. F. Zhou, "Numerical study of non-uniqueness of the factors influencing relative permeability in heterogeneous porous media by lattice Boltzmann method," *International Journal of Heat and Fluid Flow*, vol. 42, p. 23–32, 2013.

[22] H. Warda, S. Haddara, E. Wahba and M. Sedahmed, "Lattice Boltzmann simulations of the capillary pressure bump phenomenon in heterogeneous porous media," *Journal of Petroleum Science and Engineering*, vol. 157, p. 558–569, 2017.

[23] A. Fager, B. Crouse, G. Sun, R. Xu and D. Freed, "Evaluation of Directly Simulated WAG Hysteresis at Pore Scale and its Effect on Injectivity Index," in *SPE Offshore Europe Conference and Exhibition*, 2019.

[24] M. N. Nemer, P. R. Rao and L. Schaefer, "Wettability alteration implications on pore-scale multiphase flow in porous media using the lattice Boltzmann method," *Advances in Water Resources*, vol. 146, p. 103790, 2020.

[25] A. F. Matias, R. C. Coelho, J. S. Andrade Jr. and N. A. Araújo, "Flow through time-evolving porous media: Swelling and erosion," *Journal of Computational Science*, vol. 53, no. 101360, 2021.

[26] L. Zheng, T. Lee, Z. Guo and D. Rumschitzki, "Shrinkage of bubbles and drops in the lattice Boltzmann equation method for nonideal gases," *PHYSICAL REVIEW E*, vol. 89, no. 033302, 2014.

[27] Z. Li, J. McClure, J. P. Middleton, T. K. Varslot and A. P. Sheppard, "Discretization limits of lattice-Boltzmann methods for studying immiscible two-phase flow in porous media," *International Journal for Numerical Methods in Fluids*, vol. 92, no. 9, p. 1162–1197, 2020.

[28] M. L. Porter, E. T. Coon, Q. Kang, J. D. Moulton and J. W. Carey, "Multicomponent interparticle-potential lattice Boltzmann model for fluids with large viscosity ratios," *Physical Review E*, vol. 86, 2012.

[29] M. Sbragaglia, R. Benzi, L. Biferale, S. Succi, K. Sugiyama and F. Toschi, "Generalized lattice Boltzmann method with multirange pseudopotential," *Physical review E*, vol. 75, 2007.

[30] Dominique d’Humières et al., "Multiple-relaxation-time lattice Boltzmann models in three dimensions," *Philosophical Transactions of The Royal Society A Mathematical Physical and Engineering Sciences*, vol. 360, no. 1792, pp. 437-451, 2002.

[31] K. N. Premnath and J. Abraham, "Three-dimensional multi-relaxation time (MRT) lattice-Boltzmann models for multiphase flow," *Journal of Computational Physics*, vol. 224, p. 539–559, 2007.

[32] Y. Zhao, G. G. Pereira, S. Kuang and B. Shi, "On a modified pseudopotential lattice Boltzmann model for multicomponent flows," *Applied Mathematics Letters*, vol. 114, no. 106926, 2021.

[33] Q. Zou and X. He, "On pressure and velocity boundary conditions for the lattice Boltzmann BGK model," *Physics of Fluids*, vol. 9, no. 6, pp. 1591-1598, November 1997.
[34] Y. Hou, H. Deng, Q. Du and K. Jiao, "Multi-component multi-phase lattice Boltzmann modeling of droplet coalescence in flow channel of fuel cell," Journal of Power Sources, vol. 393, pp. 83-91, 2018.

[35] R. C. V. Coelho, C. B. Moura, M. M. Telo da Gama and N. A. M. Araújo, "Wetting boundary conditions for multicomponent pseudopotential lattice Boltzmann," International Journal for Numerical Methods in Fluids, vol. 93, no. 8, 2021.

[36] M. C. Sukop and D. T. J. Thorne, Lattice Boltzmann Modeling, An Introduction for Geoscientists and Engineers, Springer, 2007.

[37] S. Iglauer, C. H. Pentland and A. Busch, "CO2 wettability of seal and reservoir rocks and the implications for carbon geo-sequestration," Water Resources Research, vol. 51, p. 729–774, 2015.

[38] A. Parmigiani, "Lattice Boltzmann calculations of reactive multiphase flows in porous media. (PHD Dissertation)," ReproMail print shop, Geneva - Switzerland, 2011.

[39] B. Dong, Y. Y. Yan and W. Z. Li, "LBM Simulation of Viscous Fingering Phenomenon in Immiscible Displacement of Two Fluids in Porous Media," Transport in Porous Media, vol. 88, no. 2, pp. 293-314, 2011.

[40] S. Schmieschek and J. Harting, "Contact Angle Determination in Multicomponent Lattice Boltzmann Simulations," Communications in Computational Physics, vol. 9, no. 5. pp. 1165-1178, 2009.