Hydrodynamic behavior of the pseudopotential lattice Boltzmann method for interfacial flows


DOI: 10.1103/PhysRevE.99.053305

Document status and date:
Published: 17/05/2019

Document Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.

Link to publication

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the “Taverne” license above, please follow below link for the End User Agreement:
www.tue.nl/taverne

Take down policy
If you believe that this document breaches copyright please contact us at:
openaccess@tue.nl
providing details and we will investigate your claim.
Hydrodynamic behavior of the pseudopotential lattice Boltzmann method for interfacial flows

Daniele Chiappini*
Department of Industrial Engineering, University of Rome “Niccolò Cusano,” Via don Carlo Gnocchi 3, 00166 Rome, Italy

Mauro Sbragaglia
Department of Physics, INFN, University of Rome “Tor Vergata,” Via della Ricerca Scientifica 1, 00133 Rome, Italy

Xiao Xue
Department of Physics, INFN, University of Rome “Tor Vergata,” Via della Ricerca Scientifica 1, 00133 Rome, Italy
and Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

Giacomo Falcucci
Department of Enterprise Engineering “Mario Lucertini,” University of Rome “Tor Vergata,” Via del Politecnico 1, 00133 Rome, Italy
and John A. Paulson School of Engineering and Applied Physics, Harvard University, 33 Oxford Street, 02138 Cambridge, Massachusetts, USA

(Received 10 December 2018; published 17 May 2019)

The lattice Boltzmann method (LBM) is routinely employed in the simulation of complex multiphase flows comprising bulk phases separated by nonideal interfaces. The LBM is intrinsically mesoscale with a hydrodynamic equivalence popularly set by the Chapman-Enskog analysis, requiring that fields slowly vary in space and time. The latter assumptions become questionable close to interfaces where the method is also known to be affected by spurious nonhydrodynamical contributions. This calls for quantitative hydrodynamical checks. In this paper, we analyze the hydrodynamic behavior of the LBM pseudopotential models for the problem of the breakup of a liquid ligament triggered by the Plateau-Rayleigh instability. Simulations are performed at fixed interface thickness, while increasing the ligament radius, i.e., in the “sharp interface” limit. The influence of different LBM collision operators is also assessed. We find that different distributions of spurious currents along the interface may change the outcome of the pseudopotential model simulations quite sensibly, which suggests that a proper fine-tuning of pseudopotential models in time-dependent problems is needed before the utilization in concrete applications. Taken all together, we argue that the results of the proposed paper provide a valuable insight for engineering pseudopotential model applications involving the hydrodynamics of liquid jets.

DOI: 10.1103/PhysRevE.99.053305

I. INTRODUCTION

The development of modern applications and innovative materials involving multiphase flows [1,2] naturally sets a compelling case for the development of suitably designed numerical methods to be used in synergy with experimental investigations [3] and analytical predictions [4]. The understanding of many of such problems is routinely rationalized via the help of a continuum hydrodynamics: In a nutshell, one can say that bulk phases coexist while being separated by thin interfaces, whose width represents the smallest scale of the continuum description. Such interfaces are characterized by a nonzero surface tension, i.e., the force per unit area that is the continuum manifestation of the anisotropy of atomistic forces close to the interface. Whereas for purely analytical calculations, the zero-width limit (“sharp interface”, hydrodynamics) is most easily handable [5–7], for numerical simulations the situation is somehow more diversified [8–14]. In this landscape, increasing attention has been driven towards mesoscale simulations and, in particular, the lattice Boltzmann method (LBM) [15–20]. When solving the complex fluid dynamics of multiphase flows, the traditional advantages of the LBM (simplicity [21,22], easy handling of boundary conditions [23,24], and easy parallelization [25]) can be further enriched by a remarkable versatility in simulating non-ideal equations of state (EoS) and complex interfaces [26,27]. More precisely, LBM reproduces “diffuse” interfaces, i.e., the bulk phases are separated by a region of finite thickness where the fluid properties (i.e., density, velocity, and pressure) change continuously. The hydrodynamical behavior of the LBM is traditionally assessed via the Chapman-Enskog analysis; however, from the theoretical point of view, the main assumptions of the Chapman-Enskog analysis of having fields slowly varying in space and time may well be violated due to the presence of the interfaces and/or singular events, such as breakups [28,29]. Practically, it is also found that LBM implementations are affected by spurious contributions at the interface [30,31]. We use the term spurious meaning that they are not predicted by hydrodynamics. These spurious currents are particularly relevant close to the interfaces [32]. Consequently, the actual recovery of the LBM-hydrodynamic
“equivalence” could fail [15,33]. Natural questions then arise on the quantitative potentiality retained by diffuse interface LBM simulations of multiphase flows, especially in comparison to the analytical description of sharp interface hydrodynamics. In fact, although it is largely acknowledged in the literature [20,34–43] that the LBM is capable of reproducing static properties driven by surface tensions (i.e., Laplace pressures [44] and contact angles [45]), very rarely there have been quantitative characterizations on the recovery of time-dependent hydrodynamics with nonideal interfaces, especially in the presence of singular events. This paper aims to take a step forward in the latter direction. As a prototypical problem of a time-dependent multiphase flow with nonideal interfaces, we refer to the Plateau-Rayleigh instability [6,46–52] of a liquid ligament. The Plateau-Rayleigh instability—driven by the tendency of the interface to minimize the area at fixed available volume—causes the fragmentation of a liquid ligament into smaller droplets via breakup events. Numerical results on the breakup time show a neat asymptotic behavior when the interface width is much smaller than the ligament size. These asymptotic results are compared with the theoretical predictions of sharp interface hydrodynamics; moreover, our observations are also enriched with a side-by-side comparison of two different LBM collision operators, namely, the single relaxation time (SRT) with shifted equilibrium [30] and the multiple relaxation times (MRT) with Guo-like forcing [53]. Numerical simulations show that the distribution of velocity at the interface in the vicinity of the pinch-off region is different, causing different breakup processes. A very preliminary investigation on some of the results presented in this paper is also available in a recent conference proceedings [54].

The paper is organized as follows. In Sec. II, we recall the basic features of the numerical methodology used; in Sec. III, we report on the setup used for the numerical simulations; results will be presented in Sec. IV, and in Sec. V, conclusions will be drawn.

II. NUMERICAL MODELS

In this section, we briefly highlight the important features of the numerical methodology based on the LBM [15,19]. For extensive technical details, the interested reader is referred to the papers cited in the following. The LBM is a mesoscale numerical approach for the study of fluid dynamics, which has been successfully employed to dissect complex phenomena of scientific and technical interest in recent years [20,23,27,37,40,55,56].

The LBM is grounded on an optimized formulation of Boltzmann’s kinetic equation in which particle distribution functions \( f_\alpha(x,t) \) stream and collide on a lattice characterized by a finite set of velocities \( c_\alpha = 0, \ldots, 18 \) in our case, according to the following dynamics:

\[
\Delta_t f_\alpha(x,t) = f_\alpha(x + c_\alpha \Delta t, t + \Delta t) - f_\alpha(x,t) = -\Omega_{\text{coll}}[f_\alpha(x,t) - f_{\alpha,\text{eq}}(x,t)].
\]  

In Eq. (1), \( \Omega_{\text{coll}} \) represents the collision operator, which can be written as follows:

\[ \Omega_{\text{coll}} = \Delta t/\tau \quad (\text{SRT}), \]

\[ \Omega_{\text{coll}} = MA M^{-1} \quad (\text{MRT}), \]

\( \tau \) represents the (single) relaxation time towards local equilibrium [19]; \( M \) and \( A \) are the transformation matrix and the (diagonal) matrix of the relaxation parameters, respectively. For the details on their formulation, the reader is addressed to Ref. [43]. More specifically, the \( A \) vector has \( s_2 = s_{10} = s_{12} = s_{14} = s_{15} = s_{16} = \omega = \frac{2c_s^2}{\nu} \), and all the other free parameters equal to 1, where \( \nu \) is the kinematic viscosity and \( c_s^2 \) is the squared lattice speed of sound. No special adjustments have been considered here because modifications on the \( A \) vector should not affect hydrodynamic behavior of the employed method. For both the SRT and the MRT formulations, the term \( f_{\alpha,\text{eq}}(x,t) \) in Eq. (1) represents the distribution of (local) Maxwellian equilibrium, which is given by

\[
f_{\alpha,\text{eq}}(x,t) = \frac{c_\alpha - \mathbf{u}(x,t)}{2c_s^2} + \frac{c_\alpha \cdot \mathbf{u}(x,t)}{2c_s^2} \cdot \left( \frac{|\mathbf{u}(x,t)|^2}{2c_s^2} \right). 
\]

in which \( \rho(x,t) \) and \( \mathbf{u}(x,t) \) are the hydrodynamic macroscopic density and velocity, respectively, and \( w_\alpha \) represents the set of weights for the D3Q19 lattice [15,33]. From Eq. (1), macroscopic fluid density and velocity may be derived through the zeroth and the first population momenta, respectively, as follows:

\[
\rho(x,t) = \sum_{\alpha=0}^{N_{\text{pop}}-1} w_\alpha f_\alpha(x,t), \quad \mathbf{u}(x,t) = \sum_{\alpha=0}^{N_{\text{pop}}-1} c_\alpha w_\alpha f_\alpha(x,t). 
\]

One among the main interesting \textit{atouts} of the LBM lies in its effectiveness in dealing with nonideal multiphase flows [20]: The forcing term can be conveniently implemented in Eq. (1) to account for the phase interactions that trigger the macroscopic phase segregation. Among the various approaches proposed in the literature, we focus on the single-belt formulation of the pseudopotential Shan-Chen forcing [34,57], whose force reads

\[
\mathbf{F}(x,t) = -G_0 \psi(x,t) \sum_{\alpha=0}^{N_{\text{pop}}-1} \psi(x + c_\alpha \Delta t, t) \mathbf{c}_\alpha w_\alpha. 
\]

In Eq. (4), \( G_0 \) is the basic parameter which rules the interparticle interaction and \( \psi(x,t) \) is the \textit{pseudopotential}, a local functional of the fluid density [58],

\[
\psi(x,t) = \rho_0 \left[ 1 - \exp \left( -\frac{\rho(x,t)}{\rho_0} \right) \right]. 
\]

In this paper, we have fixed the reference density \( \rho_0 = 1.0 \): With this assumption, the interparticle strength \( G_0 \) is the only free parameter which fixes both the density ratio and the surface tension. Forcing schemes are different for the two collision operators; more in detail, for the SRT, starting from Eq. (4), the component of the interaction force along each direction can be evaluated and then used to shift the macroscopic velocities before evaluating the equilibrium distribution functions,

\[
\mathbf{u}^*(x,t) = \mathbf{u}(x,t) + \frac{\mathbf{F}(x,t) \tau}{\rho(x,t)}. 
\]
On the other hand, for the MRT scheme, we adopted the forcing scheme proposed in Refs. [38,42] where we compute the equilibrium momentum by means of the velocity evaluated as follows:

\[ u^0(x, t) = u(x, t) + \frac{F(x, t)}{2\rho(x, t)}. \]  

(6)

For both considered collision operators, the EoS of the system may be written as follows:

\[ P(\rho) = \rho c_s^2 + \frac{\rho^2 G_0}{2} \psi^2. \]  

(7)

Before ending this methodological section, some remarks on the models used are in order. The main difference in between the two collision operators is that the SRT is solved into space, whereas the MRT projects the distribution functions into momentum space by means of the matrix product. This technical passage allows for increasing the stability and robustness of the method itself. Regarding the equilibrium properties (i.e., density ratio, surface tension, etc.), it is well known that the basic Shan-Chen formulation is affected by some pathologies (i.e., density ratio, surface tension, etc.), it is well known that the basic Shan-Chen formulation is affected by some pathologies.

### III. SIMULATIONS SETUP

We have performed the LBM simulations in a three-dimensional (3D) box of \( L_x L_y L_z \) lattice sites. The Plateau-Rayleigh instability is triggered through a sinusoidal perturbation with a fixed amplitude and a constant wavelength (see Fig. 1). More specifically, the initial condition for the ligament radius is \( \delta(x) = R_0 + \delta \sin \left( \frac{\pi x}{L_x} \right) \), where \( R_0 \) is the unperturbed ligament radius. The domain size and the ligament radius are chosen to accommodate roughly two wavelengths of the most unstable mode of the instability [6]. The perturbation \( \delta \) is assigned the three different values of \( R_0/30, R_0/20, \) and \( R_0/10 \). The breakup phenomenon is driven by some characteristic parameters, and between them, the Ohnesorge number (Oh)

#### TABLE I. Main simulation parameters at \( G_0 = -5.3 \) and \( \text{Oh} = 0.1 \) as a function of ligament radius for the SRT.

<table>
<thead>
<tr>
<th>( R_0 ) (LU)</th>
<th>14</th>
<th>28</th>
<th>42</th>
<th>56</th>
<th>70</th>
<th>84</th>
<th>98</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L_x )</td>
<td>256</td>
<td>512</td>
<td>768</td>
<td>1024</td>
<td>1280</td>
<td>1536</td>
<td>1792</td>
</tr>
<tr>
<td>( L_y = L_z )</td>
<td>96</td>
<td>192</td>
<td>288</td>
<td>384</td>
<td>480</td>
<td>576</td>
<td>672</td>
</tr>
<tr>
<td>( \tau )</td>
<td>0.67926</td>
<td>0.76297</td>
<td>0.83053</td>
<td>0.90311</td>
<td>0.97021</td>
<td>1.03776</td>
<td>1.10647</td>
</tr>
<tr>
<td>( t_{\text{cap}} )</td>
<td>335</td>
<td>912</td>
<td>1611</td>
<td>2380</td>
<td>3189</td>
<td>4015</td>
<td>4846</td>
</tr>
<tr>
<td>( \rho_i )</td>
<td>2.1167</td>
<td>2.1254</td>
<td>2.1348</td>
<td>2.1450</td>
<td>2.1557</td>
<td>2.1666</td>
<td>2.1775</td>
</tr>
<tr>
<td>( \rho_0 )</td>
<td>0.0836</td>
<td>0.0900</td>
<td>0.0974</td>
<td>0.1059</td>
<td>0.1156</td>
<td>0.1264</td>
<td>0.1383</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>0.05345</td>
<td>0.05775</td>
<td>0.06277</td>
<td>0.06848</td>
<td>0.07491</td>
<td>0.08206</td>
<td>0.08991</td>
</tr>
</tbody>
</table>

#### TABLE II. Main simulation parameters at \( G_0 = -5.3 \) and \( \text{Oh} = 0.1 \) as a function of ligament radius for the MRT.

<table>
<thead>
<tr>
<th>( R_0 ) (LU)</th>
<th>14</th>
<th>28</th>
<th>42</th>
<th>56</th>
<th>70</th>
<th>84</th>
<th>98</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L_x )</td>
<td>256</td>
<td>512</td>
<td>768</td>
<td>1024</td>
<td>1280</td>
<td>1536</td>
<td>1792</td>
</tr>
<tr>
<td>( L_y = L_z )</td>
<td>96</td>
<td>192</td>
<td>288</td>
<td>384</td>
<td>480</td>
<td>576</td>
<td>672</td>
</tr>
<tr>
<td>( \tau )</td>
<td>0.67293</td>
<td>0.74445</td>
<td>0.79942</td>
<td>0.84575</td>
<td>0.88667</td>
<td>0.92350</td>
<td>0.95745</td>
</tr>
<tr>
<td>( t_{\text{cap}} )</td>
<td>347</td>
<td>981</td>
<td>1803</td>
<td>2775</td>
<td>3878</td>
<td>5098</td>
<td>6424</td>
</tr>
<tr>
<td>( \rho_i )</td>
<td>2.1086</td>
<td>2.1086</td>
<td>2.1086</td>
<td>2.1086</td>
<td>2.1086</td>
<td>2.1085</td>
<td>2.1085</td>
</tr>
<tr>
<td>( \rho_0 )</td>
<td>0.0778</td>
<td>0.0779</td>
<td>0.0779</td>
<td>0.0779</td>
<td>0.0778</td>
<td>0.0778</td>
<td>0.0778</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>0.04951</td>
<td>0.04952</td>
<td>0.04952</td>
<td>0.04955</td>
<td>0.04953</td>
<td>0.04953</td>
<td>0.04954</td>
</tr>
</tbody>
</table>
study at changing the ligament radius (lattice units hereafter), which allows a fair grid convergence instability [6].

and the capillary time $t_{\text{cap}}$ are defined as follows:

$$
\text{Oh} = \frac{\mu}{\sqrt{\rho_l \sigma R_0}}, \quad t_{\text{cap}} = \sqrt{\frac{\rho_l R_0^3}{\sigma}},
$$

(8)

where $\rho_l$ is the liquid density, $\mu$ is the dynamic viscosity, and $\sigma$ is the surface tension. For our numerical simulations, the interparticle strength $G_0$ [27,37] has been fixed to $-5.3$ LU (lattice units hereafter), which allows a fair grid convergence study at changing the ligament radius $R_0$ from values comparable to the interface thickness to values much larger. Regarding the choice of the Ohnesorge number, a few remarks are in order. According to the literature on the breakup of liquid ligaments [62–64], it is known that, for Oh $< 1$, instability phenomena of the liquid jet start to take place, causing the formation of pinched regions, which, eventually, lead to the breakup of the liquid column. To accomplish our analysis in the LBM framework, we have fixed Oh $= 0.1$, which is a well-established value on the pinching breakup regime [65]. Moreover, through such a value, it is possible to have a set of corresponding numerical viscosities that grant the numerical stability of the LBM algorithm [15,33] as explained in the following. The ligament radius $R_0$ has been varied in the range of 14–98 LU. Table I reports the corresponding values of density ratio and surface tension retrieved with the SRT approach for the different values of $R_0$. To accurately evaluate the surface tension $\sigma$ as a function of the ligament radius, we first carried out a set of steady-state simulations to perform the well known Laplace test [66]. With the SRT collision operator, the Laplace test requires accounting for the natural adaptation of $\sigma$ to the kinematic viscosity value [57], whereas in the MRT framework, such an effect is absent. To retrieve a reliable value for the surface tension for all ligament radii reported in Table I, we have implemented an iterative procedure aimed at providing stable values for $\sigma$. More specifically, we chose a first attempt estimation for the viscosity, aimed at ensuring numerical stability; with the corresponding $\tau$, we have performed the Laplace test according to three values of the static droplet radius, obtaining a first estimate of $\sigma$. By using the obtained value of surface tension in Eq. (8), we find the new viscosity value that meets the $\text{Oh} = 0.1$ target: Since the values of $\sigma$, $\rho_l$, and $\rho_v$ (vapor density) are intimately connected to that of $\tau$ in the SRT approach, we have iterated the above-described procedure until the relative error on two consecutive values of surface tension was less than 5%. For the MRT, no such procedure was needed as viscosity variations have a negligible impact on the algorithm. Once we acquired the asymptotic surface tension value for both collision operators, we performed simulations with flat interfaces to find the correct liquid and vapor densities corresponding to the simulation parameters. Finally, after this last set of simulations, we obtained all the input data needed to perform the ligament simulations. Table II displays the values of density ratio and surface tension obtained with the MRT collision operator: As is apparent from the comparison between Tables I and II, the values provided by the MRT display a negligible dependence of the physical properties on the employed computational grid.

Before closing this section, we notice that the breakup of a thin ligament has already been studied by means of an axisymmetric LBM formulation in Refs. [67–71]; in this paper, we extend the results already available in the literature by performing a 3D grid convergence analysis by analyzing the effect of different collision operators on the predictions of hydrodynamics and by performing a more detailed analysis on the properties of the breakup process.

IV. RESULTS

According to the parameters reported in Tables I and II, we have performed the numerical simulations for the breakup of the liquid ligament for $\delta = R_0/10$. In Fig. 2, we report results on the time evolution (up to the breakup point) and the breakup times $t_{\text{break}}$ at changing the grid resolution. Note that the breakup time has been made dimensionless with respect to the capillary time $t_{\text{cap}}$. For both collision operators, we observe a very neat trend of the breakup time increasing with the simulation resolution and, thus, with the initial radius $R_0$, in line with the numerical results in Ref. [72]. In our working conditions, sharp interface hydrodynamics predicts a dimensionless breakup time that is a function only of the Oh and $\delta$ (see Ref. [73] and references therein). Since the Oh and $\delta$ are fixed, the observed grid dependency cannot be explained in terms of sharp interface hydrodynamics, and it is an effect induced by the finite width of the interface. It naturally becomes the question of how much these finite width effects are hydrodynamical. To cope with this issue, one would need to use a diffuse interface hydrodynamic solver for the corresponding hydrodynamic equations predicted by the LBM [15,33]. Finite width effects are expected to be negligible for large resolutions, and one can use the results of sharp interface hydrodynamics (see Ref. [73] and references therein) for comparison. For the Ohnesorge number used $\text{Oh} = 0.1$, the breakup process is known to produce two mother droplets and two satellite droplets. In Fig. 2(b), the cases in which stable secondary droplets are found are reported with filled symbols. We would like to stress that only stable droplets have been considered, that is, secondary droplets that live for a period of time, at least, comparable to the capillary time $t_{\text{cap}}$. It is known, in fact, that, in the pseudopotential framework of LBM multiphase flows, small droplets tend to be reabsorbed in the vapor phase as discussed in Refs. [40,74]. In our simulations, the SRT provides stable secondary droplets for $R_0 \geq 70$ LU, whereas the MRT collision operator provides
secondary droplets that live considerably less than a single capillary time. Such a short-living feature is due to their initial diameters, which tend to be smaller with the MRT than with the SRT. By comparing the diameters obtained with the two collision operators to the analytic, numerical, and experimental results in the literature [50,75,76], we find that the SRT approach provides more accurate predictions. This surely calls for a careful comparison with the existing LBM data in the literature. Earlier investigation by Premnath and Abraham [67] used an axisymmetric LBM formulation with source terms embedded in the LBM dynamics in the Bhatnagar-Gross-Krook (BGK) approximation. The Carnahan-Starling EoS was used with a dynamic viscosity ratio of 4 between the liquid and the vapor phase. The authors report the formation of satellite droplets with an initial cylinder radius of 50 grid points (their Fig. 7), hence well below our largest resolutions used. Srivastava et al. [68] proposed an axisymmetric LBM formulation with the Shan-Chen force and the forcing scheme provided by the equilibrium shift, essentially the same as our forcing scheme for the SRT simulations. For $\text{Oh} = 0.09$, they reported the formation of satellite droplets with a dynamic viscosity ratio of about 30, which is consistent with our results. Another axisymmetric LBM formulation proposed by Liang et al. [70] makes use of a phase field van der Waals model and adds the forcing term as a source to the BGK evolution. They use an initial cylinder radius with 60 grid points and report the presence of satellite droplets with a dynamic viscosity ratio of about 16.6. In the recent investigation by Liu et al. [71], the authors report numerical simulations with an axisymmetric LBM with a color-gradient model and a MRT collision operator, reporting the formation of satellite droplets. Finally, in the recent simulations by some of the authors with the Shan-Chen force for a multicomponent fluid and a MRT forcing scheme, the emergence of the satellite droplets was found [77]. These facts said, it is likely that the missed formation of satellite droplets in our MRT simulations originates from the chosen EoS and the choice of a viscosity ratio that sensibly differs from one.

Although at a very qualitative level, results in Fig. 2 provide a clue to a physically different behavior of the two collision operators with the SRT looking “more physical” than the MRT. This result is strange and counterintuitive since the Chapman-Enskog analysis predicts that SRT is affected by extra forcing-dependent stress contributions, which are large at large forces (i.e., close to interfaces). These observations stimulated further analysis on the quantitative comparisons between the numerical simulations and the theoretical predictions. To this aim, we kept the resolution fixed to the largest used in Fig. 2 and investigated the breakup time at changing $\delta$. In Fig. 3, results of the numerical simulations are compared with the predictions of sharp interface hydrodynamics from Ref. [52] and linear stability analysis. Regarding the latter, the growth rate $\omega$ is considered as a function of both the wave number and the Ohnesorge number (see Eq. (28) in Ref. [6]). Knowing the growth rate, the breakup time in the linear approximation can be calculated from $T_{\text{break}} = \ln(R_0/\delta)/\omega$.
We note that the MRT collision operator is well aligned with linear stability analysis reported in Ref. [49], whereas the SRT is practically overlapped with result presented in Ref. [52] where computation fluid dynamics Navier-Stokes (NS) simulations have been used for the same test case. In view of the results displayed in Figs. 2 and 3, one then asks where the mismatch between the two collision operators emerges, i.e., whether it is in the initial stage (where we are linearly unstable) or later at the pinch-off stage. To answer this question, we inspected the perturbation growth rate in the initial stage of the ligament destabilization and considered the ligament *silhouettes* for the whole dynamics up to breakup. The results are reported in Fig. 4. We observe that the initial destabilization process is the same and well in line with the prediction of sharp interface hydrodynamics.

The difference between the two dynamics rather lies in the pinching regime. To have a deeper understanding of the ligament deformation near the breakup, we also look at the nondimensional “minimum” ligament radius as a function of the nondimensional time. Results are reported in Fig. 5. The minimum ligament radius is defined as the smallest radial coordinate in a configuration at a given time. We further make this quantity dimensionless by normalizing with the initial ligament radius. Note that sharp interface hydrodynamics predicts a linear trend of the minimum ligament radius [5,78] and the linear trend is more in line with the SRT dynamics than the MRT. It is worth noting that the above presented method is characterized by a diffuse interface which tends to occupy few sites but some technicalities have been developed so to reduce the number of nodes occupied by the interface. Moreover, this thickness cannot be zero, such as a sharp interface solver, and, its tuning will represent an additional degree of freedom while approaching these simulations. In the present paper, we have decided to modify the ligament radius while keeping

![Figure 4](image1.png)

**FIG. 4.** Panel (a): Normalized perturbation with respect to the initial perturbation value at $x \approx L_x/2$ (and $x = L_x/8$ in the inset) as a function of nondimensional time. Panel (b): Three snapshots of interface evolution at $t^* = 7–9$ both for the SRT and for the MRT.

![Figure 5](image2.png)

**FIG. 5.** Normalized minimum ligament height near the breakup time.
unchanged the interface thickness rather than modify the lattice sites occupied by the interface with the same ligament radius. To delve deeper into the problem, we compare the velocity profiles for the ligament during the time evolution of the surface instability leading to the liquid column breakup. Results are displayed in Fig. 6. The figure displays the dimensionless velocity magnitude $v^* = \frac{\mathbf{u} \cdot \mathbf{v}}{R_0/t_{cap}}$ for both collision operators for selected times. To facilitate a comparison between the velocity distribution and the curvature profile, we compare the spatial distribution of the velocity field in both the MRT and the SRT at similar interface morphology. We observe that the dimensionless velocity profiles are different for the MRT and the SRT, both in spatial distribution and in magnitude. This difference in velocity greatly pertains to the vapor phase, and the velocity distributions are differently correlated to the curvature: whereas, for the SRT, the velocity localizes in the region of maximum curvature, for MRT, it localizes in the regions of maximum curvature changes. Moreover, when curvature increases, the velocity contributions increase. A quantitative assessment of how much the observed velocity distribution is spurious would require the solution of the full hydrodynamic equations in the presence of a vapor phase [6]. Nevertheless, the difference between the SRT and the MRT emerging from Fig. 6 suggests that both collision operators lead to spurious contributions that develop “dynamically” and whose spatial localization is different for the same curvature profiles. Specifically, if the spurious currents on the MRT are more localized at the pinch-off region, this can cause the breakup time to be different and the satellite droplets to be smaller after breakup. One could then reconsider the comments on the hydrodynamic recovery via the Chapman-Enskog theory: Although the SRT has extra terms with respect to the MRT in its Chapman-Enskog expansion, the mismatch may be originated by the fact that the impact of spurious currents is more effective in the present MRT implementation. In other words, the bulk equations are more correct in the MRT than in the SRT, but the interface boundary conditions are dynamically more spurious in the MRT than in the SRT. One could think of readsorbing this effect of spurious current in a modified stress tensor so that the dynamics of the MRT would be that of a system with a slightly different Ohnesorge number. At the largest resolution analyzed, however, this would not be possible: We do not observe any steady satellite droplets, whereas theory predicts them to exist [64]. Summarizing, for the specific test case analyzed, the pinching of the interface generates momentum, and it is significantly influenced by the distribution of spurious currents. As we may observe from Fig. 6, the MRT with this specific set of parameters shows a stronger concentration of velocities in the pinching region, whereas the SRT presents weaker interference. We think this is the reason why the breakup dynamics captured from the SRT better matches the expected results, despite presenting some possible lacks of consistency while reconstructing the NS equation.

V. CONCLUSIONS

We have investigated the dynamics of a liquid ligament perturbed via a Plateau-Rayleigh instability by means of the LBM. More specifically, we have considered two LBM collision operators, the SRT and the MRT, implemented in a multiphase numerical scheme based on the Shan-Chen EoS [34,36,57]. We have seen that numerical simulations display a neat asymptotic behavior in the limit where the interface thickness is sensibly smaller than the characteristic radius of the liquid ligament. Such behavior has been compared with the predictions of sharp-interface hydrodynamics [5,78] for both LBM environments. Adopting the same EoS, the two collision operators displayed a different behavior with the SRT providing results more adherent to the theoretical and experimental evidence from the literature, compared to the MRT. In particular, even if the breakup dynamics presents a very similar trend between the two collision operators in the early stages of the instability, the SRT provides a pinching evolution closer to the theoretical predictions with the eventual formation of a long-living secondary droplet after the ligament breakup, which we have not detected in the MRT environment. This difference is traced back to the dynamic distribution of spurious currents rising in the pinching region.
For the specific realizations of EoS adopted, the MRT—
despite a higher numerical stability granted in the set of
hydrodynamical parameters characterizing the simulation—
displays a spurious currents pattern localized towards the flex
of the ligament silhouette in the pinching region; the SRT,
on the other hand, is characterized by a different distribution
of the spurious velocities, which appear to be localized away
from the pinching region, hence the dynamics of the ligament
breakup is less affected by such a spurious pattern and pro-
vides results closer to the sharp-interface hydrodynamics.

On a more general perspective, some comments are in or-
der. Our results show that, whenever spurious currents effects
are weak in the pinching region, the LBM results can quan-
titatively match the ones obtained through the sharp-interface
hydrodynamics from the initial perturbation destabilization up
to the breakup point. The fact that our simulations with the
SRT perform better than the MRT may well depend on the
specificity of the parameters chosen here, causing dynamical
spurious currents to distribute less in the pinching region.
Although the issue of spurious currents has been pretty well
detailed for “static” problems [27,32,60,79–81], very little is
known about dynamical problems. Hence, we do not want to
promote a collisional operator rather than the other; instead,
we want to point out that different dynamical distributions of
spurious currents may produce quantitatively different results.

Of course, this is just a macroscopic property which obviously
hide many nontrivial dependencies on the parameters and
technical details of the models used. This also opens up
future perspectives in determining the impact of the different
parameters or choices at hand (e.g., EoS, thermodynamic
consistency, surface tension coupling with EoS, collisional
scheme, interface width, Knudsen effects, etc.) to obtain a
“unifying view” on what are the causes behind the emergence
of dynamical spurious currents.

ACKNOWLEDGMENTS

The numerical simulations were performed at the Zeus
High Performance Computing (HPC) Facility at the
University of Naples “Parthenope;” the Zeus HPC
has been realized through the Italian Government Grant
No. PAC01_00119 “MITO-Informazioni Multimediali per
Oggetti Territoriali” with Professor E. Jannelli as the
Scientist Responsible. This project has received funding
from the Italian Government Program PRIN Grant No.
20154EHYW9. M.S. and X.X. thank the European Union’s
Horizon 2020 Research and Innovation Programme under the
Marie Skłodowska Curie Grant Agreement No. 642069 for
support.

[1] G. H. Yeoh, Handbook of Multiphase Flow Science and
Atomization and Drop Burning Phenomena (American Institute
of Aeronautics and Astronautics, Reston, VA, 1996).
(2007).
(2010).
(1989).
(2010).
(2017).
Preskininzi, C. Barroo, D. C. Bell, M. M. Biener, J. Biener, B.
[24] G. Di Ilio, D. Chiappini, S. Ubertini, G. Bella, and S. Succi,
(2010).
[27] M. Sbragaglia, R. Benzi, L. Biferale, S.ucci, K. Sugiyama,
Matter 8, 3798 (2012).
[33] T. Krüger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva,
and E. M. Viggen, The Lattice Boltzmann Method (Springer,