Many-body Dissipative Particle Dynamics simulation of capillary pinch-off

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Abstract

The MDPD method provides a mesoscale description of the liquid-gas interface where molecules can be thought of as grouped in particles with modeled Brownian and dissipative effects. No liquid-gas interface is explicitly defined; surface properties, such as surface tension, result from the MDPD interaction parameters. In this paper, the mesoscale character of MDPD is demonstrated in the context of jet pinch-off by comparison with the asymptotic scaling predictions for large, intermediate and low Ohnesorge numbers. We observe that the predominant behavior at a large Oh number tends to be dominated by thermal fluctuations, whereas at smaller Oh a viscous-inertial and even an inviscid flow behavior can appear. One MDPD simulation in particular displays all the three regimes. The fact that eventually the final stage of pinch-off follows the stochastic scaling suggests that a stochastic element cannot be completely neglected in continuum discretizations. We also clarify in what sense MDPD results for multiphase flow are convergent, that is, independent from the coarse-graining level. Finally, the thickness of the micro-bridge that forms just before capillary pinch-off is discussed with and without the interaction with a still gas.
Introduction

In the study of free-surface flows, the advantage of methods like Dissipative Particle Dynamics (DPD) resides in the simplicity of the underlying algorithm of particle interaction under a soft repulsive potential. While substantially less expensive than Molecular Dynamics (MD), DPD can be formally constructed from coarse-graining of Lennard-Jones clusters [1]. DPD has been used to investigate phase separation in immiscible binary liquid mixtures [2], [3] [4], droplet deformation and rupture in shear flow [5], and droplets on surfaces under the influence of shear flow [6]. The standard DPD method presents, however, a fundamental limitation, in that in single-species fluid flows the repulsive soft potential alone cannot reproduce surface tension. In fact, the DPD potential leads to a predominantly quadratic pressure-density equation of state (EOS) [7], while a higher-order pressure-density curve is necessary for the coexistence of the liquid and vapor phases.

Single-species phase coexistence in a liquid occurs in the range of densities $\rho_V < \rho < \rho_L$ where $\rho_V$ and $\rho_L$ are the pure vapor and liquid number densities. In that state, surface tension emerges from the asymmetry of the intermolecular forces acting on a layer of molecules at the liquid-vapor interface. As this asymmetry causes larger intermolecular distances in the outer layer than in the liquid bulk, the forces in that layer act to contract the interface.

In the Many-body DPD (MDPD) method by Pagonabarraga and Frenkel [8], the amplitude of the soft repulsion is made proportional to the local density of the particles, thus achieving a cubic pressure-density relation, and an attractive force is added. A similar approach was introduced by Nugent and Posch in the context of Smoothed Particle Hydrodynamics (SPH) [9]. MDPD has been extensively investigated by Warren [10] and Trofimov et al. [11].

In this paper, the MDPD technique is applied to the study of liquid thread pinch-off. The dependence of surface tension on the interaction parameters in relation with the bulk density of the fluid was clarified by Arienti et al. [12]. Here, an example illustrates the link between the interaction forces and the fluid properties. The sense in which an MDPD simulation can converge to a time-dependent solution is also explained in this introductory section. The main body of the paper demonstrates the ability of MDPD to capture the complete sequence of scaling behaviors – inviscid, inertial-viscous and stochastically dominated – that the asymptotic analysis of slender jets has identified. Simulations are carried out for different viscosities of the fluid and also in the presence of a DPD gas.

MDPD scheme

MDPD inherits the three pairwise-additive inter-particle forces formulation of the standard DPD scheme. The conservative, dissipative and random forces are defined, respectively, as

$$F_{ij}^C = F_{ij}^C(r_{ij})\hat{r}_{ij}$$  \hspace{1cm} (1)

$$F_{ij}^D = -\gamma \omega_p(r_{ij}) (v_{ij} \cdot \hat{r}_{ij})\hat{r}_{ij}$$  \hspace{1cm} (2)

$$F_{ij}^R = \Theta(\xi \omega_r(r_{ij}) \hat{r}_{ij})$$  \hspace{1cm} (3)

where $\hat{r}_{ij} = r_{ij}/|r_{ij}|$ and $v_{ij} = v_i - v_j$.

Warren’s approach [13] is pursued for the conservative term. The repulsive force depends on a weighted average of the local density, whereas the attractive force is density-independent:

$$F_{ij}^C = A_{ij}\omega_c(r_{ij}) + B_{ij}(\bar{\rho}_i + \bar{\rho}_j)\omega_d(r_{ij})$$  \hspace{1cm} (4)

The weight functions $\omega_c(r) = (1 - r/r_c)$ and $\omega_d(r) = (1 - r/r_d)$ vanish for $r > r_c$ and $r > r_d$, respectively. Since a DPD method with a single range may not have a stable interface [9], in Equation (4) the repulsive contribution is set to act at a shorter range $r_d < r_c$ than the soft
pair attractive potential. The many-body repulsion is derived from a self-energy per particle which is quadratic in the local density, 
\[ B_i(\bar{\rho}_i + \bar{\rho}_j)\omega_d(r_{ij}) \], where \( B > 0 \). The MDPD number density is defined as
\[ \bar{\rho}_i = \sum_{j \neq i} \omega_d(r_{ij}) \]  
(5)
and its weight function \( \omega_d \) is
\[ \omega_d(r) = \frac{15}{2\pi r_d^3}(1 - r/r_d)^2. \]  
(6)
This kernel vanishes for \( r > r_d \) and is normalized for convenience: \( \int d^3r \omega_d(r) = 1 \).

The MDPD thermostat is the same as the DPD thermostat. It consists of random and dissipative forces, which maintain the equilibrium temperature \( T \) through the condition posed by the fluctuation-dissipation theorem
\[ \xi^2 = 2\gamma k_b T, \]  
(8)
with \( (\omega_d^2) = \omega_d^D \). \( k_b \) is the Boltzmann constant. \( \mathbf{F}_{ij}^d \) is modeled as a Gaussian distribution with zero first moment and second moment proportional to the temperature. Thus, the dissipative force \( \mathbf{F}_{ij}^d \) acts to reduce the kinetic energy of the particle and is compensated by the random motion induced by the stochastic part, \( \mathbf{F}_{ij}^R \). The weight function for the dissipative force is
\[ \omega_d(r) = (1 - r/r_c)^2 \]  
(9)
Details about the choice of \( \xi \) and \( \gamma \) can be found in [13]. The simulations presented in this work are carried out with the velocity Verlet algorithm of Groot and Warren [13] using the empirical parameter value of 1/2.

Since the random and dissipative forces of MDPD are common with DPD, particles from the two schemes can be easily combined. This enables the simulation of more complex flows, for instance the inclusion of a surrounding gas. Table 1 offers an example of two different sets of parameters: the first row corresponds to an MDPD fluid, the second to a DPD gas. In the latter, the sign of the coefficient \( A \) is switched and there is no density-dependent term. An example of MDPD-DPD interaction will be presented later.

We conclude this Section by mentioning that the simulations are enabled by the particle dynamics software code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [14], to which a new MDPD class was added. The computationally scalable implementation of LAMMPS guarantees the optimization of the interaction calculation through an efficient neighbor list algorithm, and will not be discussed here.

**MDPD properties**

Conventionally, dissipative particle dynamics methods operate in reduced units, so that length is measured in units of \( r_c \) and mass in units of \( m \), the mass of a single particle. Choosing the physical units of length (\( L_{DPD} \)), mass (\( M_{DPD} \)), and time (\( T_{DPD} \)) allows one to obtain a specific set of MDPD properties, for instance in relation with the properties of a real liquid.

Let us consider the set of interaction parameters \( A = 40, B = 25, r_d = 0.75 \); see Table 1. The number density \( \rho \), the kinematic viscosity \( \nu \) and the surface tension coefficient \( \sigma \) are not simulation inputs, but they can be evaluated with simple numerical tests. For instance, by applying the Young-Laplace relation to a spherical drop in equilibrium we find \( \rho = 6.1 \) and \( \sigma = 7.3 \); see Ref. [12] for a systematic study of the dependence of surface tension on the interaction parameters. Viscosity can be assessed in a different test, for instance one where a doubly periodic Poiseuille (DPP) flow is established. The description of a convenient procedure for creating two opposite Poiseuille flows can be found in Ref. [15]. In the example that follows, the kinematic viscosity is determined by the choice of \( \gamma = 0.005 \) and \( \xi = 0.1 \).
If the same properties of surface tension coefficient, density and viscosity are expressed in physical units and labeled with an asterisk, dimensional analysis yields to

\[
M_{\text{DPD}} = L_{\text{DPD}}^3 \frac{d^*}{d}, \quad T_{\text{DPD}} = \left( \frac{M_{\text{DPD}} \sigma}{\sigma^*} \right)^{1/2}, \quad \frac{L_{\text{DPD}}^2}{T_{\text{DPD}}} = \frac{\nu^*}{\nu} \tag{10}
\]

From these equations, the properties of water at ambient conditions \((d^* = 998 \text{ kg/m}^3, \sigma^* = 0.0720 \text{ N/m}, \text{ and } \nu^* = 1.00 \cdot 10^{-6} \text{ m/s})\) are matched by taking \(M_{\text{DPD}} = 3.94 \cdot 10^{-18} \text{ kg}, \quad T_{\text{DPD}} = 7.32 \cdot 10^{-7} \text{ s}, \quad \text{and } L_{\text{DPD}} = 3.18 \cdot 10^{-6} \text{ m}.\) The number of molecules per MDPD particle is obtained directly from \(M_{\text{DPD}}\) divided by the mass of a water molecule; it is \(n = 1.47 \cdot 10^7.\)

The set of equations (10) reveals the link between the viscosity of the system and \(L_{\text{DPD}}\): everything else being the same, the smaller is \(\nu^*\), the greater is the coarse-graining. Other properties however, such as the non-dimensional isothermal compressibility \(\kappa^{-1} = (\partial P/\partial \rho)_T/k_B T\), will not in general coincide with the properties of the reference liquid. For this MDPD fluid, we find \(\kappa^{-1} \approx 50\) (based on the generalized equation of state proposed by Warren [10]), whereas the actual value for water is \(\kappa^{-1} = 16.\) Thus, the operation of matching surface tension coefficient, density and kinematic viscosity of a liquid may lead to different interaction parameters than the ones obtained by imposing equal compressibility.

It is to be noted that the MDPD kinematic viscosity can be changed by varying the dissipation coefficient \(\gamma.\) This operation can be carried out while keeping the temperature of the fluid the same, as long as Equation (8) is satisfied. Tables 2 illustrates the results for an MDPD system where \(\gamma = 72, 0.5 \text{ and } 0.005.\) The first column (viscosity \(\nu = 0.96\)) was calculated instead for a DPD system with parameters \(A = 10, B = 0, r_d = 0,\) and with particle mass \(m = 0.00647.\) With these parameters, the number density is 0.935 particles per unit cube and the compressibility is \(\kappa^{-1} \approx 1 + 0.202 \cdot \rho_G / k_B T = 1.19,\) according to the empirical relation by Warren [10]. The DPD parameters are listed at the bottom row of Table 1 and will be used for an MDPD/DPD simulation later on.

**Table 1.** Example of parameter sets for DPD and MDPD fluids.

<table>
<thead>
<tr>
<th>(m)</th>
<th>(A)</th>
<th>(r_c)</th>
<th>(B)</th>
<th>(r_d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-40</td>
<td>1</td>
<td>25</td>
<td>0.75</td>
</tr>
<tr>
<td>0.00647</td>
<td>10</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 2.** Kinematic viscosity of DPD and MDPD fluids at \(k_B T = 1.\)

<table>
<thead>
<tr>
<th>(\gamma)</th>
<th>(\nu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.96</td>
</tr>
<tr>
<td>72</td>
<td>2.8</td>
</tr>
<tr>
<td>0.5</td>
<td>0.93</td>
</tr>
<tr>
<td>0.005</td>
<td>0.072</td>
</tr>
</tbody>
</table>

**MDPD coarse-graining**

MDPD is proposed as a truly mesoscopic method that can bridge the gap between the atomistic scale (in the range of nanometers and nanoseconds) that is accessible by molecular dynamics (MD) simulations and the macroscopic scale (in the range of micrometers and milliseconds) considered by continuum descriptions. To this end, it is important to define in what sense a simulation is independent from a specific level of coarse-graining.

Of the various approaches that have been proposed, the one by Füchslin [16] for a DPD system is particularly instructive. Let us consider a system whose particle number \(N\) has been scaled by a factor \(\phi\) while keeping the domain size constant. Denoting with a prime the new equivalent system, so that \(N' = N/\phi\)
and \( m' = m \phi \), the scaling relations in three dimensions are \( r_c' = r_c \phi^{1/3} \) and \( t' = t \phi^{1/3} \). The first relation maintains the fractional particle overlap in the change of the coarse-graining level, while the second ensures that velocity increments calculated during one time step are the same for the two systems. The interaction parameters require to be modified as a function of the coarse-graining level:

\[
A' = A \phi^{2/3} \quad (11) \\
\gamma' = \gamma \phi^{2/3} \quad (12) \\
\xi' = \xi \phi^{2/3}. \quad (13)
\]

This procedure can be extended to MDPD [12] by adding the primed parameters

\[
r_d' = r_d \phi^{1/3} \quad (14) \\
B' = B \phi^{5/3} \quad (15)
\]

Scale independence holds for bulk interactions because the energy associated with an individual particle is made proportional to the number of molecules it represents. It is noted, however, that, while the stress tensor terms are unaffected by coarse-graining, the kinematic viscosity scales like \( \phi^{1/3} \). Thus, for an increased coarse-graining \( N'/N > 1 \) (so that \( \phi < 1 \)), the viscosity, \( \nu' = \nu \phi^{1/3} \), decreases. Similarly, even if \( \sigma' = \sigma \phi^{1/3} \), the surface tension is invariant (\( \phi^{1−1/3−2/3} = \phi^0 \)).

Coarse-graining is illustrated in Figure 1. The jet, repeated periodically in the axial direction, is 10 DPD units long. A small axial perturbation is applied to the jet with wavelength \( \lambda = 10 \). The jet radius is chosen so that \( \lambda/R = 9.01 \). This length-to-radius ratio corresponds to the fastest growing rate of capillary instability according to linear analysis. The wavelength corresponds to 31.8 \( \mu m \) in the physical units from the previous section, and \( R = 7.07 \mu m \). A preliminary series of calculations at a larger radius (not shown here) confirms that the Plateau condition on the minimum surface energy for pinch-off is respected.

![Figure 1](image)

**Figure 1.** Convergence study of jet pinch-off. See text for details.
independently from coarse-graining [12]: the jet returns to the equilibrium cylindrical shape if the jet radius \( R \) is larger than \( \lambda/2\pi \).

Each snapshot in Figure 1 shows a slice of a liquid jet immediately after pinch-off. The calculation in frame (a) is carried out with the MDPD parameters listed on the first row of Table 1 and with \( \xi = 72 \) from Table 2. The time step is \( \Delta t = 0.001 \). The calculation is repeated for \( \phi = 1/8 \) in frame (b), but with the new parameter values reduced according to Equations (11) to (15). This approach is repeated for \( \phi = 1/64 \) in frame (c), and for \( \phi = 1/512 \) in frame (d). The baseline simulation has 287 particles and takes less than a minute to run on a single-core CPU. The number of particles increases then by a factor 8 in each of the following calculations, while the interactions become correspondingly more distributed. As the coarse-graining is reduced, the development of a thin liquid bridge that rapidly retreats toward the newly formed drops becomes more defined. The shape of the pinched thread can be said to be converged at \( \phi = 1/64 \) since there are minimal differences with the \( \phi = 1/512 \) calculation. The extended thin long thread before pinch-off is in agreement with the deterministic approximation to the Navier-Stokes equations [17]. Overall, no qualitative differences are observed between the different levels of coarse-graining; particularly, the pinch-off is symmetric and no satellite drops are formed in this configuration.

**Local dynamics near pinch-off**

A number of authors have carried out local analyses of the Navier–Stokes equations for pinching threads; see, for instance, Ref. [17]. To establish a connection with the theory, the minimum thread radius \( h_{\text{min}} \) from the simulation is plotted as a function of the time to breakup, \( \tau \). Even if in reality every MDPD simulation has its own specific trajectory, this plot is expected to follow a specific power law depending on the Ohnesorge number of the flow, \( \text{Oh} = \rho^{1/2} \nu / (R \sigma)^{1/2} \).

According to the analysis of the Navier–Stokes equations, pinch-off asymptotically proceeds (in the absence of an outer fluid) according to a solution that balances surface tension, viscous, and inertial forces. However, for sufficiently small values of Oh, viscosity drops out of the description; it follows from dimensional analysis that \( h_{\text{min}} \sim (\sigma \tau^2/\rho)^{1/3} \sim \tau^{2/3} \). Viscous effects eventually become important as the minimum radius continues to decrease and becomes of order \( \text{Oh}^2 \). At that point, the flow transitions to an inertial-viscous regime where the scaling is \( h_{\text{min}} \sim \tau \).

On even smaller scales, it can be postulated that the driving force leading to pinch-off consists of thermal fluctuations at the molecular level. The relevant length scale appears from the comparison of the thermal energy with the surface energy,

\[
\ell_T = \sqrt{k_B T / \sigma}.
\]  

In this regime, fluctuations speed up the breakup process, dominating over the effect of surface tension.

The domain concerned by thermal fluctuations (up to a few hundreds of nanometers) has been recently probed by Molecular Dynamics simulations of nanojets [18]. From an analysis standpoint, a set of one-dimensional dynamical equations can be derived from the Navier-Stokes equations in the limit of a thin layer of liquid where inertia, the component of velocity normal to the surface, and the in-plane derivatives are neglected. These “lubrication equations” are fully deterministic, but stress fluctuations can be added via a stochastic term [19]. The flow obeying to the Stochastic Lubrication Equations (SLE) exhibits a self-similar profile resembling two cones joined at their apexes (called the double-cone profile) and leading to a symmetric pinch-off. The relation between \( h_{\text{min}} \) and \( \tau \) is described by a power law with exponent 0.418, found by numerical integration [20].

According to theory then, it should be possible to observe in a logarithmic plot of
$h_{\text{min}}(\tau)$, the 2/3 slope first, then the slope 1, and finally the 0.418 slope. However, spanning the three scaling behaviors in a single pinch-off simulation has so far proven computationally prohibitive. This is because the first transition from inviscid behavior depends on Oh, but the second occurs for $h_{\text{min}} \sim \text{Oh}^2$, at sub-micron scales for most liquids. In the following example we will demonstrate that such a simulation is possible with MDPD. To this end, instead of changing the domain scale, we take a constant reference jet radius, as well as given fixed values of surface tension and density, and decrease the viscosity of the fluid until all the three regimes appear.

The simulation takes place in a $40^3$ periodic cube. To track the minimum jet radius as a function of time, it is necessary to post-process several snapshots of particle positions according to the following procedure. The computational domain is first axially divided into 50 bins; then the center of mass of each slice of the jet is calculated. This is a crucial step in measuring the radius profile because the liquid thread can oscillate during the pinch-off process. For each bin, an histogram of number density is constructed in annular rings with a radial increment of $10^{-3}$ units. The surface of the liquid slice is identified at a position such that 1% or less of the particles of the bin lie outside the surface. This small number of particles is assumed to belong to the vapor phase – a threshold consistent with almost no vapor phase. The pinch-off time is established as the instant when one of the bins becomes empty. The time to pinch-off $\tau$ is normalized by the capillary time scale $(\rho R^3/\sigma)^{1/2}$, whereas $h_{\text{min}}$ is normalized by $R$.

The log-log plot of $h_{\text{min}}(\tau)$ in Figure 2 corresponds to the kinematic viscosity $\nu = 2.8$ (Oh=1.2). It shows a noise-dominated behavior where most of the tracked points are aligned along the slope 0.418. The plot ends with substantial noise just before pinch-off. At a smaller value of viscosity, $\nu = 0.93$ (Oh=0.41), the inertial-viscous slope 1 begins to appear (Figure 3), with a transition roughly located at $h_{\text{min}}/R \sim 0.1$. At an even smaller viscosity, $\nu = 0.072$, the 2/3 power inviscid scalings also appears, albeit briefly (Figure 4). The transition from inviscid to viscous-inertial takes place at $h_{\text{min}}/R \sim 0.5$, whereas the transition from viscous-inertial to stochastic remains at $h_{\text{min}}/R \sim 0.1$. The MDPD system consists of 14776 particles and the simulation takes a few hours on an eight-core Linux machine. As mentioned above, the simulation achieves the result of showing the complete sequence of scaling behaviors that lead to pinch-off.

**Figure 2.** Variation of $h_{\text{min}}$ with $\tau$ when Oh = 1.2 ($\nu = 2.8$).

**Figure 3.** Variation of $h_{\text{min}}$ with $\tau$ when Oh = 0.41 ($\nu = 0.93$).
It can be expected that, when the characteristic size of the flow is much larger than the thermal length scale, the break-up process is dominated by deterministic factors and the pinch-off profile is characterized by long threads. For a liquid with the properties of water, stochastic effects begin to appear when the liquid thread reaches a radius of 0.1\( R \), corresponding to 1.2 \( \mu m \) in this case. Equation (16) also gives \( \ell_T = 0.37 \) DPD units, that is, \( \ell_T = 1.2 \mu m \). This suggests that a stochastic element should not be completely neglected in high-fidelity calculations of spray formation.

When the size of the flow is comparable to the thermal length scale, the pinch-off profile resembles a double-cone [17]. A remainder of this shape is perhaps visible at the tips of the separating ligament threads in Figure 1. A similar conical shape also appears when studying the effect of the ambient gas on the dynamics of pinch-off, as we shall see now.

The presence of a gas surrounding a capillary thread can be neglected until \( h_{\text{min}} \sim M \) Oh\(^2 \), where \( M \) is the ratio of the viscosity of the ambient gas to that of the liquid [21]. We add now to the MDPD fluid a DPD gas using the parameters listed on Table 1, bottom row. The values are selected to obtain the density ratios of water with respect to air: \( (m \rho)_G / (m \rho)_L = 998 \). The dissipation parameters are set so that \( v_G / v_L = 13 \). Finally, we choose the inter-particle DPD-MDPD parameters to be the same as the DPD parameters: \( A = 10, r_c = 1, B = 0, rd = 0, \gamma = 2 \) and \( \xi = 2 \). The repulsive force coefficient between the liquid and the gas is \( A_{12} = 10 \). This value avoids inter-penetration of the two species, but no studies are presently available to define how \( A_{12} \) should be calculated; it is reasonable to take \( B_{12} = 0 \).

A snapshot of the simulation is shown in Figure 5, where the denser fluid jet after pinch-off is clearly distinguishable from the surrounding DPD gas. The plot of \( h_{\text{min}}(\tau) \) is in Figure 6. Both figures indicate that the effective behavior of the MDPD fluid becomes

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**Figure 4.** Variation of \( h_{\text{min}} \) with \( \tau \) when \( \text{Oh} = 0.032 \) (\( \nu = 0.072 \)).

**Figure 5.** MDPD fluid pinch-off in a still DPD gas.

**Figure 6.** Variation of \( h_{\text{min}} \) with \( \tau \) when \( \text{Oh} = 0.032 \) in the presence of a DPD gas (\( v_G / v_L = 13 \)).
more viscous in the presence of the gas even if the Oh number is small. The jet profile is close to the double-cone self-similar profile of SLE, which has been recently observed in MD simulations of nanojets [18]. This is an interesting but very preliminary result; the interaction of an MDPD fluid with a surrounding gas will be the matter of further investigations.

Conclusions

The spatial and temporal mesoscales (within 10 and 1000 nm and within 1 ns and 10 ms) that are captured by coarse-graining particle techniques can significantly extend the reach of molecular dynamics (MD) simulations while keeping the fundamental viewpoint that fluid properties arise from elementary particle interactions. In particular, the MDPD scheme provides a viable mesoscale description of free-surface flow of single-species fluid.

This paper shows how matching the surface tension coefficient, the density and the kinematic viscosity of a given liquid with the properties of a system of MDPD particles determines all the interaction parameters. In a convergence study applied to jet pinch-off, the occurrence and shape of a thin liquid thread are shown to become independent from the level of coarse-graining when the number of molecules per particles is sufficiently small.

The principal result of this paper is to show that MDPD simulations agree with the asymptotic scaling predictions for large, intermediate and low Oh number. Particularly, the behavior at large Oh is dominated by thermal fluctuations, whereas at smaller Oh a viscous-inertial and even an inviscid flow behavior can appear. One simulation displays all three regimes, proving the truly mesoscopic range of MDPD.

It can be argued that, independently from the reference Oh number, a point is reached in the simulation when any fluctuation towards a smaller neck radius accelerates the pinch-off more effectively than surface tension. This behavior, previously observed in nanojets, can also be thought of as the final state of jet rupture in the micrometer range.

A simple demonstration of a two-species flow concludes this work. It is natural to use MDPD to model a liquid and DPD to model a gas, since both techniques use the same thermostat. Future work will concentrate on imposing a flow rate on the gas field, so that pinch-off under shear can be simulated.

Acknowledgements

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Nomenclature

\begin{align*}
A & \quad \text{MDPD attractive force coefficient; DPD repulsive force coefficient} \\
B & \quad \text{MDPD repulsive force coefficient} \\
d & \quad \text{fluid density} \\
F_c^{ij} & \quad \text{inter-particle conservative force} \\
F_d^{ij} & \quad \text{inter-particle dissipative force} \\
F_r^{ij} & \quad \text{inter-particle stochastic force} \\
h_{\text{min}} & \quad \text{minimum thread radius} \\
k_B & \quad \text{Boltzmann constant} \\
\ell_T & \quad \text{thermal length } \sqrt{k_B T/\sigma} \\
L_{\text{DPD}} & \quad \text{DPD unit length} \\
m & \quad \text{mass of an MDPD particle} \\
M & \quad \text{ratio of gas to liquid viscosity} \\
M_{\text{DPD}} & \quad \text{DPD unit mass} \\
n & \quad \text{number of molecules per particle} \\
N & \quad \text{number of particles in the system} \\
\text{Oh} & \quad \text{Ohnesorge number } \rho^{1/2} \nu / (\sigma \nu)^{1/2} \\
R & \quad \text{reference jet radius} \\
r_c & \quad \text{cut-off distance} \\
r_d & \quad \text{cut-off distance of repulsive core} \\
T & \quad \text{temperature} \\
t & \quad \text{time} \\
T_{\text{DPD}} & \quad \text{DPD unit time} \\
\phi & \quad \text{scaling factor } m'/m \\
\gamma & \quad \text{coefficient in dissipative force} \\
\kappa^{-1} & \quad \text{compressibility } (\partial P/\partial \rho)_T/k_B T, \\
\lambda & \quad \text{wavelength of axial perturbation} \\
\nu & \quad \text{kinematic viscosity}
\end{align*}
\( \theta_{ij} \) random number drawn from a Gaussian distribution
\( \rho \) number density
\( \sigma \) surface tension coefficient
\( \tau \) time to pinch-off
\( \xi \) coefficient in stochastic force
\( \omega \) weight function

Subscripts
12 MDPD-DPD particle interaction
G gas
L liquid phase
V vapor phase

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