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Numerical simulations of multi-phase electro-hydrodynamics flows using a simple incompressible smoothed particle hydrodynamics method

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Abstract

Practically, every processing technology deals with complex multi-phase flows and predicting the fluid flow behaviour is crucial for these processes. Current study discusses the application of a mesh-less numerical methodology, i.e. Incompressible Smoothed Particle Hydrodynamics (ISPH) to investigate the behaviour of different multi-phase flow systems. This works is presented in a coherent way with increasing test problem difficulties and their concerned physical complexities. A wide range of problems including Laplace's law, bubble rising, bubble suspension under an external electric field are considered for a code validation purpose, while the numerical results manifest very good accordance with the experimental and theoretical data. Finally, we show the effectiveness of using an external electric field for controlling a complex problem such as Couette flow for a range of electrical permittivity and electrical conductivity ratios. It is noted that the Electrohydrodynamics (EHD) effect on a suspended droplet in Couette flow case is simulated for the first time using the SPH method.

Keywords: Smoothed Particle Hydrodynamics (SPH), Meshless methods, ElectroHydrodynamics (EHD), Multi-phase flow, Couette flow

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1 I. Introduction

Predicting the behaviour of multi-phase flow systems has attracted for decades the atten-2 3 tion of many industries due to their wide ranges of applications in the chemical engineering, aerospace engineering and renewable energy sectors, among others [1, 2, 3]. In multi-phase sys-4 tems two or more fluids share interfaces which can deform/ migrate as outcome of exerted forces 5 and constitutional laws. Some applications of multi-phase systems include boiling, condensa-6 tion, water purification and petroleum refinement processes where these phenomena have been 7 investigated mostly experimentally and theoretically. However, with the ever-increasing power 8 of Computational Fluid Dynamics (CFD) methods, numerical simulations of these systems be-9 came of great interest among researchers [4, 5, 6]. 10 Smoothed Particle Hydrodynamics (SPH) is a relatively recent and promising mesh-less La-11 grangian method which discretizes the domain into a set of nodes, known as material particles. 12 These particles can freely move inside the computational domain subject to an external force or 13 particle-particle interactions. Initially introduced by Gingold and Monaghan [7], and Lucy [8]14 for astrophysics applications, SPH was soon found to be suitable for fluid dynamics problems, 15 where complex geometries [9, 10, 11], large deformations [12, 13, 14], multi-phase [15, 16, 17] and 16 multi-physics problems [18, 19, 20] are involved. A recent overview for the application of SPH 17 can be found in [21]. 18 One of the most important engineering problems which involves many of above cases is the 19

Electrohydrodynamics (EHD) one, where hydrodynamics of a fluid system is coupled with its 20 response to an external electric field. In EHD problems, one may control the interface between 21 the two fluids (here, the droplet and the bulk fluid) by controlling the flow conditions and fluid 22 properties [22, 23]. In such problems, the coupling may lead to a large interfacial deformation 23 (i.e. merge/breakup) or migration. Indeed, EHD is a very complex problem including multi-24 phase, multi-physics and multi-scale phenomena with strong topological changes of the interface 25 shape [24, 25]. Although, there are many experimental and theoretical studies available in the 26 literature on the coupled modeling of EHD problems [26, 27, 28]. Nevertheless, some discrep-27 ancies between experiments and analytical data still exist 28. As such, numerical simulations 28 have been developed to tackle these difficulties and provide insight into EHD problems. 29 Considering the numerical simulations of EHD using SPH method, Shadloo et al. [29] were 30 the first group to provide a model for such problems. They validated their code with the simple 31 EHD deformation of droplets suspended in a neutrally buoyant Newtonian fluid. Rahmat et 32 al. have proposed a multi phase ISPH method based on the lubrication theory and the drainage 33 model to simulate droplet electro-coalescence for wide ranges of simulation conditions. [30, 31]. 34 Rahmat et al. [32] also provided the first simulation results for the Rayleigh-Taylor instability 35

³⁶ under the combined effect of electric field and gravitational forces. Yet, step-by-step validation of

the SPH method for each individual force using the same methodology is not well-documented.
Additionally, numerical simulation of a multi-phase flow under the effects of an electric field

using various scenarios ranging from low to high deformations, droplet migration, and effect of
shear flow on the droplet's deformation would provide a broader perspective into the capabilities
of the SPH method for such applications. To this end, this article aims at introducing a mesh-less
numerical methodology, i.e. Incompressible SPH (ISPH) approach, to deal with such complex
problems. Additionally, we verify the applicability of some of the used algorithms for a range of
problems including hydrodynamic, capillary, gravity, shear and EHD forces.

This article is organized as follows: First, we introduce the mathematical formulation of the 45 SPH method as well as the numerical discretization scheme. Then, we incorporate the governing 46 equations of the multi-phase system including the conservation equations for mass, momentum 47 and electrical charges in a Lagrangian form. Thereafter, a code validation and numerical conver-48 gence study is asserted in the absence of electric field. Numerical results cover solutions with 49 and without electric filed sections. Additionally, the effect of surface tension through Laplace 50 law, the effect of gravitational force, and the Couette flow for a multi-phase system are examined 51 and validated against analytical solution and available numerical data in the literature. Finally, 52 conclusions are provided in the last section. 53

54 2. Mathematical Formulation of SPH

The idea of SPH comes from the fact that any field variable f(x) can be calculated by an exact mathematical relation as

$$f(x) = \int_{\Omega} f(x')\delta(x')dx'.$$
 (1)

⁵⁷ Upon approximating $\delta(x')$ by an interpolation function W(x - x', h), this equation can be for-⁵⁸ mulated as

$$f(x) = \int_{\Omega} f(x')W(x - x', h)dx',$$
(2)

where x and x' are the position vectors and h is the smoothing length. In our case, $h = \zeta dx$ where $\zeta = 1.6$ is a constant value, and dx is the initial particle spacing. The interpolation function, also known as smoothing function or kernel function, should have, among others, the following properties [33]

- Normalized over the domain

$$\int_{\Omega} W(x - x', h) dx = 1.$$
(3)

- Produces δ function for a small enough smoothing length

$$\lim_{h \to 0} W(x - x', h) = \delta(x'). \tag{4}$$

- Remains monotonically decreasing throughout the entire domain.

- Has a compact support, meaning that for |x - x'| > kh

$$W(x - x', h) = 0.$$
 (5)

- Is a symmetric function.

Initially, the kernel functions were defined such that each particle should have interactions with all others [7]. By introducing the concept of Neighboring particles¹, kernel function affect only a compact support around it were substituted (see Eq. (5)). Depending on the smoothing length parameter h, only a few number of particles in the entire space affect the approximated value of the kernel function (around 25 to 35 in 2D). In the current work, a cubic spline kernel function is used both for the balk fluid and the interface modeling while taking harmonic average.

$$W_{ij} = A \begin{cases} 2/3 - (r/h)^2 + 1/2(r/h)^3 & r/h \in [0,1) \\ 1/6(2 - r/h)^3 & r/h \in [1,2). \\ 0 & r/h \ge 2 \end{cases}$$
(6)

75

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Hereafter, W(x - x', h), will be shown by W_{ij} and $A = \frac{15}{7\pi h^2}$. Also, i, j, and r represent the index of the particle of interest, the index of its neighbors, and the smoothing radius.

To calculate the SPH gradients, one can show that it is sufficient to differentiate the kernel function W(x - x', h). In other words, in SPH there is no need to differentiate the field function f(x); instead one can differentiate the kernel function. The latter is one of the fascinating features of the SPH method which distinguishes this method from other mesh-based techniques. In this work, we use an improved version of the first derivative, presented in [34] as

$$\frac{\partial f_i^m}{\partial x_i^k} a_i^{kl} = \sum_j \frac{1}{\psi_j} (f_j^m - f_i^m) \frac{\partial W_{ij}}{\partial x_i^l}.$$
(7)

Also, the derivatives for vectorial and scalar quantities are calculated, respectively, as follows:

$$\frac{\partial^2 f_i^m}{\partial x_i^k \partial x_i^k} a_i^{ml} = 8 \sum_j \frac{1}{\psi_j} (f_i^m - f_j^m) \frac{\partial W_{ij}}{\partial x_i^l} \frac{r_{ij}^m}{r_{ij}^2},\tag{8}$$

¹particles that are located within the range of the kernel function with respect to the particle of interest. Outside of this range, the kernel function has already dropped to zero.

86 and

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$$\frac{\partial^2 f_i}{\partial x_i^k \partial x_i^k} (2 + a_i^{kk}) = 8 \sum_j \frac{1}{\psi_j} (f_i - f_j) \frac{\partial W_{ij}}{\partial x_i^k} \frac{r_{ij}^k}{r_{ij}^2},\tag{9}$$

where ψ is the particle number density and a_i^{kl} represents a corrective second rank tensor to avoid particle inconsistencies[9].

90 3. Governing Equations

Assuming an immiscible two-phase Newtonian, viscous, incompressible, isothermal fluid system, the corresponding mass and momentum conservations in a Lagrangian formulation are given as follows

$$\frac{D\rho}{Dt} = -\rho \nabla. \vec{V},\tag{10}$$

94 and

$$\rho \frac{DV}{Dt} = \nabla \mathcal{T} + \vec{f}^b + \vec{f}^s + \vec{f}^e, \tag{II}$$

⁹⁵ where, ρ is the fluid density, $\frac{D}{Dt}$ is the material time derivative operator², $\nabla . \vec{V}$ is the divergence ⁹⁶ of the velocity vector, \mathcal{T} is the total stress tensor which is defined as $\mathcal{T} = -pI + \tau$ where p is the ⁹⁷ static pressure, I is the identity matrix and $\tau = \mu (\nabla \vec{V} + (\nabla \vec{V})^T)$ is the viscous dissipation term ⁹⁸ for μ being the dynamic viscosity.

Additionally, $\vec{f}^b = \rho \vec{g}$ is the body force due to gravity and \vec{f}^s is the surface tension which can be calculated using the volumetric force proposed by Brackbill [35], so called the Continuum Surface Force (CSF) method, as

$$\vec{f}^s = \gamma \kappa \vec{n} \delta^s. \tag{12}$$

Here, γ is the surface tension coefficient, $\kappa = -\nabla . \vec{n}$ is the interface curvature, $\vec{n} = \frac{\nabla C}{|\nabla C|}$ is the unit vector normal to the interface, and $\delta^s = |\nabla C|$ is surface Dirac-delta function, and finally, \vec{f}^e is the electric field force.

To avoid sharp discontinuities at the interface, the smoothed color function of the particle iis defined as

$$C_i = \frac{\sum_j W_{ij} c_j}{\sum_j W_{ij}},\tag{13}$$

where the color function *c* assigns a unit value to one phase and zero to the other phase in a two-phase system such that

²The material time derivative is a directional time derivative for a fixed point.

$$c_j = \begin{cases} \mathbf{I}, & \text{fluid A} \\ \mathbf{o}, & \text{fluid B} \end{cases}.$$

Furthermore, this approach provides a clear definition for the volume fraction of each fluid, i.e. $C_i^A = C_i$ and $C_i^B = 1 - C_i$ define the volume fraction corresponding to the fluid A and fluid B, respectively, such that $\sum_n C_i^n = 1$ for all *n* phases, here n = 2.

As mentioned before, in this study the electrostatics and the hydrodynamics are coupled together. This coupling is achieved through the Maxwell stress tensor. Maxwell equations provide a mathematical framework for the interaction and the connection between the electric and the magnetic fields [36]. Here, the EHD part of the system can be regarded as quasi-static model, and dynamic currents values are so low, hence the induced magnetic field effects are negligible. Therefore, the contribution from the induced magnetic field is neglected. Consequently, the volumetric electric force can be written as

$$\vec{f}^e = \nabla.T^E. \tag{14}$$

In case of an application of the external electric field on a multi-phase fluid flow, this new term for the electric force, will be added to the right hand side of the momentum equation (see Eq. (II)), where the Maxwell's stress tensor defines as

$$T^{E} = \vec{D}\vec{E} - \frac{1}{2}(\vec{D}.\vec{E})$$
I, (15)

where \vec{E} is an external electric field, $\vec{D} = \epsilon \vec{E}$ is the dielectric displacement vector, and ϵ is the electrical permittivity. Also, based on the Gauss's law [36]

$$\nabla . \dot{D} = q^{\nu}, \tag{16}$$

where q^{ν} is the free electric charge density.

126 Application of Eqs. (15) and (14) will result in

$$\vec{f}^e = q^v \vec{E} - \frac{1}{2} \vec{E} \cdot \vec{E} \nabla \epsilon.$$
(17)

In this work both fluids are considered to be leaky dielectric, (i.e. electric relaxation time is much shorter compared to its viscous counterpart or $t^e \ll t^{\nu}$).

129 4. Time integration

We apply a predictor-corrector scheme to advance the governing flow equations in time considering a first-order Euler approach. The time-step is selected based on Courant-Friedrichs-Lewy (CFL) condition in which $\Delta t = C_{CFL}h/V_{max}$, with V_{max} being the largest magnitude of

109

particle velocity and the C_{CFL} is the constant taken as 0.25. During the predictor step, we first advance all the variables to an intermediate value denoted by (*), from the variables' value at the *n*-th time-step denoted by superscript (*n*), as

$$\vec{r}_{i}^{*} = \vec{r}_{i}^{(n)} + \vec{V}_{i}^{(n)} \Delta t + \delta \vec{r}_{i}^{(n)}, \tag{18}$$

136

$$\vec{V}_{i}^{*} = \vec{V}_{i}^{(n)} + \frac{RHS}{\rho_{i}^{(n)}} \Delta t,$$
 (19)

137

$$\psi_i^{(*)} = \psi_i^{(n)} - \Delta t \psi_i^{(n)} (\nabla . \vec{V}_i^*).$$
(20)

RHS denotes the right hand side of Eq. (II), $\psi_i = \sum_j W_{ij}$, is the number density associated with the particle of interest *i*, which is calculated from the summation of kernel function at all neighboring particles *j*, δr_i is the artificial particle displacement, defined as $\delta r_i^k = \alpha \sum_{i}^{N} (r_{ii}^k/r_{ii}^3) r_{io}^2 V_{max} \Delta t$, and its constant α is set to 0.05 according to [34].

These intermediate values will then be used to solve the Poisson equation which gives the pressure value at the next time-step (n + 1). Using this pressure, new velocity and displacement vectors are updated as following

$$\nabla \cdot \left(\frac{1}{\rho_i^*} \nabla p_i^{(n+1)}\right) = \frac{\nabla \cdot \vec{V}_i^*}{\Delta t},\tag{21}$$

145

$$\nabla . \vec{V}_{i}^{(n+1)} = \vec{V}_{i}^{*} - \frac{1}{\rho_{i}^{*}} \nabla p_{i}^{(n+1)} \Delta t, \qquad (22)$$

146

$$\vec{r}_i^{(n+1)} = \vec{r}_i^{(n)} + 0.5(\vec{V}_i^{(n)} + \vec{V}_i^{(n+1)})\Delta t + \delta \vec{r}_i^{(n)}.$$
(23)

147 5. Results

148 5.1. Validation and convergence

To ensure a suitable particle resolution based on the numerically computed pressure jump 149 across the interface, in Fig.2 the data is represented for 60×60, 100×100 and 140×140 grids. To 150 study numerical convergence, a droplet with the radius of r = 0.01 [m] is situated at the center 151 of a square domain, *i.e.* $x_o/r = y_o/r = 2$, with the side lengths of x/r = y/r = 4 (see Fig. 152 1). While the Dirichlet (no-slip) boundary condition is set for the velocity at all four boundaries, 153 namely, BC-X1, BC-X2, BC-Y1, and BC-Y2, the Neumann boundary condition is applied for the 154 pressure field. As for the hydrodynamics properties, we keep both viscosity and density ratios 155 equal to unity such that $\rho_1 = \rho_2 = 1000 \, [\text{kg/m}^3]$ and $\mu_1 = \mu_2 = 0.1 \, [\text{Pa.s}]$ and set the 156 surface tension to $\gamma = 0.01$ [N/m], given neither electrical nor gravitational force. 157



Figure (1) Schematic of the test case for validation and numerical convergence test, bubble rising as well as bubble deformation under the effect of electrohydrodynamics (EHD). For the first test case $\vec{g} = 0$ and $\vec{E} = 0$, for the second one $\vec{g} \neq 0$ and $\vec{E} = 0$ while for the third one $\vec{g} = 0$ and $\vec{E} \neq 0$

This problem, known as Young-Laplace problem, has an analytical solution which is $\Delta p =$ 158 $p_i - p_o = \gamma/r = 1$. As can be seen in Fig.2-Left, the pressure oscillations decrease by increasing 159 the resolution from the coarser to the finest and the results, converging towards the analytical 160 solution. It is noted that the relative error is less than 1% for the intermediate particle resolution. 161 Therefore, we chose the 100×100 resolution for our simulations as it provides accurate results 162 with reasonable computation cost. Similar simulations, with different surface tension coefficient 163 are tested, while putting r = 0.5 |m| and keeping x/r and y/r ratios constant to validate the 164 accuracy of the used method. As can be seen in Fig.2-Right, the pressure jump increases by an 165 increment in the surface tension confirming the capability of the method to capture the physical 166 jump across the interface. Once more for the reported simulations, the relative error is less than 167 1% when the numerical results are compared to the Laplace's law. 168

It is noteworthy to discuss the reason behind the different values obtained for the theoretical 169 and numerical pressure jump at the interface. As mentioned before, the pressure and other flow 170 field variables (velocity, color function, etc.) are approximated using the numerical smoothing 171 scheme which converts the sharp values at the interface to smoother ones resulting in a loss of 172 accuracy and introduction of spurious oscillations near the surface of the droplet. Furthermore, 173 it is found that these spurious currents are generated because of an inappropriate evaluation of 174 the curvature of the circular droplet due to unreliable values for the unit normal vector (\vec{n} = 175 $\frac{VC}{|\nabla C|}$ in the surface tension force calculation [37]. 176



Figure (2) Comparison of (left) the pressure jump across the droplet interface for three particle resolutions and (right) its comparison with the theoretical pressure jump, *i.e.* Laplace's law, for different cases.

177 5.2. Bubble rising

In this section, the ISPH method is applied to test and to validate the simulation of the 178 bubble rising problem due to the gravitational force. The computational geometry for this test 179 case is similar to the one shown in Fig. 1 except that the domain size is increased in the normal 180 direction (orthogonal), *i.e.* x/r = 6 and y/r = 12, and the bubble is initially placed such 181 that $x_o/r = 3$ and $y_o/r = 2.4$. The grid resolution is set to 240×480 in x and y direction, 182 respectively. The velocity boundary conditions are set to be free slip for BC - X1 and BC - X2, 183 and no slip for BC - Y1 and BC - Y2. Also, pressure boundary conditions are set to be Dirichlet 184 with a constant value at $BC - Y^2$ and Neumann for the other three boundaries ($\nabla p \cdot \vec{n} = 0$) 185 where \vec{n} is normal direction to the given boundary. 186

Here, both bubble and bulk phases are set to have stationary conditions at initial time step.
 The bubble starts to rise during the simulation due to the gravitational forces. This problem can
 be characterized by Reynolds and Bond numbers defined as following:

$$Re = \frac{\rho_2 g^{0.5} (2r_o)^{1.5}}{\mu_2},\tag{24}$$

190 and

$$Bo = \frac{\rho_2 g(2r_o)^2}{\gamma}.$$
 (25)

¹⁹¹ respectively.

For the first simulation, a case with low density and viscosity ratios and high surface tension is considered, where $\rho_2/\rho_1 = 10$ with $\rho_1 = 100$ [kg/m₃], $\mu_2/\mu_1 = 10$ with $\mu_1 = 1$ [Pa.s], and surface tension coefficient is $\gamma = 24.5$ [N/m]. Additionally, the gravity is set to be $\vec{g} =$



Figure (3) Time evolution of bubble rising problem with the density ratio of $\rho_1/\rho_2 = 0.1$ and viscosity ratio of $\mu_1/\mu_2 = 0.1$ at different dimensionless times $t^* = 0.5$, $t^* = 18.5$, $t^* = 37$ and $t^* = 64.8$. Here the dimensionless time is defined as $t^* = t\sqrt{(g/D)}$ and Reynolds and Bond numbers are Re = 35 and Bo = 10, respectively. The left half of each snapshot shows the velocity streamlines in black and the droplet interface in red, while the right half shows the velocity magnitude's to highest levels' contour in the range of [0, 4.5] [m/s].

-1[m/s2] in y direction such that it produces Reynolds number Re = 35, and the Bond num-195 ber Bo = 10 for this case. The time snapshot of this test case for dimensionless times of $t^* = 0.5$, 196 $t^* = 18.5, t^* = 37$ and $t^* = 64.8$ are shown in Fig. 3. As observed in this figure, the bubble 197 starts to rise straight upwards due to the gravity, while its velocity increases from zero to 0.36 198 [m/s] and remains constant until it feels the pressure coming from the stationary upper-wall. 199 Additionally, the bubble shape is changing from circular shape to a quasi elliptical one due to 200 hydrodynamic pressures on its tip. The final shape comes from the competition among surface 201 tension, gravitational, and viscous forces. As it is observed, the shape remains unchanged after 202 some time steps which is the main reason for the bubble's almost constant terminal velocity. 203

Fig. 4 shows the mean migration velocity and the position of the droplet with respect to dimensionless time $t^* = t\sqrt{(g/D)}$, which are in agreement with the results of [31] and [38]. Here, the velocity gradient near the stationary wall starts to deviates at the final times which could be due to the confinement effects.

To show the applicability of the proposed algorithm for capturing larger deformations and breakups, we perform a second bubble rising test case. This time, the computational domain size is x/r = 6 and y/r = 10 with the particle resolution of 240×400 . The bubble is initially placed at $x_o/r = 3$ and $y_o/r = 2$. Here, all four boundaries have no slip boundary condition for



Figure (4) The average normalized central position of the droplet, \bar{y} (top) and its average vertical migration velocity, \bar{y} (bottom) as a function of dimensionless time, t^* .

velocity. However, the pressure boundary conditions are kept the same as before. The gravity is selected as $\vec{g} = -1$ [m/s2] in y direction, while the surface tension coefficient is set to be $\gamma = 20$ [N/m]. Additionally, the density and viscosity ratios are $\rho_2/\rho_1 = 1000$ and $\mu_2/\mu_1 =$ 2.828/10 with $\rho_1 = 1$ [kg/m3] and $\mu_1 = 1$ [Pa.s], respectively. These choices are for mimicking the test case presented in [15] in order to produce the fluid flow system with Reynolds and Bond numbers of Re = 1000 and Bo = 200, respectively.

The snapshots of our current simulations are illustrated (middle) in Fig. 5 for the dimensionless times between $t^* = 3.2$ and $t^* = 5.6$ with a time increment of $\Delta t^* = 0.4$. These snapshots are compared to their experimental (top) and Volume of Fluid method (bottom) counterparts, presented in [39] and [40], respectively. As can be seen, the proposed ISPH approach can predict the large deformation and bubble breakup as accurate as its well establish mesh based method. The presented Volume of fluid (VoF) method uses a hybrid VoF-level-set method [40] to accurately capture the interface.



Figure (5) Comparison of bubble rising and break up due to gravitational and hydrodynamic forces using experiment [39], SPH method and Volume of Fluid method [40], respectively from top to bottom rows. Here, the density ratio $\rho_2/\rho_1 = 1000$ and viscosity ratio $\mu_2/\mu_1 = 10$ are applied. Reynolds and Bond numbers, as previously defined, are Re = 1000 and Bo = 200, respectively. The dimensionless time is defined as $t^* = t\sqrt{g/r_o}$, starting from $t^* = 3.2$ at the very fist frame on the left, up to $t^* = 5.6$, with a time increment of 0.4 per frame.

225 5.3. EHD droplet deformation

In this section, we consider a suspended circular droplet under the effect of an external ap-226 plied electric field. The schematic of the computational domain is similar to what is presented 227 in Fig. 1 with an increment in the size of the domain. Here, we double the domain size in each 228 direction, *i.e.* x/r = 8 and y/r = 8, in order to reduce the confinement effect. In Fig. 6-left, 229 a particle resolution of 240×240 is used with a circular droplet initially placed at the center of 230 computational domain. The initial zero velocity are assigned to both fluids and wall particles. 231 Density ratio and viscosity ratio are set to unity with values of $ho_1 =
ho_2 = 1000$ [kg/m³] and 232 $\mu_1 = \mu_2 = 1$ [Pa.s]. The surface tension coefficient $\gamma = 1$ [N/m]. The velocity and pressure 233 boundary conditions are exactly the same as those imposed in section 5.1. The electrical bound-234 ary conditions are Dirichlet ($\varphi = cte$.) and Neumann boundary ($\nabla \varphi \cdot \vec{n} = 0$) conditions for 235 horizontal (*i.e.* BC - Y1 and BC - Y2) and vertical walls (*i.e.* BC - X1 and BC - X2), respec-236 tively, where \vec{n} is normal direction to the given boundary. 237

The deformation of a suspended circular droplet under such conditions is a commonly utilized test case for validation of a EHD solver, where two theories are available in the literature. Taylor [41] estimates the droplet deformation D_T as

$$D_T = \frac{9f_{dT}E_o^2\epsilon_2 r_o}{8(2+R)^2\gamma},\tag{26}$$

where f_{dT} is the discriminating function evaluated as

$$f_{dT} = R^2 + 1 - 3.5S + 1.5R.$$
⁽²⁷⁾

For the same problem, Feng [42] suggests the following relation

$$D_F = \frac{f_{dF} E_o^2 \epsilon_1 r_o}{3(1+R)^2 S \gamma},\tag{28}$$

where f_{dF} is estimated from

$$f_{dF} = R^2 + 1 - 3S + R.$$
⁽²⁹⁾

In Eqs. (26) and (28), r_o is the initial droplet radius before its deformation and E_o is the electric field intensity in vertical direction which is calculated from $E_o = (\varphi^+ - \varphi^-)/H$, H being the domain height. Additionally, the permittivity ratio and the conductivity ratio of droplet to the balk are called S and R, presented as

$$S = \frac{\epsilon_1}{\epsilon_2}, \quad R = \frac{\sigma_1}{\sigma_2},$$
 (30)

where ϵ and σ are the electrical permittivity and conductivity, respectively. Also the subscripts 1 and 2 show, droplet and bulk medium properties, respectively.

Another point in the theory of droplet deformation is to investigate the velocity recirculation 250 vectors inside and outside of the droplet when a vertical electric field is applied. The relative 251 differences in the electric permittivity and conductivity of both constituent phases define the 252 direction of the flow rotation in either phase. This is shown for two cases in Fig. 6. On the left 253 side test case is adopted for S = 0.5 and R = 0.05 with the electrical permittivity of the droplet 254 (ϵ_1) being 0.5 [F/m] which is half of that of the bulk fluid. Also, the electrical conductivity of 255 the droplet (σ_1) is set to 150 [S/m] which is three-times more than the background fluid. On 256 the right side of Fig. 6, the test case has S = 0.5 and R = 3 with $\epsilon_1 = 0.5$ and $\sigma_1 = 1$. As can 257 be seen in the left sub-figure, the re-circulation zone in the first quarter (i.e. the top-right quarter 258 inside the droplet) of the droplet orients clockwise. This should be the case for S > R and is 259 consistent with the results of [29]. The opposite flow circulation pattern should be expected for 260 the case of S < R as it also presented on the right side of the same figure. 261

Additionally, Eqs. (27) and (29) define the sign of Eqs. (26) and (28), respectively. The positive sign, so called prolate deformation, indicates that the droplet is elongated in the direction parallel to the electric field. The positive sign, so called oblate deformation, shows the droplet elongation in the opposite direction. For the comparison with the simulation results, we define the numerical deformation as

$$D_N = \frac{A - B}{A + B},\tag{31}$$



Figure (6) Deformation of a suspended droplet in response to an external vertical electric field in the steady-state simulation for the cases with (left) S = 0.5, R = 0.05 and (right) S = 0.5, R = 3.

where A and B are the elliptic droplet diameters, parallel and perpendicular to the direction of the external electric field, respectively, at the steady state condition. When this parameter is equal to zero, the droplet keeps its initial circular shape. On the other hand, more deviation from zero indicates more deformation from its initial shape.

Fig. 7 provides comparison between the current ISPH results and the two aforementioned 271 theories for multiple cases. As can be seen, numerical data reasonably follow the available the-272 ories. However, in most of the cases, an over-prediction is reported by the simulations. Some 273 might be some possible reasons for such behaviour can be mentioned: (i) in the theory it is as-274 sumed that the droplet remains circular even after applying the electric field. This means the 275 change in the curvature is not integrated in the deformation equation, but only the surface ten-276 sion coefficient. (ii) Another reason might be due to the confinement effect. In theories, it is 277 assumed that the droplet is suspended in an unbounded domain for simplicity. However, pro-278 viding such domain numerically, or even with twice larger computational domain, is very ex-279 pensive computationally. Finally, the hydrodynamical properties of droplets such as density and 280 viscosity are not taken into account theoretically and the problem is considered to be inviscid. 281

282 5.4. Couette Flow

This section investigates the deformation of a droplet suspended between two parallel plates subjected to a constant shear. The flow configuration, known as Couette flow, is presented in Fig. 8. In this case, the flow is driven by viscous forces or pressure gradients [43]. Different cases



Figure (7) Comparison of deformation for all cases. permittivity ratio, conductivity ratio and surface tension coefficient of each simulation, S, R, γ , respectively, mentioned below or above the corresponding case.

with and without an external electric field with the magnitude of unity perpendicular to the flow
direction are simulated.

The computational domain consists of a rectangle box with the size of x/r = 16 and y/r = 16288 4 discretized by a set of initially equally spaced 400×100 particles, arranged in a Cartesian grid. 289 The two-phase system contains a droplet with the initial radius of r_o , placed in the middle of the 290 domain, and the balk fluid with the same density of $\rho_1 = \rho_2 = 1000 \, [\text{kg/m}^3]$ and the dynamic 291 viscosity of $\mu_1 = \mu_2 = 0.2$ [Pa.s]. The velocity boundary conditions are set to Dirichlet (no-292 slip) on the plates (*i.e.* BC-Y1 and BC-Y2) and periodic for the inlet and outlets (*i.e.* BC-X1293 and $BC - X^2$). The pressure boundary conditions is Dirichlet $BC - Y^2$ and Neumann for the 294 rest of boundaries. Also, the boundary conditions for electrical potential are of Dirichlet at the 295 walls (*i.e.* $\varphi = cte$ in BC - Y1 and BC - Y2) and periodic for the two other sides (*i.e.* BC - X1296 and BC - X2). 297

Initially, the upper and the lower wall velocities are set to $U_o/2$ and $-U_o/2$, respectively, where $U_o = 0.02$ [m/s]. Additionally, particles inside the droplet are initialized to be at rest, while background fluid particles having undisturbed Couette flow velocity. The simulations are performed for a range of electrical permittivity and electrical conductivity ratios shown as (S, R), while neglecting the gravity and keeping the surface tension coefficient constant $\gamma =$ 0.02 [N/m]. The droplet radius is a quarter of the distance between two parallel plates (i.e. r = H/4). The dimensionless Reynolds, Weber and Electroinertial numbers, respectively, are



Figure (8) Schematic of the Couette flow test case.

305 as follows

$$Re = \frac{\rho_2 U_o r_o}{\mu_2}, \qquad We = \frac{\rho_2 U_o^2 r_o}{\gamma}, \qquad Ei = \frac{\rho_2 U_o^2}{\epsilon_2 E_o^2}, \tag{32}$$

where Re = 1, We = 0.2, and Ei = 50.

Fig.9 shows the time evolution of the droplets' deformation under the same external electric field and the shear stress conditions, but for different working fluids having different electrical permittivity and conductivity ratios (*i.e.* only a change in *S* and *R* is considered here). In this figure, the dimensionless time is defined as $t^* = tU_o/r_o$, while the droplet deformation is calculated from

$$D_f = \frac{L_{max} - L_{min}}{L_{max} + L_{min}},\tag{33}$$

where L_{max} and L_{min} are major and minor droplet diameters, respectively. As can be seen in 312 this figure, the droplet deformation increases when an external electric field is applied regardless 313 of S and R. Additionally, at the constant electrical permittivity ratio, larger deformations can 314 be achieved by an increment in the electrical conductivity ratio when S > R. However, for 315 the similar condition (*i.e.* S = cte.), smaller deformations are seen by an increment in the 316 electrical conductivity ratio when S < R. Similarly, at constant electrical conductivity ratio 317 larger electrical permitivities result in larger droplet deformations for R < S, while decreases the 318 same for S < R. It is noted that the (5.0, 0.2) and (5.0, 0.5) test problems did not reach a steady 319 profile during the simulation time, here fixed at $t^* = 1$ due to large computational costs. Fig. 320 10 provides a comparison on the interface shape in the absence (in blue) and the presence of the 321 electric field (in black) at this time. Following the previous figure, it can be seen that the droplets 322 are more slender for larger deformation factors. 323



Figure (9) Numerical deformation for twelve cases (Left), a close-up look at the rate of deformation at the steady state (Right). Cases without electric field are denoted by a black + sign. The pair number on the legend box, corresponds to the electrical permittivity and electrical conductivity (S, R), respectively.

It is notable that the angle between the major axis of the elliptic droplet and the stream-wise direction become smaller with an increment in the conductivity ratio, while the cases of (5.0, 0.2) and (5.0, 0.5) are immediately distinguishable due to their larger deformations. This elongation is due to the suppression of surface tension forces which is the result of the larger electric field force at higher electrical conductivity ratios. It is also noted that the droplet is no longer elliptical and is suspected to have the breakup at larger time steps.

Finally, the time snapshot of an extreme test case with the electrical permittivity ratio of S =330 10 and the electrical conductivity ratio of R = 0.2 is illustrated in Fig. 11 to show the ability of 331 the presented method to capture very large deformations with the interfacial topological change. 332 Here, the interface is represented by red color, while the velocity streamlines and electrical vectors 333 are represented by blue and black arrows, respectively. In this case, the circular droplet becomes 334 elliptical soon after the start of the simulation. The elliptical interface is elongated in the stream-335 wise axis direction due to the four re-circulation zones in the bulk flow just next to the interface. 336 Soon after that, pairs of re-circulation merge with each other at the both tips of the droplet and 337 cause the creation of the third re-circulation in its center. By time, the droplet gets folded in 338 four different places and new re-circulation zones appear close to the interface which makes the 339 droplet very susceptible to breakup. As can be seen, this is a promising test problem to show 340 the ability of the present ISPH code to treat the complex multi-phase fluid behavior under an 341 extreme EHD conditions with large interfacial deformation. 342



Figure (10) Bubble interface at $t^* = 1$. The pair number above each case corresponds to the electrical permittivity and electrical conductivity (S, R), respectively. If zero, the electric field is not applied.



Figure (II) Deformation of a suspended droplet in Couette flow with S = 10 and R = 0.2 subject to electric field at $t^* = 0$, $t^* = 0.4$, $t^* = 0.8$, $t^* = 1.2$ and $t^* = 1.6$, respectively, from top to bottom where dimensionless time is defined by $t^* = tU_o/r$. The velocity streamlines (in blue), the electric field vectors (in black) and the droplet interface (in red) are shown at five moments.

343 6. Summary

In this work, we presented an effective multi-phase Incompressible Smoothed Particle Hy-344 drodynamics (ISPH) approach to simulate complex multi-physics electrohydrodynamics (EHD) 345 problems. We showed a step-by-step validation of the multiphase code for surface tensions, hy-346 drodynamic forces and electric forces, respectively, by solving Laplace's law, bubble rising and 347 buoyant droplet deformation under an applied electric field problems. Results are validated 348 either against available analytical or numerical results. An overall satisfactory agreement were 349 found. Finally, we presented, for the first time, results of droplet deformation under sheared 350 Couette flow with external electric field for a range of simulation parameters. Different parame-351 ters such as time resolved topological changes, droplet deformation magnitudes as well as velocity 352 field and electrical potential vectors were presented and compared with each other. It was shown 353 that the current ISPH approach is able to be easily adopted for different multi-physics problems. 354 It is also capable of predicting large interfacial topological changes such as folding and breakup. 355 In future, our strategy would be to include more complex transport and multi-physics phenom-356 ena. 357

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