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Numerical simulation of the electrically induced deformation of a water-oil interface

J.-L. Reboud, J. Raisin and P. Atten

Abstract — As a part of a study of electrocoalescence of water droplets in oil, the electrically induced deformations of water-oil interfaces are studied. Cases of large deformations of the interfaces involve the strong coupling of hydrodynamics and electrostatics, in which cases numerical simulation is needed. The paper presents different numerical simulations performed using the commercial software COMSOL MULTIPHYSICS™ in cases of water-air or water-oil configurations with axial symmetry. Electrohydrodynamics problems are solved using ALE approach in deforming meshes. Comparisons are presented with the results of analytical developments, asymptotic approaches or experiments.

Index Terms— Electrohydrodynamics, fluid-fluid interfaces, drop deformation, coalescence, numerical simulations.

I. INTRODUCTION

¹Electrocoalescence is the phenomenon of merging droplets of conducting liquid suspended in an insulating liquid (or gas), under the action of an electric field [1]. This phenomenon is important for the petroleum industry as it is used to increase the size of water droplets suspended in crude oils and, therefore, to drastically reduce the time required to separate water and oil phases under the gravity effect. Now, compact electrocoalescers that promote electrocoalescence in a very limited time are often used [2]. But the control and increase of their efficiency are sometimes very difficult as the numerous processes involved in electrocoalescence are far from being fully understood. Other cases where this phenomenon of drops merging under the action of an electric field might be used are observed in the lab-on-a-chip domain devoted to various

chemical or biological analyses on very small amounts of products.

The action of an electric field on a water-in-oil emulsion is, first, to polarise the conducting water droplets and to promote an attraction between them. For nearly contacting droplets pairs the attraction force is strong; it induces a deformation of the droplets facing parts and often results in their merging. It is therefore necessary to distinguish the stage of build-up of drops pairs by the fluid motion (during which some droplets are brought in very close proximity), from the second stage, the coalescence itself, during which the interfaces deform and disrupt [3]. The determination of the probability of coalescence of two nearly colliding droplets as a function of the main parameters of the problem (electric field, drops size distribution, water volume fraction and flow properties) is a difficult problem. A pre-requisite is a good description of the interfaces disruption mechanism and the determination of the electrocoalescence critical conditions.

Cases of large deformations of the interfaces involve the strong coupling of hydrodynamics and electrostatics. In such cases numerical simulation is needed. Therefore, different approaches have recently been developed, as illustrated for example in [4-6]:

- Boundary element methods which allow exact description and adapted discretization of the interfaces. Meshing only the boundaries is worthwhile but restricts in practice the model to inviscid fluid flows. Merging or splitting interfaces remains challenging.
- Arbitrary Lagrangian-Eulerian (ALE) methods which associate deformation of interfaces and resolution of electrostatics and fluid dynamics equations in moving meshes. Treatment of merging or splitting interfaces is impossible and simulations should be stopped before.
- Volume of Fluid / Level set methods which involve front tracking of interfaces across fixed meshes, allowing the simulation of complete sequences including topological changes in the interface. Accuracy of interfaces location and curvature strongly depends of the initial mesh and surface forces should be transformed in volume terms.

This paper presents different numerical simulations, using 2D axisymmetric geometries, performed with the commercial software COMSOL MULTIPHYSICS™ in cases of water-air and water-oil configurations. Electrohydrodynamics problems are solved by using an ALE approach for mesh deformation that allows tracking and parameterization (surface tension and electrostatic pressure) of the fluid-fluid interfaces.

This work was developed in the framework of a collaborative research between the French CNRS and the Consortium working on the project "Electrocoalescence – Criteria for an efficient process in real crude oil systems"; co-ordinated by SINTEF Energy Research (contact person is L.E. Lundgaard). The project is supported by The Research Council of Norway, under the contract no: 169466/S30, and by the following industrial partners: Vetco Aibel AS, Aker Kvaerner Process Systems AS, StatoilHydro ASA, BP Exploration Operating Company Ltd, Shell Technology Norway AS, Petrobras..

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In the first part, basic validations of the model are presented: free oscillations of an initially elongated droplet and transient elongation of a conducting droplet in an electric field are compared with analytical results: respectively frequency and damping of oscillations, and final electrically induced elongation.

The second part concerns the deformation and instability of a horizontal interface between water and an insulating fluid, electrically influenced by a metallic sphere located just above it. Comparisons with results of experiments performed in our laboratory in the case of water-air interfaces are presented.

Finally, we investigate the deformation and coalescence of two closely spaced drops of conducting liquid suspended in an insulating fluid under the action of an electric field. The initial case deals with two facing drops anchored on capillary tubes at different electric potential. The critical conditions, corresponding to the maximum potential difference that can be applied before coalescence for a given spacing between the drops, are widely studied and compared with the results of an asymptotic approach in the common range of application.

II. MODEL

We study the deformation of the interface between a perfectly conducting liquid (water) and a dielectric one (air or oil), under the effects of an electric field. From an electrostatics point of view, the Laplace equation has to be solved to obtain the electric potential in the domain occupied by the dielectric fluid. A perfect conductivity is assumed for the conducting fluid and is implemented by prescribing a uniform potential at the interface. Electrostatic pressure acting at the interface is then equal to $\varepsilon E^2/2$ (ε : fluid permittivity, E : electric field magnitude). Velocity fields are computed by solving the time dependent Navier-Stokes equations in the water (NS1) and in the dielectric fluid (NS2) media. Because the two fluids are incompressible, the volume of the closed domains (droplets) is automatically conserved. These fluid dynamics equations are solved taking into account the boundary conditions at the fluid-fluid interface imposing the continuity of the velocity fields and the pressure drop due to electrostatic pressure and surface tension effects:

$$p_{\text{in}} - p_{\text{out}} = T \left(\frac{1}{R_1} + \frac{1}{R_2} \right) - \frac{1}{2} \varepsilon E^2 \quad (1)$$

here R_1 and R_2 are the principal radii of curvature and T the surface tension.

Cases of large deformations of the fluid-fluid interface involve the strong coupling of hydrodynamics and electrostatics. The accurate location of the water-dielectric fluid interface, and mainly the resulting curvature, has a major influence on the local electric field and resulting electrostatic forces, and on surface tension effects.

That is why we chose the Arbitrary Lagrangian-Eulerian formulation: starting from the initial position of the interface the boundary is deformed in a Lagrangian way with respect to the velocity fields of the two phases. Hydrodynamics is

coupled with the successive solutions of the Laplace equation when the interface is deformed, the electrostatic pressure serving as coupling variable.

To obtain static solutions for the deformed interface, the voltage applied as boundary condition of the electrostatics problem should be varied very slowly in time so that the inertial and viscous terms of the hydrodynamics problems remain in practice negligibly small. On the other hand transient problems can be studied by starting with non balanced force fields or by imposing very fast rise of the applied voltage. All the test cases were computed considering axial symmetry, and, in the particular cases of two droplets of same radius, taking into account the plane of symmetry between the drops. Computing more than one drop on the same axis is possible by solving the Navier-Stokes equations in each supplementary domain. The main modification of the standard software COMSOL MULTIPHYSICSTM concerns the computation of the interfacial forces performed through a weak formulation of the fluid dynamics equation [7] adapted to the axial symmetry conditions.

In water-oil test cases, boundary conditions imposed for Navier Stokes equations in the two liquid domains are:

- i) Static pressure is imposed at external boundary of the oil domain. The pressure computed in oil (NS2 equations on fig. 1), modified by electrostatic pressure $P_{elec} = -\varepsilon E^2/2$, is applied as boundary condition at the interface for the water domain. Interfacial tension T and local curvature involved in equation (1) are implemented indirectly through the weak formulation.
- ii) The velocity field computed within the water domain (NS1), ensuring the volume conservation in the case of drops, is, in turn, applied as boundary condition at the interface for the oil domain.
- iii) Liquid velocity at the water-oil interface is applied in a Lagrangian way to move the boundary.

In water-air test cases, the model was simplified by imposing a constant pressure in the air domain and neglecting the air flows.

III. TEST CASES

A. Free oscillations of liquid drop in air

As first test of the hydrodynamic model including the implementation of surface tension, we studied the time-dependent relaxation of an initially elongated liquid drop, in air. Under the effects of surface tension, transient evolution toward spherical shape is observed, with damped oscillations.

The frequency and damping characteristic time of these oscillations are compared with analytical results obtained for the first mode of drop surface deformation [8]. Results are presented in Table 1 for the following conditions: surface tension $T = 0.07$ N/m; density $\rho = 1000$ kg/m³; drop volume $Vol = 30$ and 0.3 mm³ (corresponding to sphere equivalent radii $R_0 = 4.2$ and 0.42 mm) and viscosity $\mu = 0.01$ and 0.001 Pa.s.

TABLE I

Comparison between numerical and analytical results for frequency and damping characteristic time of oscillation of single liquid drop in air.

Vol (mm ³)	μ (Pa.s)	f_{th} (Hz)	f_{exp} (Hz)	τ_{th} (s)	τ_{exp} (s)	Err/f %	Err/ τ %
30	0.01	14.08	14.09	0.345	0.344	0.03	0.21
30	0.001	14.09	14.09	3.45	3.39	0.02	1.51
0.3	0.01	443.1	441.8	0.0034	0.0032	0.29	7.72
0.3	0.001	445.5	447.1	0.034	0.035	0.36	1.82

The mesh of one half of a circular disk in the meridian plane is defined by about 1000 triangular elements. The initial amplitude of oscillation was set to 10% which is the upper limit for the validity of linear analysis [8]. Oscillation frequencies are found to be in very good agreement with analytical results. The viscous damping of the oscillations is quantified by the damping characteristic time τ which is compared with the irrotational approximation proposed by Lamb [8]. The damping characteristic time is in good agreement with theory, the relative error being smaller than 2%, except for the small drop with large viscosity, where the non dimensional viscosity $\mu/(\rho TR_0)^{1/2} = 0.06$ reaches the limit of validity of linear irrotational approximation [9].

B. Transient elongation of a conductive drop in oil.

The complete model has been tested by computing the transient evolution and final elongation of a water drop in oil

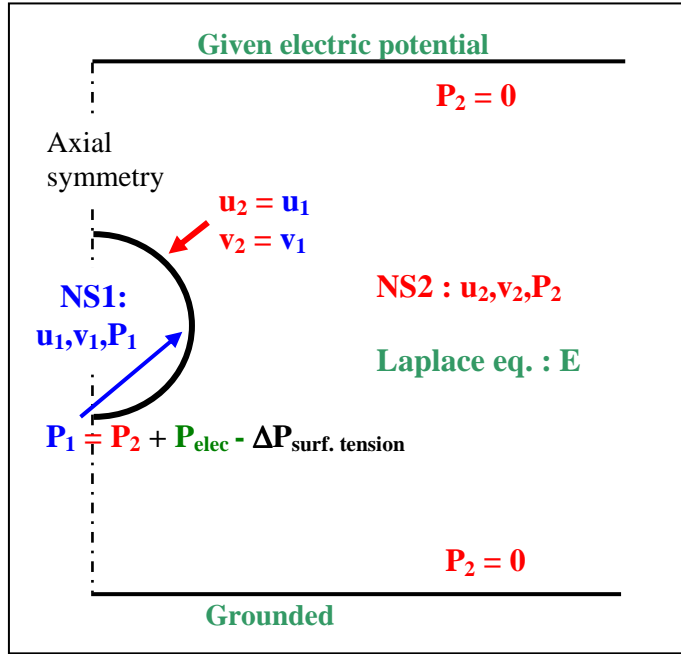


Fig. 1. Elongation of water drop in oil : boundary conditions for the two Navier-Stokes and the Laplace problems..

under the influence of an electric field imposed by two parallel electrodes (the spacing between the electrodes is 10 times greater than the initial drop diameter). Numerical simulations have been performed with water drop in toluene, the viscosity of which is close to that of water ($\mu_{toluene} : 0.0006$ Pa.s).

A constant electric potential difference imposed between the electrodes generates an initial uniform electric field E_0 . A spherical conducting droplet of radius R_0 is placed between the electrodes: initially it is in non equilibrium state and damped oscillations of the drop are observed up to final elongated shape.

Assuming an ellipsoidal shape for the deformed drop, Taylor related the static elongation of the ellipsoid a/b (a is the large axis, perpendicular to the electrodes, b is the small one), to the non dimensional uniform electric field $E_0 (2 R_0 \epsilon / T)^{1/2}$ [9], and found the static stability limit for $E_0 (2 R_0 \epsilon / T)^{1/2} = 0.65$.

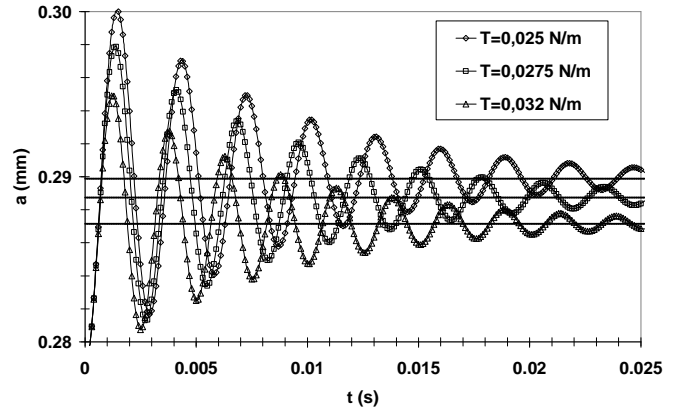


Fig. 2. Oscillations and final elongation of water drop in oil: effect of surface tension (condition $R_0 = 0.279$ mm, $E_0 = 0.45$ kV/mm). Horizontal full lines indicate the results of Taylor's model (steady state).

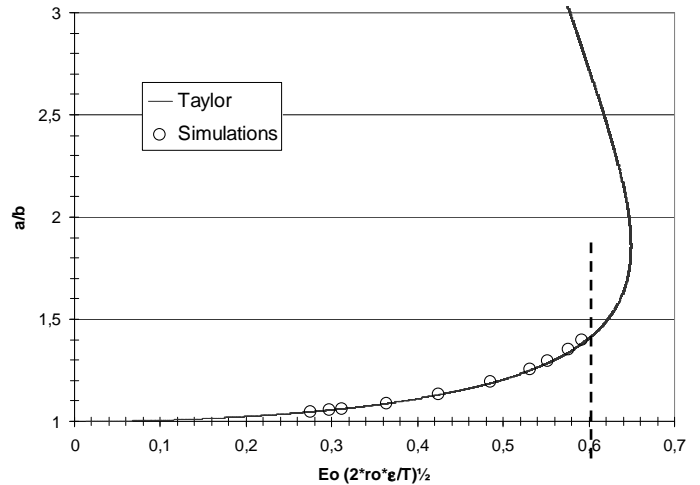


Fig. 3. Elongation of water drop in oil : comparison of final elongation with Taylor model. The vertical dotted line illustrates the numerical stability limit observed for water drop in toluene.

damping of the oscillations, as a result of combined action of Numerical simulations have been performed using the boundary conditions summarized on Fig. 1. The resulting oscillations of the drop are illustrated on Fig. 2 for three different values of the surface tension coefficient. The water and oil viscosities, can be quantified by the damping characteristic time τ .

The ALE approach gives results very close to Taylor's solution when damping of the oscillation is observed (Fig. 3). The numerical stability limit appears smaller than Taylor's because of the transient behavior: the amplitude of the first oscillation observed in Fig. 2 depends on the viscosity of the fluids and should not exceed the stability limit.

IV. SPHERE-PLANE CONFIGURATION

The problem of instability of a horizontal interface between water and an insulating fluid, electrically influenced by a metallic sphere located just above it, is considered here with its relevance to the basic electrocoalescence phenomenon of small water droplets suspended in an insulating medium near a much larger drop. Indeed, in that case, the deformations of the small drop are negligible compared to those of the large one.

The used experimental set-up is presented on Fig. 4. Initial spacing S_0 between the sphere and the free surface is varied in the range 0.03 to 3 mm. The sphere diameter is equal to $D_0 = 8$ mm. The electric potential is raised progressively and the quasi steady water surface rise h along the axis of symmetry is measured from visualisation. The results presented here were obtained with air as insulating fluid.

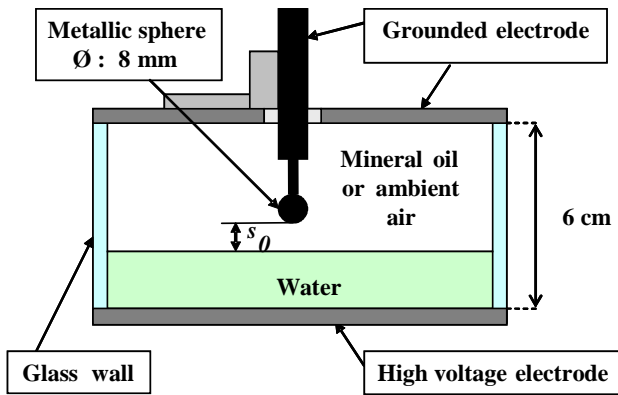


Fig. 4. Sphere-plane configuration: experimental set-up

Numerical simulations of transient surface rise with slowly increased electric field have been performed (Fig 5) taking into account the gravity effect in the Navier Stokes equations.

As we studied the quasi steady surface deformation, the water viscosity was artificially raised to increase the damping

of free surface oscillations. The final non dimensional surface rise at the axis of symmetry: $f_0 = h/S_0$ is drawn on Fig.6 as a function of the square of the electric potential difference ΔV^2 . Stable deformation of the free surface is obtained up to a non dimensional level rise a little smaller than 50%. This stability limit tends to decrease with increasing initial spacing S_0 . Interface disruption is observed above, stopping the computation.

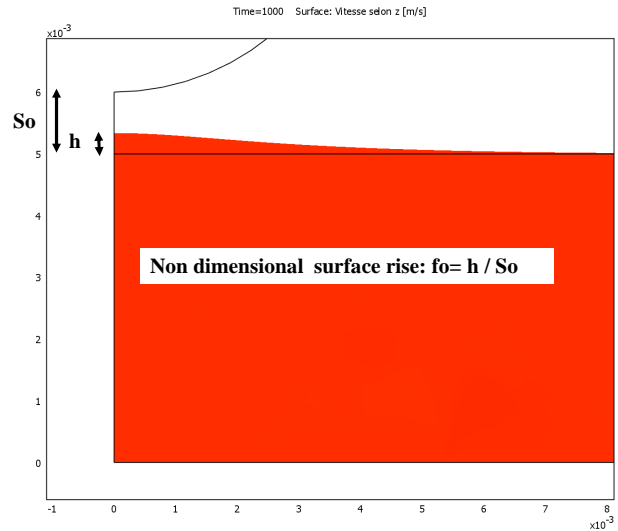


Fig.5. Sphere-plane configuration: final rise of water free-surface.

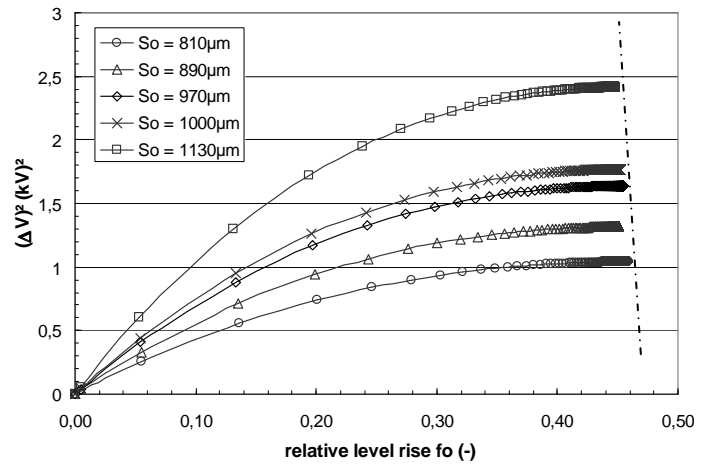


Fig. 6. Sphere-plane configuration: Relative level rise of the free surface versus sphere potential squared ΔV^2 for different values of the initial spacing S_0 . Dotted line shows the limit of stability of the computations.

Initial spacing S_0 and corresponding maximum potential difference ΔV_{crit} are used to build a critical electric Bond number Be_{crit} :

$$Be_{crit} = \frac{1}{2} \varepsilon (\Delta V_{crit}/S_0)^2 / (T/R_0)$$

On Fig. 7, Be_{crit} is drawn as a function of Bond number Bo :

$$Bo = \rho g S_0 / (T/R_0).$$

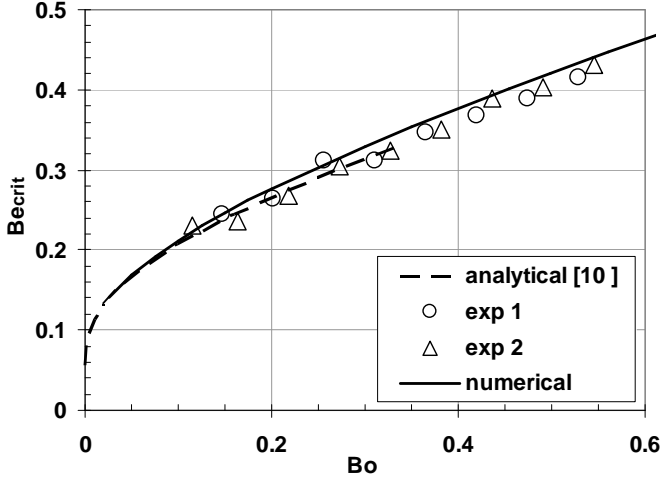


Fig. 7. sphere-plane configuration: $Be_{crit} = \frac{1}{2} \varepsilon (\Delta V_{crit}/S_0)^2 / (T/R_0)$ vs $Bo = \rho g S_0 / (T/R_0)$.

Numerical results are compared with measurements. Analytical results obtained by asymptotic approach for small values of S_0/R_0 [11] are also reported. A general good agreement is found in a large range of Bond number Bo . Numerical and asymptotic results coincide for small Bond numbers, while experimental Be_{crit} seems slightly over estimated. In the case of water-oil experiments, surface tension T is approximately three times smaller $T \approx 0.025$ N/m. Similar values of Bond number can be obtained but with smaller initial spacing S_0 and small influence of non linear effects can be observed according to the difference of ratio S_0/R_0 .

V. ANCHORED DROPLETS

We consider now two water drops of radius R_0 with a spacing S_0 immersed in oil (insulating fluid) at the end of capillary tubes (Fig. 8). The application of a potential difference ΔV between the drops induces an electric field E and an electrostatic pressure at the interfaces. The problem is to determine the subsequent deformation of the drops and, in particular, of the facing zones of the interfaces. As in the sphere-plane case, the critical potential difference ΔV_{crit} corresponds to the stability limit beyond which coalescence of the two droplets is observed.

For small enough droplets the gravitational force is negligible. Initial spacing of the droplets is S_0 . The angle θ_m

characterises the initial shape of the drop at the end of the capillary tubes: θ_m equals 90° for hemispherical drops and θ_m is larger than 90° when the drops diameter is larger than the diameter of capillary tube as illustrated in Fig. 8.

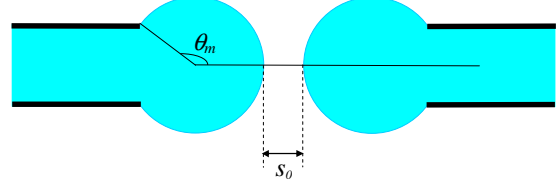


Fig. 8. Drops anchored at the end of capillary tubes.

Asymptotic approach is presented in [11] for $\sigma = S_0/R_0 \ll 1$ and numerical simulation aims to extend the analysis to large deformations and non linear behaviours. Numerical simulations presented here have been performed in the case of two drops of same radius, taking into account the plane of symmetry. Transient calculations have been performed with a slow rise of the voltage: $\Delta V/\Delta t = 0.1$ V/s.

Fig. 9 illustrates the instantaneous shape of a deforming droplet and the associated fields, for ΔV very close to the critical potential difference ΔV_{crit} . The parameter $\sigma = S_0/R_0$ is here much higher than the limit of validity of the asymptotic case approach, with simple electric field approximation. Electric field lines are drawn in the oil domain to illustrate the point. A small pressure gradient can be seen inside the water, due to increasing electrostatic pressure on the interface and the subsequent interface deformation and flows of liquids. Variation of the spacing S is drawn on Fig. 10 as a function of potential difference ΔV

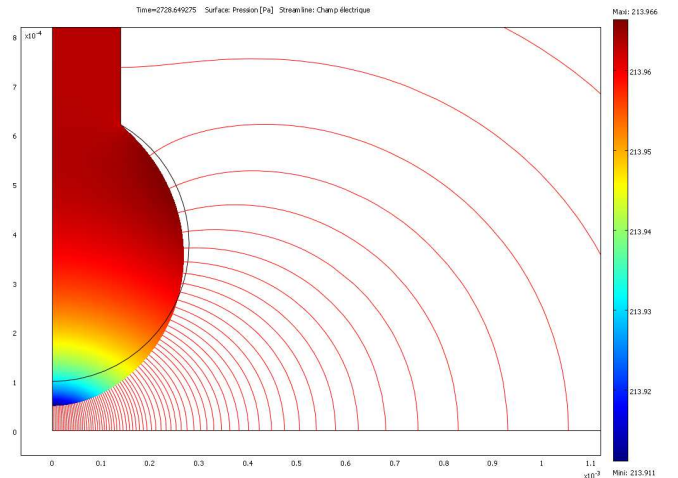


Fig. 9. Deformation of droplet shape in conditions close to the critical ones, : electric streamlines in the outer domain (oil), pressure field in the water (full color scale: 0.05 Pa). $\theta_m = 150^\circ$, $R_0 = 0.28$ mm, $\sigma = S_0/R_0 = 0.7$, $T = 25$ mN/m, $\varepsilon = 21.2$ pF/m.

It can be seen that the appearance of the interfacial instability corresponds to a very sharp drop of the curve that provides an accurate evaluation of ΔV_{crit} .

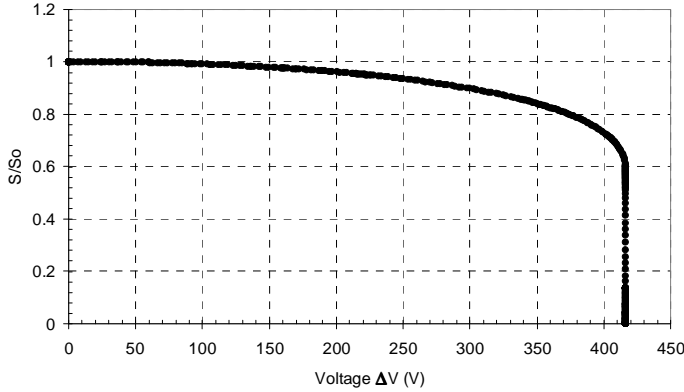


Fig. 10. Time-dependent relative spacing S/S_0 vs increasing voltage ΔV . $\theta_m = 90^\circ$, $R_0 = 0.28$ mm, $\sigma = S_0/R_0 = 0.7$, $T = 25$ mN/m, $\epsilon = 21.2$ pF/m ; result gives $Be_{crit} = (\epsilon/2) \Delta V^2 / s_0^2 (R_0 / T) = 0.512$.

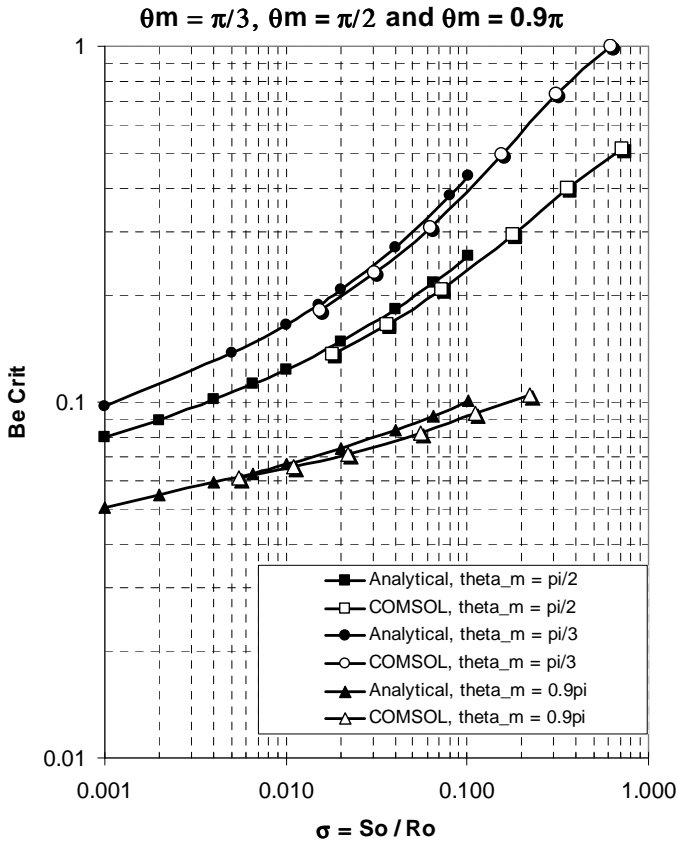


Fig.11. Critical value of the electric Bond number Be_{crit} as a function of the relative initial spacing σ . Asymptotic and numerical approaches.

The critical spacing S_{crit} appears to be slightly larger than $0.6 S_0$. The difference with the value close to $0.5 S_0$, obtained by the asymptotic approach [11] (and also in the sphere-plane configuration), can be mainly attributed to the non linear effects due to the large ratio S_0/R_0 . Results of the asymptotic and numerical approaches are plotted on Fig. 11 as a function of the relative spacing $\sigma = S_0/R_0$. In the range $\sigma = 0.01 - 0.1$, there is a good agreement between the numerical and asymptotic models, validating the numerical approach proposed here. As expected, the difference between results given by the two methods increases with σ . The general numerical method gives critical values slightly lower than the asymptotic ones because the real electric field on the interface is slightly higher than the uniform field retained in the asymptotic approach, thus requiring a slightly lower applied voltage. Finally let us note that the influence of relative spacing σ on the critical condition becomes stronger when σ is increased.

VI. CONCLUSION

Numerical simulations of electrically induced deformations of water-air and water-oil interfaces are presented using the commercial software COMSOL MULTIPHYSICS™ in 2D axisymmetric cases. Electrohydrodynamics problems are solved by using an ALE approach for mesh deformation. This method allows us to account, with a good accuracy, for non linear effects and large deformations.

Results of the numerical simulations are compared with those of analytical developments, asymptotic approaches and experiments. A good agreement is found between numerical and theoretical models in the validity range of linear approaches. The numerical method proves its ability to extend the previous results to a wider range of parameters. Experimental results are well predicted in the case of sphere-plane configuration. Other experiments are in progress and the accuracy of the numerical model will be analysed more in detail in the near future.

As a first case for further work, the interaction of two conducting droplets in a stagnant dielectric fluid was simulated with an electric field parallel to the axis of symmetry. Under the effect of the electrostatic forces, one could observe a first stage where fast deformation of the facing surfaces occurs, as in the case of anchored droplets, and a second stage of progressive drift of the two droplets due to their attraction. In that second stage the inertial effects and the draining of the oil film between the drops seem to control the approaching velocity and the resulting coalescence.

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