Smoothed particle hydrodynamics-based numerical investigation on sessile, oscillating droplets

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Forced oscillations in sessile droplets can be exploited in electrowetting mixing of fluid fractions. The necessary complex flows and large shape deformations require a numerical investigation of fluid dynamics in the transient regime. We provide a means to characterize oscillations qualitatively and quantitatively with the goal to examine and to classify flow patterns occurring inside. A superposition of different harmonic excitation patterns gives the possibility to control the convective flow. In this investigation, we apply a generic and accurate multi-phase smoothed particle hydrodynamics model to a two-dimensional three-phase flow and consider an oscillating droplet sitting on a substrate and immersed in a fluidic phase. These vibrations are investigated in two ways: the analysis of a step response due to an abrupt change of the contact angle is applied to identify the resonance frequencies. Secondly, the time evolution of the shape of the droplet in terms of harmonic functions is determined. Their amplitudes are examined in the time and frequency domain. This gives the possibility to relate resonance frequencies to mode shapes and to detect a coupling between them. Our approach is successfully applied to different numerical case studies.

Keywords: multi-phase flow; smoothed particle hydrodynamics; sessile droplet; vibration; normal mode analysis; electrowetting

1. Introduction

Oscillations in liquid, viscous droplets have been considered both analytically and numerically [1–4]. The corresponding solution of an eigenvalue problem was limited to small shape deformations of the linearized Navier–Stokes equation. With the prospect of lab-on-a-chip applications, forced droplet oscillations by the electrowetting (EW) effect have been studied experimentally [5–7]. The droplets perform self-excited oscillations that were compared for small amplitudes with the aforementioned linearized models. An investigation on droplet shapes with respect to EW actuation and surface tension models can be found in Lienemann et al. [8] where suggestions are given on how to improve EW-induced actuation.

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For an accurate analysis of the transient regime, including large amplitudes and
different transport properties, a multi-phase capable numerical model is needed.
For simulating sessile droplets, an adjustable surface tension between the different
phases allows for setting an apparent contact angle of the liquid phase.

An investigation of droplet oscillations requires stability over a large number
of time steps, computational efficiency, as well as long-term numerical stability
of the interface. Thus, conventional Eulerian methods like the finite-element
method or the finite-volume method are challenged: rapid changes in the topology
require frequent and expensive remeshing. A further transport equation for the
phases like in a phase-field model has to be solved and smears the interfaces in
the long run: phase fractions are transported cell-wise and spread by numerical
diffusion. Lagrangian, meshless methods, on the other hand, are well suited for the
requirements above. The discretization points, the particles, carry the information
to which phase they belong and allow for sharp interfaces, even in the long run.
From the different meshless methods, smoothed particle hydrodynamics (SPH)
seems to be especially attractive for being relatively well explored and cheap.

Oscillations of a two-dimensional droplet with a given contact angle are
excited by abruptly changing the wetting properties of the substrate. Thereby,
all eigenfrequencies are excited, the eigenspectrum is obtained and an estimate of
the resonance frequencies can be given. For measuring mode shapes, the surface
of the droplet is represented in terms of spherical harmonics. We calculate the
mode in the time and frequency domain, relate the resonance frequencies to mode
shapes and identify mode coupling.

2. Model and analysis

We compute a multi-phase flow of a liquid and a vapour phase on a solid substrate
by solving the Navier–Stokes equations with a multi-phase SPH model. By
introducing different surface energies between the phases involved, corresponding
contact angles arise. This is illustrated in figure 1 for contact angles of 60° and
120°. By changing the surface energy between solid and liquid phase, vibrations
are induced in the droplet.

(a) Governing equations

We consider the isothermal and incompressible Navier–Stokes equations in
Lagrangian form

\[ \frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v} \]  

(2.1)

and

\[ \frac{d\mathbf{v}}{dt} = -\frac{1}{\rho} \left( \mathbf{F}^{(p)} + \mathbf{F}^{(sf)} + \mathbf{F}^{(v)} \right) + \mathbf{g}, \]  

(2.2)

with velocity \( \mathbf{v} \), density \( \rho \), pressure force \( \mathbf{F}^{(p)} \), surface tension force \( \mathbf{F}^{(sf)} \), viscous
force \( \mathbf{F}^{(v)} \) and gravitational acceleration \( \mathbf{g} \). For incompressible media, the viscous
part of the momentum equation with a dynamic viscosity $\eta$ simplifies to

$$
\mathbf{F}^{(v)} = \eta \nabla^2 \mathbf{v}. \quad (2.3)
$$

Incompressibility is approximated by a stiff equation of state (EOS), which relates pressure $p$ to density and allows us to keep density fluctuations small [9],

$$
p = p_0 \left( \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right), \quad (2.4)
$$

where $p_0$ represents a reference pressure, $\rho_0$ a reference density and $\gamma$ depends on the phase, where a usual choice is 7 for liquids and 1.4 for gases. The continuum surface force (CSF) model from Brackbill et al. [10] gives

$$
\mathbf{F}^{(sf)} = - (\alpha \kappa \mathbf{n} + \nabla_s \alpha) \delta_{sf}, \quad (2.5)
$$

with the surface tension coefficient $\alpha$, the curvature $\kappa$ and the surface normal $\mathbf{n}$. The surface delta function $\delta_{sf}$ describes the narrow transition band between two phases and in the limit approaches the Dirac delta function representing a spatial phase jump. The equilibrium contact angle of the liquid phase that arises is given by the Young equation, which relates surface energies to a contact angle,

$$
\gamma_{sl} - \gamma_{sv} = - \cos(\phi) \gamma_{lv}, \quad (2.6)
$$

where $\gamma_{ij}$ is the surface energy between two phases $i$ and $j$, $\phi$ is a contact angle and $s$, $l$, $v$, respectively, label the solid, liquid or vapour phase.

(b) Smoothed particle hydrodynamics multi-phase model

For zeroth-order consistency, we use a normalized smoothing function [11],

$$
\chi_i(r) = \frac{W(r - r_i, h)}{\sum_k W(r - r_k)} = \frac{W_i}{\sigma}, \quad (2.7)
$$

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where $W$ is a generic SPH smoothing kernel, $h$ is the smoothing length and $\sum_k$ is a global sum contributing only within the support of $W$. The usual SPH density equation [12] then reads
\[ \rho_i = m_i \sum_j W_{ij} = m_i \sigma_i, \quad (2.8) \]
so that the density of a particle $i$ does not depend on the mass $m_j$ of surrounding particles, but only on its specific volume $V_i = \sigma_i^{-1}$. For continuity at interfaces, we use an expression suggested by Hu & Adams [13] for a particle-averaged spatial derivative
\[ \nabla \Phi_i \approx \sigma_i \sum_j \left( \frac{1}{\sigma_i^2} + \frac{1}{\sigma_j^2} \right) \Phi_{ij} \frac{\partial W}{\partial r_{ij}} e_{ij} = \sigma_i \sum_j A_{ij} \Phi_{ij} e_{ij}, \quad (2.9) \]
of a quantity $\Phi_i$, where $A_{ij} = (\sigma_i^{-2} + \sigma_j^{-2}) \partial W / \partial r_{ij}$, $\Phi_{ij}$ is an interparticle average and $e_{ij}$ is a unit vector pointing from particle $i$ to particle $j$.

The mass in equations (2.1) and (2.8) is inherently conserved by the Lagrangian nature of our approach. The pressure force with the interparticle pressure $\tilde{p}_{ij} = (p_i + p_j) / (\rho_i + \rho_j)$ is discretized as
\[ \left( \frac{d\mathbf{v}}{dt} \right)^{(p)} = -\frac{1}{\rho_i} \nabla p_i = -\frac{1}{m} \sum_j A_{ij} \tilde{p}_{ij} e_{ij}, \quad (2.10) \]
Secondly, the shear stress contributes to the momentum equation and for different viscosities $\eta^k$ and $\eta^l$ in different phases $k$ and $l$, the interparticle-averaged shear stress can be written as
\[ \tilde{N}^{(v)}_{ij} = \frac{2 \eta^k \eta^l}{r_{ij}(\eta^k + \eta^l)} (e_{ij} v_{ij} + v_{ij} e_{ij}), \quad (2.11) \]
when assuming that the phase interface is centred between two particles. For incompressible flow, the following expression is found [11]:
\[ \left( \frac{d\mathbf{v}}{dt} \right)^{(v)} = \frac{1}{m_i} \sum_j \frac{2 \eta_k \eta_l}{(\eta_k + \eta_l)} A_{ij} \frac{v_{ij}}{r_{ij}}, \quad (2.12) \]
 Furthermore, the surface tension force of the CSF model contributes to the momentum equation. A colour index is defined for each phase. A corresponding colour function $C_i^s$ defined on each particle $p_i$ is 1 if particle $i$ belongs to phase $s$, otherwise it is 0. The gradient of the colour function for a particle $i$ in phase $k$ between two phases $k$ and $l$ can be written as
\[ \nabla C_i^{kl} = \sigma_i \sum_j \left( \frac{C_j^l}{\sigma_i^2} + \frac{C_j^k}{\sigma_j^2} \right) \frac{\partial W}{\partial r_{ij}} e_{ij}, \quad (2.13) \]
where an interparticle average is avoided. Considering equation (2.5), a straightforward SPH discretization for the calculation of the interface curvature $\kappa = \nabla \cdot ((\nabla C) / |(\nabla C)|)$ is cumbersome for high curvatures [14] and a tensorial description that avoids direct computation of second derivatives is used instead.

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$$
\Pi_{kl}^{(sf)} = a_{kl}^{(s)} \frac{1}{\sqrt{C_{kl}^{(s)}}} \left( \frac{1}{d} \mathbf{I} |\nabla C_{kl}^{(s)}|^2 - \nabla C_{kl}^{(s)} \nabla C_{kl}^{(s)} \right),
$$

(2.14)

where $\mathbf{I}$ is the unit tensor, $d$ the dimensionality, $\Pi_{kl}^{(sf)} = \sum_{k \neq l} \Pi_{kl}^{(sf)}$ is the global surface stress and $\mathbf{F}^{(sf)} = -\rho^{-1} \nabla \Pi^{(sf)}$, which we adopt.

(c) Mode shape detection and modal analysis

We express the radius of a droplet with respect to its mass centre, which is projected onto the substrate’s surface, by a superposition of spherical harmonics functions

$$
f(\vartheta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{lm} Y_{lm}(\vartheta, \varphi),
$$

(2.15)

with the inclination $\vartheta$, the azimuth $\varphi$, a spherical harmonics function $Y_{lm}$ and its attributed amplitude $c_{lm}$. For our analysis, we interprete two-dimensional functions as $\varphi$-symmetric. A particle is represented in spherical coordinates with the components $r, \vartheta$ and $\varphi$. The set of particles forming the droplet is situated on a half sphere with the angular range $\cos(\vartheta) = [-1;1]$. We divide the sphere into equally sized bins $\vartheta_i$ and $\varphi_i$, $i = 1, \ldots, n$, with the corresponding particle subsets $\mathcal{B}_\vartheta^i$ and $\mathcal{B}_\varphi^i$. We define a radius function to approximate the distance of a sphere segment of the droplet’s surface from its centre

$$
f_r(\vartheta, \varphi) = \max\{\mathbf{Z}_r(p) | p \in \mathcal{B}_\vartheta^i \cap \mathcal{B}_\varphi^i\},
$$

(2.16)

where $\mathbf{Z}_r$ returns the radial component of a particle $p$. The coefficients $c_{lm}$ of the individual spherical harmonics for the projection of equation (2.16) and expansion with equation (2.15) are calculated by

$$
c_{lm} = \int_{\varphi=0}^{2\pi} \int_{\vartheta=0}^{\pi} Y_{lm}^*(\vartheta, \varphi)f_r(\vartheta, \varphi) \sin \vartheta \, d\vartheta \, d\varphi,
$$

(2.17)

with $Y_{lm}^*$ being the conjugate complex of $Y_{lm}$.

Figure 2a shows a droplet described with particles. Figure 2b,c shows extracted surface and continuous representation by spherical harmonics with $l_{\text{max}} = 5$ or $l_{\text{max}} = 35$, respectively.

To determine the eigenspectrum, the initial surface energy $\alpha_{s,l}$ is changed abruptly to $\alpha_{d,s}$ corresponding to a step excitation and the step response is measured. The approach of applying the Fourier transformation $\mathcal{F}(\mathbf{r}_i(t))$ on the trajectory $\mathbf{r}_i(t)$ of individual particles was useful for obtaining the eigenspectrum when integration errors were substantially lowered by tremendously reducing the time-step length. Transforming the expansion of the surface of the droplet by equation (2.15) is numerically more efficient. Only the noise inherent in the trajectories of surface particles contributes to errors and as a further benefit, the number of expensive Fourier transformations is thereby decreased.
3. Numerical results

The simulations in this section were performed on a rectangular periodic domain \([-0.5;0.5] \times [-0.4;0.4]\) filled with 2880 particles having initial positions on a regular lattice, a quintic smoothing kernel with the smoothing length \(h = 0.016\) and a support of \(3h\), equal viscosities \(\eta = 0.05\) and densities \(\rho_0 = 1\) for all phases and an artificial speed of sound of \(v_s = 100\). Initial surface tension coefficients were chosen as \(\alpha_{sl} = \alpha_{lv} = \alpha_{sv} = 1\). All simulations ran with a time step of \(\Delta t = 10^{-6}\) and for about \(4 \times 10^6\) time steps. For all simulation runs, we calculated a maximum Reynolds number of \(Re_{\text{max}} = 10\) and Weber numbers in the range of \(We = [0.5;1.5]\).

(a) Step response

We change the solid–liquid surface energy abruptly from 0.5 to 1.5 which corresponds to steady-state contact angles of 60° and 120°, respectively. The surface of the droplet is described by equation (2.16). The expanded droplet’s radius from equation (2.15) is then Fourier transformed.

In figure 3a, we observe some peaks in the spectrum for lower frequencies at about \(f \approx 2\) Hz, \(f \approx 5\) Hz and \(f \approx 7\) Hz. In the calculated sample, numerical noise appears to inhibit the detection of lower amplitude eigenfrequencies. A higher sampling rate, as well as repeated excitation, might improve results. The latter is presented in figure 3b by a squarewave excitation with identical system configuration and improved methodology.

(b) Mode shapes

Now, we consider individual mode shapes in the time and frequency domain. The droplet is excited with different patterns, where \(\alpha_{sl,0}\) corresponds to a constant surface energy term, \(\alpha_{sl,A}\) to an amplitude, and \(\text{sgn}\) stands for the signum function,

\[
\alpha_{sl}(t) = \alpha_{sl,0} + \alpha_{sl,A} \cos(2\pi ft)
\]  

and

\[
\alpha_{sl}(t) = \alpha_{sl,0} + \alpha_{sl,A} \text{sgn}(\cos(2\pi ft)).
\]

All steady surface energies were set to \(\alpha_{sl,0} = \alpha_{lv} = \alpha_{sv} = 1\), corresponding to a contact angle of 90°. The excitation frequency was set to \(f = 5\) Hz.
Owing to enforced quasi-incompressibility, the $Y_{00}$ mode is approximately constant, presented for both patterns in figure 3b: the small deviations reflect the stiffness of the EOS. For symmetry reasons, odd modes do not change substantially. Figure 4a shows first interesting amplitudes $c_{20}$, $c_{40}$ and $c_{60}$ for a harmonic excitation by equation (3.1), and figure 4c for the square wave excitation by equation (3.2). In both figures, the $c_{20}$ amplitude slowly increases, indicating resonance behaviour. This corresponds to the peaks detected in §3a and observed in the eigenspectrum in figure 3a.
Figure 4b,d shows the $c_{lm}$ in the frequency domain. The peak at $f = 5$ Hz for all modes corresponds to the excitation frequency. For both excitation patterns in the $c_{lm}$ spectra, a contribution to resonance is visible for $c_{20}$ at $f \approx 2$ Hz. The amplitude for the square wave excitation is however slightly higher, which might be caused by the higher amount of energy brought into the system. A further correspondence to the eigenspectrum is observable at a frequency of $f \approx 7$ Hz, where different modes show contributions.

We finally relate our results to an analytical model [15], which gives resonance frequencies $f^2 = \frac{s(l^2 - l)}{((r_d + r_e)r_0^3)}$ for small amplitude oscillations of cylindrical droplets in an external fluid. $r_d$ and $r_e$ are corresponding densities, $l$ stands for the mode number, $\sigma$ for the droplet’s surface tension and $r_0$ for the radius of the unperturbed sphere. For the meaningful second mode, the model predicts $f = 10.54$, which is in fair agreement with our result from a damped system.

4. Concluding remarks

We have presented an SPH-based normal mode analysis of a sessile, oscillating droplet and provided a means to extract and to represent its shape in terms of spherical harmonics functions. The presented approach for estimating resonance frequencies and measuring mode shapes in the time and frequency domain is broadly applicable, as the multi-phase scheme applied allows for different transport properties in the individual phases. Numerical case studies were performed and compared with resonance frequencies in order to relate individual mode shapes. An extension to complex flows is straightforward and makes possible meaningful parameter studies for industrial applications beyond analytical scope.

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References


