Modeling of surface cleaning by cavitation bubble dynamics and collapse
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ABSTRACT
Surface cleaning using cavitation bubble dynamics is investigated numerically through modeling of bubble dynamics, dirt particle motion, and fluid material interaction. Three fluid dynamics models; a potential flow model, a viscous model, and a compressible model, are used to describe the flow field generated by the bubble all showing the strong effects bubble explosive growth and collapse have on a dirt particle and on a layer of material to remove. Bubble deformation and reentrant jet formation are seen to be responsible for generating concentrated pressures, shear, and lift forces on the dirt particle and high impulsive loads on a layer of material to remove. Bubble explosive growth is also an important mechanism for removal of dirt particles, since strong suction forces in addition to shear are generated around the explosively growing bubble and can exert strong forces lifting the particles from the surface to clean and sucking them toward the bubble. To model material failure and removal, a finite element structure code is used and enables simulation of full fluid–structure interaction and investigation of the effects of various parameters. High impulsive pressures are generated during bubble collapse due to the impact of the bubble reentrant jet on the material surface and the subsequent collapse of the resulting toroidal bubble. Pits and material removal develop on the material surface when the impulsive pressure is large enough to result in high equivalent stresses exceeding the material yield stress or its ultimate strain. Cleaning depends on parameters such as the relative size between the bubble at its maximum volume and the particle size, the bubble standoff distance from the particle and from the material wall, and the excitation pressure field driving the bubble dynamics. These effects are discussed in this contribution.

1. Introduction
Non-chemical submerged surface cleaning is accomplished through application of shear forces at the surface to be cleaned large enough to lift adhered particles [1–4]. This can be achieved by using liquid jets or high frequency acoustic waves (ultrasonic, megasonic). Acoustic fields generate highly unsteady pressures and liquid motions, which exert high drag forces on solid contaminants and dislodge them from the surfaces being cleaned. Cleaning can also be achieved through generation of cavitation driven by intense pressure amplitude cycling between high negative and high positive pressures. Industrial scale implementation of ultrasonic cleaning covers many applications including cleaning of machine parts, jewelry, surgical instruments, laboratory equipment, textile, oil pipes, filter membranes, and semiconductor substrates [5–10]. Submerged liquid cavitating jets are also widely used for cleaning, cutting, drilling [11–13], and for controlled evaluation of materials' resistance to cavitation erosion [14–16]. Cavitation intensity produced by submerged jets can be varied in a very wide range through adjustment of the jet velocity, diameter, angle and standoff distance relative to the exposed surface, and the ambient pressure in which they are discharged [15].

Even though application of the above techniques is very widespread, the understanding of the physical phenomena involved is still limited due to the complexity and the multiple widely different scales of the mechanisms involved. The cleaning process involves activation and dynamics of sub-micron bubbles, which grow and collapse emitting shock waves and forming fast micro-jets in the micro- and milli-second time scales. In addition, the small spatial and fast temporal scales hinder clear visualization of the physical processes. However, various theoretical, experimental, and computational contributions have been made toward understanding cleaning processes involving cavitation. For example, the problem of surface contamination of silicon wafers in the microelectronic industry was studied in [17], which showed how removal efficiency varied with sonication time, temperature and particle size. High speed photography was used to understand

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the complex mechanisms (e.g. [5,18–22]). Collective bubble dynamics effects were considered in general in [23–28] and particularly for the mechanism of cleaning particles adhered to a solid substrate in [29]. The shock waves generated at bubble collapse also play an important role in the cleaning process. For instance, the pressures generated on the wall due to collapse of a bubble in a megasonic field were computed in [30,31] and other under various conditions in (e.g. [32,33]). One has to be careful, however, with this effect to not actually result in damaging the material surface being cleaned [15,32,39]. Another important mechanism for cleaning is to trigger oscillations of stable bubbles close to surface, which results in bubble translation near the surface and cleaning [34–38].

Cavitation is due to the local pressure in the liquid dropping below a critical pressure (often quoted to be the liquid vapor pressure for studies investigating bubble surface tension), which drives omnipresent nano- and micro-bubble nuclei in the liquid to grow explosively [15,42,43]. When the pressure returns to a high value, bubble implosion occurs and generates high pressure pulses and shock waves. Many pioneering studies [44–47] have shown, experimentally as well as analytically, that the collapse of these cavitation bubbles near a rigid boundary results in high-speed reentrant liquid jets, which penetrate the bubbles and strike the nearby boundary generating water hammer like impact pressures. The high speed flow field, the large pressure variations, and the shock waves produce high local stresses on the adjacent material surface and are responsible for material micro-deformation, damage and failure, and high forces dislodging nearby particles or material layers to remove.

Simulation of the collapse of bubbles near boundaries has been an active research area since the pioneering work of [45]. The resulting reentrant jet has been found to play an important role in hydrodynamics and ultrasonic cavitation, as well as in large-scale underwater explosion problems [20,48–53] and in small-scale medical applications [54]. Modeling approaches started with incompressible potential flow methods using the observation that the dynamics of the concerned bubble is highly inertial where liquid viscosity influence is very low, while liquid velocities remain smaller than the sound speed enabling the inertial where liquid viscosity influence is very low, while liquid observation that the dynamics of the concerned bubble is highly

2.1. Boundary element model

The potential flow model used in this study is based on a Boundary Element Method (BEM) [49–54]. The Laplace equation, \( \nabla^2 \phi = 0 \), is solved for the velocity potential, \( \phi \), defined through \( \mathbf{u} = \nabla \phi \), where \( \mathbf{u} \) is the velocity vector. A boundary integral method based on Green's theorem:

\[
\int_{\Sigma} (\phi \nabla^2 G - G \nabla^2 \phi) \, d\Omega = \int_{\Sigma} \mathbf{n} \cdot (\mathbf{u} \nabla G - G \nabla \mathbf{u}) \, dS,
\]

is used to solve the Laplace equation. In this expression \( \Omega \) is the domain of integration having elementary volume \( d\Omega \) and \( \Sigma \) includes all boundary surfaces of \( \Omega \) such as the surface of the modeled bubble, the nearby surface to be cleaned, and the dirt particles. \( \mathbf{n} \) is the local normal unit vector, \( G = -1/|\mathbf{x} - \mathbf{y}| \) is Green's function, where \( \mathbf{x} \) corresponds to a fixed point in \( \Omega \) and \( \mathbf{y} \) is a field point on the boundary surface \( \Sigma \). Eq. (1) reduces to Green's formula

\[
\alpha \pi \phi(x) = \int_{\Sigma} \left[ \phi(y) \frac{\partial G}{\partial n}(x, y) - G(x, y) \frac{\partial \phi}{\partial n}(y) \right] dS,
\]

where \( \alpha \pi \) is the solid angle under which \( \mathbf{x} \) sees the domain, \( \Omega \). Eq. (2) provides a relationship between \( \phi \) and \( \partial \phi/\partial n \) at the boundary surface \( \Sigma \). Thus, if either of these two variables (e.g. \( \phi \)) is known everywhere on the surface, the other variable (e.g. \( \partial \phi/\partial n \)) can be obtained.

To solve (2) numerically, the surfaces of all objects in the computational domain are discretized into triangular panels. To advance the solution in time, the coordinates of all surface nodes, \( \mathbf{y} \), are advanced according to \( d\mathbf{y}/dt = \nabla \phi \). The velocity potential on the bubble surface nodes is obtained through the time integration of the material derivative of \( \phi \), i.e. \( d\phi/dt \), which can be written as

\[
\frac{d\phi}{dt} = \frac{\partial \phi}{\partial t} + \nabla \phi \cdot \nabla \phi,
\]

where \( \partial \phi/\partial t \) can be determined from the Bernoulli equation:

\[
\rho \left( \frac{d\phi}{dt} + \frac{1}{2} \nabla \phi \cdot \nabla \phi + g \mathbf{z} \right) + p_l = p_n.
\]

2. Modeling approaches

The modeling of bubble dynamics near boundaries uses our general bubble dynamics and free surface modeling code, 3DYNAFS©. Four modules are used in the study presented here and described below.
$p_\infty$ is the hydrostatic pressure at infinity at $z = 0$ where $z$ is the vertical coordinate. $p_l$ is the liquid pressure at the bubble surface, which balances the internal pressure and the surface tension,

$$p_l = p_g + p_s - \sigma,$$

where $\sigma$ is the surface tension, and $C$ is the local bubble wall curvature. The bubble internal pressure is composed of $p_l$, the vapor pressure and $p_g$ the gas pressure. $p_g$ is assumed to follow a polytropic law, which relates the gas pressure to the gas volume, $V$, and reference value, $p_{0g}$, and $V_0$,

$$p_g = p_{0g} \left( \frac{V}{V_0} \right)^k,$$

where $k$ is a gas compression constant; $k = 1$ corresponds to isothermal compression, while $k = c_p/c_v$ corresponds to adiabatic compression.

### 2.1.1. Accounting for background shear flow

To study bubble dynamics in a non-uniform flow field, $\mathbf{u}_b$, we consider Helmholtz decomposition of any velocity field as the sum of the gradient of a scalar potential, $\phi_b$, and the curl of a vector potential, $\mathbf{A}$, with $\nabla^2 \mathbf{A} = -\mathbf{m}$,

$$\mathbf{u}_b = \nabla \phi_b + \nabla \times \mathbf{A}.$$  

Here, we consider the case where the “basic flow” of velocity $\mathbf{V}_b$, is known and satisfies the Navier Stokes equations. In the presence of oscillating bubbles, the total velocity field is given by $\mathbf{u}_t$ and we can define bubble flow velocity and pressure variables respectively as $\mathbf{V}_b$ and $P_b$:

$$\mathbf{V}_b = \mathbf{u}_t - \mathbf{V}_b, \quad P_b = P_1 - P_0.$$  

The bubble generated flow field, $\mathbf{V}_b$, can be assumed as a potential field, and we can use the BEM model to study the dynamics, provided that $P_b$ is computed properly accounting for the basic flow. This is achieved by subtracting the Navier Stokes equations for each $\mathbf{u}_t$ and $\mathbf{V}_b$ to obtain [57–59]:

$$\nabla \left[ \frac{\partial \phi_b}{\partial t} + \frac{1}{2} \mathbf{V}_b^2 + \mathbf{V}_b \cdot \nabla \phi_b + \frac{P_b}{\rho} \right] = \mathbf{V}_b \times (\nabla \times \mathbf{V}_b).$$

This equation, once integrated, is to be compared with the classical unsteady Bernoulli equation. In the case of a flat wall boundary layer flow such that all velocity vectors are parallel to the wall (unit direction, $\mathbf{e}_z$), and depending only on the distance, $z$, to the wall, $\mathbf{V}_b = f(z)\mathbf{e}_z$, Eq. (9) becomes:

$$\frac{\partial \phi_b}{\partial t} + \frac{1}{2} \mathbf{V}_b^2 + \mathbf{V}_b \cdot \nabla \phi_b + \frac{P_b}{\rho} = \text{constant along the y direction}.$$  

The effects of the presence of shear on the bubble dynamics are considered in Section 3.3. In order to do so the flow field in a cavitating jet is modeled and described in Section 3.2.

### 2.2. Viscous mixture modeling

Completely accounting for viscous effects in the bubble dynamics simulations can be obtained using the following approach. For generality, we consider the case where the continuum in which the bubble dynamics is observed is a two-phase continuum formed by a bubbly mixture with gas volume fraction, $\alpha$. The density, $\rho_m$, and kinematic viscosity, $\mu_m$, are related to properties of the gas, $\rho_g$ and $\mu_g$, and those of the liquid, $\rho_l$ and $\mu_l$, through:

$$\rho_m = (1 - \alpha) \rho_l + \alpha \rho_g, \quad \mu_m = (1 - \alpha) \mu_l + \alpha \mu_g.$$  

The unsteady continuity and momentum conservation equations for the liquid–gas mixture are as follows:

$$\frac{\partial \rho_m}{\partial t} + \nabla (\rho_m \mathbf{u}_m) = 0,$$  

$$\frac{\partial \rho_m \mathbf{u}_m}{\partial t} + \nabla (\rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p + \nabla \tau,$$

where $t$ is time, $\mathbf{u}$ is the mixture velocity, $p$ the mixture pressure, and $\tau$ the stress tensor.

Eqs. (12) and (13) are solved using 3DYNAS-Vis© [60–62], which is based on the artificial-compressibility method [66], where a derivative of the pressure in the pseudo time, $\tau$, is added to (12) as:

$$\frac{1}{\beta} \frac{\partial \rho_m}{\partial \tau} + \frac{\partial \rho_m \mathbf{u}_m}{\partial \tau} + \nabla (\rho_m \mathbf{u}_m) = 0,$$

where $\beta$ is an artificial compressibility factor.

Eqs. (13) and (14) form a hyperbolic system of equations and are solved using a time marching scheme in the pseudo-time, $\tau$. To obtain a time-dependent solution, a Newton procedure where pseudo-time iterative stepping in $\tau$ is used at each physical time step, $\tau$, enables one to satisfy the continuity equation.

The numerical scheme uses a finite volume formulation. A first-order Euler implicit difference scheme is applied to the time derivatives. The spatial differencing of the convective terms uses a flux-difference splitting scheme based on Roe’s method [67] and a van Leer’s MUSCL method [68,69] to obtain the first or third-order fluxes. A second-order central differencing is used for the viscous terms and the flux Jacobians are obtained numerically. The resulting system of algebraic equations is solved using a discretized Newton relaxation method in which symmetrical block Gauss–Seidel sub-iterations are performed before the solution is updated at each Newton iteration. 3DYNAS-Vis has been extensively validated and used to study a range of two-phase problems and its results have compared favorably with available experimental data [70].

#### 2.2.1. Lagrangian modeling of dispersed phase

To model the two-phase flow medium, an Eulerian–Lagrangian method is adopted. The equivalent continuum medium equations are solved using the approach described in the previous section. The bubbles, on the other hand, are treated in a Lagrangian fashion as point sources and dipoles, which represent the time variations of each bubble volume and translation relative to the liquid. Volume variations are obtained with a bubble dynamics equation using bubble surface averaged pressures and velocities, to account for flow non-uniformities, and an additional pressure term to account for bubble motion relative to the liquid [70,71]. The equivalent spherical bubble radius, $R(t)$, is obtained using a modified R ayleigh–Plessel–Keller–Herring equation [72], which accounts for the compressibility of the surrounding bubbly medium and for flow field non-uniformities:

$$\frac{1 - \frac{R}{c_m}}{c_m} \frac{R}{d} \left( 1 - \frac{R}{3c_m} \right) \frac{R}{c_m} - \frac{(u_{en} - u_b)^2}{4} + \frac{1}{\rho_m} \left( 1 + \frac{R}{c_m} - \frac{R}{c_m} \right) \frac{R}{c_m} \frac{d}{dt} \left[ p_s + \frac{p_{enc}}{R} \right]$$

$$\left[ p_s + \frac{p_{enc}}{R^3} - p_{enc} - 2\sigma R^{-4} \mu_m \frac{d}{dt} \right]$$

where $c_m$ is the local sound speed in the two-phase medium and $u_b$ is the bubble translation velocity. $p_{enc}$ and $u_{enc}$, the “encountered” pressure and velocity respectively, are the pressures and velocities in the two-phase medium averaged over the bubble surface. The introduction of $u_{enc}$ and $p_{enc}$ in Eq. (15) is to account for non-uniform pressures and velocities around the bubble and for slip velocity between the bubble and the host medium. Using these average values instead of the conventionally used values at the bubble center, results in a major improvement over classical models [70,71].
The bubble trajectory is obtained using the following motion equation

\[
\frac{d\mathbf{u}_b}{dt} = -\frac{3}{\rho_m} \nabla p - 2g + \frac{3}{4} \frac{C_D}{R} (\mathbf{u}_{enc} - \mathbf{u}_b) |\mathbf{u}_b| + \frac{3}{2 \pi} \frac{C_l}{R} \left( \frac{\mu_m}{\rho_m} (\mathbf{u}_{enc} - \mathbf{u}_b) \times \mathbf{\omega} \right) \sqrt{|\mathbf{\omega}|} + \frac{3}{R} (\mathbf{u}_{enc} - \mathbf{u}_b) \mathbf{R},
\]

(16)

where \(\mathbf{\omega}\) is the local vorticity, \(g\) is the acceleration of gravity, \(C_l\) is the lift coefficient, and \(C_D\) is the drag coefficient given by [73]:

\[
C_D = \frac{24}{R_{eb}} (1 + 0.197 R_{eb}^{0.63} + 2.6 \times 10^{-4} R_{eb}^{3.8}),
\]

\[
R_{eb} = \frac{2 \rho_p R |\mathbf{u}_{enc} - \mathbf{u}_b|}{\mu_m}.
\]

(17)

In Eq. (16), the added mass term is indirectly represented by \(d\mathbf{u}_b/dt\) and the first term of the right hand side where \(d\mathbf{u}_{enc}/dt\) has been replaced by the \(\nabla p/\rho_m\) term. The last term in (16) is a force due to the interaction between the bubble volume source oscillations and the surrounding flow when the bubble has a slip velocity relative to the flow [40, 41]. The time average of this last term is the so-called Bjerknes force.

2.2.2. Eulerian–Lagrangian coupling

The two-way coupling between the Eulerian continuum-based model and the Lagrangian discrete bubble model is realized following these steps:

- The volume change and the motion of the individual bubbles in the flow field are controlled by the two-phase medium local properties and flow field gradients.
- The local properties of the mixture (void fractions and local densities) are determined by the spatial distribution of the bubble and by their volumes.
- The mixture flow field with evolving mixture density distribution satisfies mass and momentum conservation.

The key to this coupling scheme is the deduction of a void fraction distribution from the instantaneous bubble sizes and locations. A Gaussian gas volume distribution scheme to smoothly “spread” a bubble volume across neighboring cells is used [28, 74].

2.3. Inclusion of liquid compressibility

The bubble dynamics cleaning problem is also addressed here using a multi-material compressible Euler equation solver based on a finite difference method [63–65]. Continuity and momentum equations for the compressible liquid can be written as follows in Cartesian coordinates:

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = S,
\]

(18)

where

\[
Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e_t \end{bmatrix}, \quad E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho uw \\ (\rho e_t + p) u \end{bmatrix}, \quad F = \begin{bmatrix} \rho v \\ \rho v u \\ \rho v w \\ \rho v w \\ (\rho e_t + p) v \end{bmatrix}, \quad G = \begin{bmatrix} \rho w \\ \rho uw \\ \rho w v \\ \rho w^2 + p \\ (\rho e_t + p) w \end{bmatrix}, \quad \text{and} \quad S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},
\]

(19)

In (19) \(p\) is the pressure, \(u, v, w\) are the velocity components in the \(x, y, z\) directions respectively, \(e\) is the specific internal energy, and \(e_t = e + 0.5(u^2 + v^2 + w^2)\) is the specific total energy. The system is closed by using an equation of state for each material, which provides the pressure as a function of the material specific internal energy and the density. Here, a \(\gamma\)-law (with \(\gamma = 1.4\)) is used for the gas–vapor mixture [75].

\[
p = \frac{p_0}{\rho_0^\gamma},
\]

(20)

and the Tillotson equation is used for water [76]:

\[
p = p_0 + \omega (e - e_0) + A \mu + B u^2 + C \mu^3, \quad \mu = \frac{p}{p_0} - 1.
\]

(21)

\(\omega, A, B, C\) are constants and \(p_0, e_0, \rho_0\) are the reference pressure, specific internal energy, and density respectively \(\omega = 0.28, A = 2.20 \times 10^5\ \text{Pa}, B = 9.54 \times 10^8\ \text{Pa}, C = 1.48 \times 10^{10}\ \text{Pa}, e_0 = 3.54 \times 10^3\ \text{m}^2/\text{s}^2, p_0 = 1.0 \times 10^5\ \text{Pa}, \rho_0 = 1000\ \text{kg/m}^3\).

The compressible flow solver uses a high order Godunov scheme. It can solve the Riemann problem and construct a local flow solution that abruptly changes between adjacent cells. The numerical method is based on a higher order MUSCL scheme and tracks each material. To improve efficiency, an approximate Riemann problem solution replaces the full problem. The MUSCL scheme is augmented with a mixed cell approach [77] to handle shock wave interactions with fluid or material interfaces. This approach uses a Lagrangian treatment for the cells including an interface and an Eulerian treatment for cells away from interfaces. A re-map procedure is employed to map the Lagrangian solution back to the Eulerian grid [63–65]. The CFL number in the solver is based on the highest value of \(|u| + c\), and the smallest grid size, \(\Delta x\). The adaptive time step is determined using:

\[
\Delta t = \text{CFL} \frac{\min(\Delta x)}{\max(|u| + c)}.
\]

(22)

2.4. Modeling of particle and layered material removal

2.4.1. Particle contact models

The displacement of a particle laying on a substrate depends on the imposed hydrodynamic or acoustic forces and on the interaction of the particle with the substrate surface. These are influenced by many factors, which include geometrical properties such as particle size, particle shape and roughness, structure and roughness of the substrate surface, material properties of both particle and substrate, the hydrodynamic and additional external loads applied. The relative geometrical arrangement of the particle and substrate determines details such as the nature and number of contact points within the contact region, which directly influence magnitudes of frictional and other surface forces generated between the two bodies. In addition, the physical configuration determines particle exposure to or sheltering from the hydrodynamic forces and once the particle is moved it can impose constraints on where the particle can relocate.

Material properties determine the nature and magnitudes of friction and other surface forces induced in and near the contact region such as capillary forces, van der Waals forces, electrostatic forces, etc., that collectively define the adhesion or ‘pinch-off’ force between the particle and the substrate surface [78]. An important aspect of the problem being studied is the modeling of adhesion forces between the dirt particle and the substrate. The model can be as simple as the Hertz model, which considers contact to be frictionless, or more complex considering friction as well as adhesive forces between the materials. A review of various contact forces is given in [82]. Contact models that incorporate particle surface roughness and deformation have also been developed.
Critical values for particle detachment have been determined by using various variants of the contact models [83]. In the examples used in this paper we have used a simple contact model, which allows sliding between the surfaces and also accounts for coefficients of static and dynamic friction, our emphasis being on the bubble dynamics and resulting loads. The model used is a rate dependent coulomb friction model where the coefficient of friction is given by:
\[
\mu = \mu_s + (\mu_f - \mu_s)\exp(-\beta V_{rel}),
\]
(23)
where \(\mu_s\) and \(\mu_f\) are coefficients of static and kinetic friction respectively. \(\beta\) is the transition coefficient which determines the rate of change from static friction to kinetic friction, and \(V_{rel}\) is the relative velocity between the two sliding surfaces. The above equation reduces to a rate independent model if \(\mu_s\) and \(\beta\) are selected to be 0. In the examples below, we used 0.2, 0.1, and 1 for \(\mu_s\), \(\mu_f\), and \(\beta\), respectively.

2.4.2. Rigid body motion
Hydrodynamic properties determine the torque, lift, and drag forces imposed on the particle, which if sufficient in magnitude can either cause the particle to roll or slide along the substrate surface. The particle–substrate system is therefore modeled using moment and force balance arguments that define translation and/or detachment of the particle from the substrate surface if the magnitudes of the hydrodynamic applied torque and forces exceed critical limit values (e.g. [2, 4, 84]).

In order to calculate the dynamics of the dirt particle its six-degree-of-freedom equations of motion (three translations and three rotations) are solved. At each time step, the pressure field along the wetted surface of the particle is calculated and integrated to obtain the resultant force and moment vectors. These are applied to the equations of rigid body motion, which are integrated to provide an updated position, orientation, and velocity of the body [85–87].

The motion of the center of mass written in the inertial coordinate system is obtained by integrating the pressures along the wetted surface of the particle and applying other forces, \(F_{ext}\) such as those due to friction, adhesion forces, and additional viscous drag:
\[
M \cdot \frac{d\mathbf{v}_c}{dt} = -\int \mathbf{p} \cdot \mathbf{n} \cdot dS + F_{ext},
\]
(24)
where \(M\) is the mass of the body and \(\mathbf{v}_c\) is the velocity vector of the center of mass.

For a solid non-deformable body the local normal velocity at the body wall velocity is related to \(\mathbf{v}_c\) and the body angular velocity, \(\mathbf{\omega}\), by:
\[
\mathbf{u}_s \cdot \mathbf{n} = \left( \mathbf{v}_c + \mathbf{\omega} \times \mathbf{R}_c \right) \cdot \mathbf{n},
\]
(25)
where \(\mathbf{R}_c\) is the vector from the body center of gravity to the point on the body surface.

The equation for conservation of angular momentum, \(\mathbf{H}\), is given by:
\[
\frac{d\mathbf{H}}{dt} = -\mathbf{\omega} \times \mathbf{H} - \int \mathbf{p} \cdot (\mathbf{R}_c \times \mathbf{n}) \cdot dS.
\]
(26)

Solution of the two equations enable update of the particle position and orientation at each time step.

2.4.3. Material deformation model
In order to examine removal of a layer of material coating on a solid substrate, we use a similar approach to that we used to study cavitation pitting on materials [14–16]. To do so, either a synthetic load representing the forces generated by the bubble dynamics or direct coupling between the fluid computations and the structure computations at each time are applied. To model the dynamics of the material, the finite element model Dyna3D is used [88]. Dyna3D is a non-linear explicit structure dynamics code developed by the Lawrence Livermore National Laboratory. Here it computes the material deformation when the loading is provided by the fluid solution. Dyna3D uses a lumped mass formulation for efficiency. This produces a diagonal mass matrix \(M\), to express the momentum equation as:
\[
M \frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}_{ext} - \mathbf{F}_{int},
\]
(27)
where \(\mathbf{F}_{ext}\) represents the applied external forces and \(\mathbf{F}_{int}\) represents the internal forces. The acceleration, \(a = \frac{d^2\mathbf{x}}{dt^2}\) of each element, is obtained through an explicit temporal central difference method.

The material motion satisfies the formal equation
\[
\rho_s \frac{d^2\mathbf{x}}{dt^2} = \nabla \cdot \mathbf{\sigma},
\]
(28)
where \(\rho_s\) is the material density, \(\mathbf{x}\) is the position vector of the material and \(\mathbf{\sigma}\) is the Cauchy stress tensor. If we denote \(\mathbf{F}\) the deformation gradient tensor, then the Cauchy stress tensor is computed by
\[
\mathbf{\sigma} = \frac{1}{J} \mathbf{FSF}^T,
\]
(29)
where \(J\) is the determinant of \(\mathbf{F}\) and \(\mathbf{S}\) is the second Piola-Kirchhoff stress tensor.

In the present study, a viscoelastic or a visco-plastic material over a non-deformable substrate is considered. For illustration, a polyurea-like material is used and is modeled as a viscoelastic material with the following time dependent values for the shear modulus, \(G\):
\[
G(t) = G_0 + (G_\infty - G_0)e^{-t/\tau},
\]
(30)
with \(G_0\) and \(G_\infty\) being the initial and long term values of the shear modulus and \(\tau\) the relaxation time. The values selected for these parameters are shown in the corresponding section below.

The second material model that we used was based on the Johnson–Cook model [95], which relates the stress, \(\sigma\), to the effective plastic strain, \(\varepsilon_p\), normalized strain rate, \(\dot{\varepsilon}_p\), and normalized temperature, \(T^*\):
\[
\sigma = [A + B\varepsilon_p^m][1 + C\ln(\dot{\varepsilon}_p)][1 - T^*].
\]
(31)

The coefficients \(A, B, n, C,\) and \(m\) can be determined, for instance, by curve-fitting with measurements obtained with Split Hopkinson Pressure Bar tests. For example Fig. 1 shows such tests obtained at different strain rates for polyurea (Versalink) [89].

The strain rate is normalized by 1 s\(^{-1}\), \(\dot{\varepsilon}_p = \dot{\varepsilon}_p\), and the normalized temperature is defined as:
\[
T^* = \frac{T - T_r}{T_m - T_r},
\]
(32)
where \(T\) is the temperature, \(T_r\) the reference temperature, and \(T_m\) the melting temperature of the material. In this material model, the shear modulus, \(G\), does not vary.

2.4.4. Fluid structure interaction coupling
Coupling between the fluid and the structure interaction is achieved as follows. The fluid (liquid and bubble) computations determine the flow field and the pressures, which apply to the surface of the modeled material structure. In response, the solid body motion or finite element structure code computes motion, deformations, and velocities in response to this loading. The new coordinates and velocities of the structure surface nodes become the new boundary conditions for the fluid code at the next time step.
The time corresponding to a single time step is split into several smaller time steps for the structural computations. Additional details on the procedure can be found in [49,52,87]. This FSI coupling procedure has only a first-order time accuracy. A predictor-corrector approach can also be exercised in the coupling to iterate and improve the solution.

3. Bubble dynamics near a flat plate

3.1. Absence of shear

It is known that microscopic or nanoscopic bubble nuclei are always present in liquids and are entrained in the flow [42]. Also, nano-cavities at the solid surfaces and solid particles in the fluid serve as nucleation sites for the formation of microbubbles under cavitation conditions [90,91]. When the local pressures decrease below a critical value, a nucleus is activated and grows until its internal pressure drops below the surrounding local pressure. It can then collapse violently when the local pressure increases again, producing intense pressures, emitting sound, and eroding any solid surfaces in its proximity.

3.1.1. Reentrant jet formation

To illustrate the dynamics of such a cavitation scenario, we consider a nucleus initially at equilibrium with the surrounding liquid and subject it to a sudden pressure drop as illustrated in Fig. 2. The bubble nucleus has an initial radius \( R_0 = 10 \mu m \) and is initially at equilibrium in the liquid at 10 atm (1 MPa). This size was selected arbitrarily to illustrate the cleaning phenomena addressed in this paper. It is within the range of bubble sizes commonly mentioned in cleaning applications [1,19]. However, the detailed quantitative results will obviously depend on this selection. The pressure then suddenly decreases to a pressure of 1 atm (0.1 MPa) for a relatively long time. Fig. 2 also shows the response of a hypothetical spherical bubble to this pressure function obtained by integrating the Rayleigh–Plesset equation. It is seen that as soon as the ambient pressure drops the bubble responds and starts growing. A maximum bubble size, \( R_{max} \approx 27 \mu m \), is reached as the bubble size overshoots and the pressure inside it drops to about 0.015 MPa, significantly below the final ambient pressure. The bubble then collapses relatively gently as this case does not correspond to a very strong cavitation bubble, where the ratio \( R_{max}/R_0 \) would be larger than 5. Study of violent bubble collapse cases can be found in [32,33] and later in Section 5.

Even though the bubble collapse is relatively slow, a well-formed reentrant jet develops when it collapses near a wall. The strength of the jet obviously depend on the standoff distance between the bubble center and the wall, \( X \), with the normalized standoff defined as \( X = X/R_{max} \). Fig. 3 shows a case where \( X = 25 \mu m \) and \( X = 0.93 \). The figure shows the evolution of the bubble contours versus time during bubble collapse. During bubble growth the shape remains almost spherical, especially on the bubble side away from the wall, while the side close to the material flattens a little but never touches the wall as a layer of liquid remains between the bubble and the wall. The time stepping in these BEM simulations is adaptive with the time step decreasing where the variations are fast. The time step typically varies between \( 10^{-7} \) ms and \( 10^{-3} \) ms. In the contour plot figures the contours are shown every 100 time steps.

These results were obtained using the BEM module of ISYNAPS with a total of 400 nodes and 800 panels.

Due to the asymmetry of the flow, the liquid pressures at the bubble interface on the side away from the wall are much higher than those near the material; thus the collapse proceeds with the far side moving toward the rigid wall. The resulting acceleration of the liquid flow perpendicular to the bubble top surface develops Taylor instability at the axis of symmetry, which results into a reentrant jet that penetrates the bubble and moves much faster than the rest of the bubble surface to impact the opposite side of the bubble and the material boundary. In the present case, as shown in Fig. 4, the jet starts with a speed of 15 m/s and accelerates to about 45 m/s at the time it impacts the opposite side of the bubble and the wall, as we can see from Fig. 3. The momentum averaged jet velocity, \( V_{mom} \), shown in Fig. 4 is the average of all velocities inside the jet volume, \( V \), using the integrated momentum of the jet divided by the mass of liquid it contains,

\[
V_{mom} = \frac{1}{V} \int V dV. \tag{33}
\]

where \( V \) is the liquid velocity at any point inside the jet. Note that the discontinuity in the jet velocity curve is due to the discretization of the jet surface and the detection of the jet volume. As the bubble shape with a reentrant jet evolves, the numerical definition of the jet volume is sometimes discontinuous when several new nodes change curvature and new panels become included as part of the jet.

Fig. 5a shows the pressure contours and velocity vectors at the time the jet impacts the opposite side of the bubble. Fig. 5b shows the corresponding velocity vectors and velocity magnitude contour levels. It is clear from this figure that the jet results from a high concentrated pressure region in the liquid behind the jet, which moves into the bubble as the bubble collapses and the reentrant jet advances to impact the wall. Also, it is important to notice that the jet speed varies continuously between the jet base and its tip, increasing toward the tip.

3.1.2. Generation of loads

As we will see in later sections, the high speed flow of the reentrant jet, introduced at a distance of the order of one or a few microns from the surface to be cleaned, is essential for particle removal as the jet speed exceeds speeds generated by acoustic or hydrodynamic means, which are significantly damped by viscous effects in the boundary layer near the wall.

In addition to the high speeds, significant pressures are also generated in the same region, as illustrated in Fig. 6 for the point on the axis of symmetry. After the liquid reentrant jet crosses the gaseous environment in the bubble it impacts the wall and...
generates a water-hammer type impact dominated by compressible effects. Under these conditions, an incompressible approach is no longer warranted and compressibility of the liquid needs to be accounted for.

In addition to solving the full problem using 3DYNAFS-Comp© or Gemini (a Navy code with more advanced capabilities [64], we have developed a hybrid method described in more detail in [32] and [33] to pursue the computations from a BEM solution selected to be at a time when the reentrant jet has sufficiently approached the opposite bubble wall. This guarantees a higher accuracy of the jet computation and faster turnaround time to obtain the solution. This incompressible/compressible link method has been applied to obtain the pressures versus time presented in Fig. 6. The pressure peak of 4.4 MPa corresponds to the jet impacting the wall. In the present weak impact case, it is followed by a simple exponential decay because, as stated earlier, the collapse is rather soft and the timing of the bubble minimal volume is very close to that of the jet impact and does not produce a second high impulsive pressure as seen in other cases later.

In more dynamic cases, such as presented in [32,33] and illustrated in Fig. 7, the collapse of the ring remaining after the jet impact generates a second impulsive pressure that could be even higher than the jet impact pressure. This case corresponds to a larger bubble initiated from a nucleus of initial radius 50 µm, which increases to a 2 mm radius bubble and then collapses due to a collapse driving pressure of 10 MPa. Fig. 7 also shows the time history of the bubble equivalent radius. One can observe the correspondence between the bubble minimum volume and the second distinct pressure peak.
addition to these two peaks, many other pressure peaks are observed due to pressure or shock waves bouncing back and forth between the cleaned surface, the bubble surface, and any other daughter bubbles in the near wall flow field. The magnitudes of these pressure peaks depend on the level of deformation of the solid material.

3.2. Shear generation by a submerged jet

So far in Section 3.1 we investigated bubble behavior in idealized near wall conditions in absence of shear. In this section we consider more realistic configurations using the cleaning in a cavitation jet as an example. We describe the macroscopic jet flow, then look at how the dynamics of a bubble would be modified by the presence of strong shear generated by the jet on the surface being cleaned. To do so, we computed the velocity and pressure fields generated by a macroscopic submerged jet (not the bubble reentrant jet) impacting on the surface to be cleaned and how cavitation modifies these fields. In an ideal axisymmetric configuration with a round jet impacting the wall with a speed $V_0$, the jet would spread out at the wall with a radial speed with the same magnitude $V_0$ (in order to conserve kinetic energy as per the Bernoulli equation). As the distance, $r$, from the axis increases, the thickness of the radial submerged jet (its height over the wall) would decrease as $1/r^2$ to conserve mass. Actually, in real fluids, viscous effects and the resulting generation of shear and vorticity change significantly the picture. The jet exiting the nozzle has a non-flat velocity profile with a higher value at the center and reduced magnitudes along the edge. In addition, viscous friction with the surrounding host liquid at the edge surface diffuses the jet, widens it, and generates vortices. These can become structured and modify significantly the flow structure. Such a behavior can be seen in the $3D$-YNAS-Vis simulated flow field displayed in Fig. 8. The jet speed is seen to form regular ‘bunching’ close to the nozzle, while the jet speed on the jet edge decay significantly. Similarly, the jet speed decays as the liquid moves away from the nozzle.

The same viscous decay effects occur also along the surface to be cleaned. Right at the wall the velocity goes to zero and then it gradually rises to the maximum value within a boundary layer, which is classical in many fluid mechanics applications [92]. The thickness of the boundary layer depends on the local Reynolds number (local liquid speed outside of the boundary layer and liquid viscosity). This has strong implications on cleaning as microscopic particles at the wall are often embedded in the very low speed boundary layer and the shear exerted on them is minuscule and is unable to dislodge these particles. This is illustrated in Fig. 9, which shows the variation of the velocity profile as the distance, $r$, form the jet axis increase. Both the thinning of the jet height, as predicted by the simple potential flow theory, and the presence of strong velocity gradient (ignored in the potential theory) due to the viscosity at the wall can be seen.

In applications requiring enhanced jet cleaning and material removal, this strong vortex generation is purposely sought and enhanced through jet nozzle design for strong acoustic resonance [11,12]. At the wall, as the incoming jet velocity fluctuates, the shear flow has also to adapt and as seen in Fig. 10, and ends up exhibiting a very intensely varying shear flow configuration in both time and space.

When the cleaning results of the jet are not satisfactory the tendency is to increase the nozzle pressure drop, $\Delta P$, (i.e. the difference between the upstream – or pump – pressure, $P_{up}$, and the pressure in the container of the surface to clean, $P_{amb}$). This also increases the flow rate and the jet velocity and thus the shear rate. However, the most important impact of doing so is the lowering of the cavitation number, $\sigma$, defined for a cavitating jet as $\sigma = (P_{amb} - P_{v})/\Delta P$, where $P_v$ is the vapor pressure. Cavitation occurs as the cavitation numbers is reduced. Microscopic bubble nuclei in the flow will grow when exiting the nozzle due to the
pressure drop and then collapse strongly in the stagnation region when the jet impacts the piece to clean. More often bubble nuclei are captured in the vortices formed in the shear layer between the jet and the host fluid, can grow significantly as they enter the vortices centers [57,71] and then again collapse intensely when they reach the cleaned surface where the pressures are much higher than those at the center of the vortices.

In order to simulate cavitation in the macro scale cavitating jet, the numerical method described in Section 2.2.2 is applied. The flow field is obtained through solution of the Navier Stokes equations and describes the jet flow exiting the nozzle, advancing in the host liquid, and then impacting on the plate. Bubble nuclei randomly dispersed in the liquid are used in the simulations. These microscopic or nanoscopic nuclei are omnipresent in any liquids [43,91] unless extreme precautions are taken to produce ultra-pure liquids, in which case there still is a chance to have undetected nanoscopic bubble nuclei. As described earlier, a Lagrangian procedure is used to track these nuclei, and determine their position and volume in space and time. This is fed back to the mixture flow and provides the void fraction at each location.

![Fig. 7. Zoom at bubble collapse of the equivalent bubble radius evolution versus time, along with the pressure recorded at the axis on the rigid wall located at a standoff of \( X = 0.75 \) for \( R_0 = 50 \mu m, R_{max} = 2 \) mm, and a collapse driving pressure of 10 MPa.](image)

![Fig. 8. (a) Axial velocity field contours normalized by the mean jet velocity for a non-cavitating flow. Wall at 13 orifice diameters from the orifice. (b) Vorticity contours when the cleaned wall is 5 orifice diameters away from the orifice.](image)
necessary to advance the solution. Knowledge of the bubble dynamics and the fluid dynamics then enables one to determine fluctuating shear and pressures at the cleaned surface.

Fig. 11 shows an illustrative result for the two-way coupled (bubbles-liquid and liquid-bubbles) simulations of a cavitating jet. The flow field near the nozzle orifice is nicely illustrated by the velocity vectors and their evolution as the distance from the nozzle increases. A more impressive illustration of the flow field is seen through the nuclei captured from the face of the nozzle into the shear layer. These nuclei grow while entering the large vortical structure at the edge of the submerged jet. These structures form two modes: an azimuthal mode resulting in vortex rings and a longitudinal mode that results in elongated vortices which join two vortical ring structures. This is very well visualized by the bubbles captured in the vortices and clearly seen in the figure. Later on as the jet advances to hit the wall (Fig. 12), the bubbles grow into larger clouds, which collapse at or near the wall. The passage of the structures and the bubbles further induces fluctuations in the wall pressures and shear. The very large difference in the generated pressure field between cavitating and non-cavitating jet is clearly seen in Fig. 13. Orders of magnitude increase relative to the non-cavitating case (red curve) in the number and amplitude of the impulsive pressures due to the collapsing bubbles can be seen in the green curve in that figure.

Understanding of the detailed mechanisms requires studying the dynamics of single bubbles in the shear layer as done in the next sections.

3.3. Bubble collapse in the shear flow over a flat plate

In order to illustrate the influence of the shear layer near a rigid wall on the dynamics of the cavitation bubbles, we reconsider the growth and collapse of the bubble case considered in Section 3.1 and account now for the presence of a shear flow at the wall. We use the modified BEM method described in Section 2.1.1. The background shear flow is such that (with the notations of Section 2.1.1) $V_{shear} = 0$ at the wall and grows following a Blasius velocity profile away from it to attain $V_{shear}$, at the location of the bubble center. In general, we can study shear effect on bubble dynamics by defining a shear parameter, $\tau$, such that:

$$\tau = \frac{V_{top} - V_{bot}}{\sqrt{\Delta P/\rho}}.$$  \hspace{1cm} (34)
where $V_{\text{top}}$ and $V_{\text{bot}}$ are the liquid velocities at the location of the top and bottom of the bubble. If the bubble is small relative to the shear layer thickness, $V_{\text{top}} - V_{\text{bot}} \approx 2 S_0 R_0$ at the beginning of the dynamics, where $S_0$ is the shear rate at location of the bubble center and $R_0$ is the initial bubble radius. $\Delta P$ is the pressure difference driving the bubble dynamics. For the case studied here and in Section 3.1, $\Delta P = P_0 - P_{\text{amb}}$. Hence, the shear parameter represents the ratio between the difference of liquid velocity between the top and bottom of the bubble and the bubble characteristic collapse velocity, $\sqrt{\Delta P/\rho}$.

Two shear conditions are used for illustration in this paper. These are shown in Fig. 14, and both cases use a Blasius profile for the boundary layer on the plate [92,93]. In one case the velocity rises from 0 m/s at the wall to 10 m/s at a distance of 200 $\mu$m (green curve). This corresponds to the results shown below in Fig. 15. In the other case the velocity rises from 0 m/s at the wall to 5 m/s but at a much smaller distance of 10 $\mu$m. This corresponds to the results shown in Fig. 16.

Figs. 15 and 16 illustrate results obtained for different values of $\tau$. Additional cases can be found in [58].
In each of the two figures four conditions are presented and correspond to different standoffs between the bubble and the plate. In an infinite medium the considered bubble grows to a maximum size of about 27 μm (see Fig. 2). This makes the three standoffs considered (15 μm, 25 μm, 40 μm, and 60 μm) close to 0.5, 1, 1.5 and 2 maximum bubble radii from the plate. Combining both cases, a range of values of τ is covered: between 0 and 0.07.

Fig. 15 shows interesting results for the bubble behavior during both bubble growth and collapse. As the shear parameter τ increases, the bubble deforms and elongates more and more during its growth. The elongated shape actually reflects properly the velocity increase rate between the wall and the bubble center or more appropriately the velocity increase between bottom and top of the bubble. For small values of τ, and smaller values of the standoff distance, X, here (as observed in the first two cases in Fig. 15), the reentrant jet angle deviates from the perpendicular to the plate, but still hits it with an angle. For larger values of τ, and larger X (e.g. Fig. 15c and d), the shear flow overpowers the pure effect of the presence of the wall on the bubble dynamics, and the re-entering jet formation is totally modified. The bubble tends to cut itself into two half-bubbles because of the development of two opposing flat jets aligning themselves in the direction of the shear.

For the cases considered in Fig. 16, the boundary layer is very thin and the three cases Fig. 16b–d have an imposed uniform flow instead of shear. The figure then actually shows the effect of the standoff distance when the bubble is almost in a uniform flow field of speed 5 m/s. As a result, the jet resulting from the presence of the wall weakens as the bubble wall distance increases. The effects of the translation speed on the jet shape are minimal under these conditions besides moving the bubble as a whole, and this affects little the bubble dynamics. This will change for higher slip velocities where the bubble forms a jet directed opposite to the direction of the flow [42].

4. Particle cleaning simulation

4.1. Near wall flow field in presence of particle and bubble

As discussed earlier, due to strong viscous effects, the velocity of the liquid in the macro scale cleaning jet drops to zero at the wall and the shear force is often unable to overcome the cohesion and friction forces of small dirt particles to remove. Fig. 17 shows the Navier Stokes simulation of a cubic particle sitting in a shear flow obtained by 3DYNAS-Vis. It is seen that the particle further reduces the magnitude of the velocities around it and generates a wake ‘shadow’ zone behind it with almost no flow in the downstream direction. This also results in the generation of a higher pressure stagnation region on the upper left corner of a cubic particle and a suction region on the upper surface of the particle and on its downstream face. For a relatively light particle and for weak adhesion and friction, this could result in tumbling the particle and getting it lifted to be entrained in the flow. For more strongly adhered particles, the pressures and flow field created by cavitation bubbles can overcome these resistance forces.

In addition to the perturbation due to the presence of particles, the flow field will be also perturbed by the presence of cavitation bubbles. Initially, during a cavitation bubble dynamics the pressure of the gas and vapor inside the bubble exceed significantly the pressure in the surrounding water, resulting in the propagation of a high pressure wave in the liquid. This wave can act as a repulsive force on an object in the vicinity of bubble. As the bubble expands, the pressure inside it decreases and the pressure around it drops below the ambient pressure and this remains for a relatively long period until an advanced stage in the bubble collapse. This is shown in Fig. 18a, when the pressure drops below 0.1 MPa. This low, relatively long duration pressure drop creates a suction force on any object in the vicinity of the bubble. The pressures, the positive pressure as the bubble expands and the suction pressure as the bubble collapses, decay with the inverse of the radial distance from the bubble interface. In the bubble near field, the pressure drops like $r^{-2}$, where $r$ is the radial distance. In the far field the pressure drops like $r^{-1}$ [97]. The spatial variations of the pressure along a line passing through the center of bubble and parallel to X-axis are shown in Fig. 18b. It is therefore expected to see a particle close to an inertial cavitation bubble be sucked toward the bubble prior to bubble collapse and then pushed away during the collapse.

4.2. Dynamics of a bubble near a responding particle

To further investigate this dynamics, we consider coupled fluid/structure interaction computations as introduced in Section 2.4.4. To remain within the same conditions as previous sections in this paper, we consider the same bubble dynamics conditions as those illustrated in Fig. 2. The initial pressure inside the bubble is 1 MPa, while the pressure in the surrounding water is 0.1 MPa.

The dynamics is simulated using 3DYNAS-Comp coupled with a rigid body motion routine as described in Section 2.4.2. The
substrate and the dirt particle are considered to be in contact initially and the contact model selected for illustration allows sliding between the surfaces and accounts for static and dynamic friction through coefficient of the model described in Eq. (23).

The results of the interaction are expected to depend on the following parameters:

(a) Relative positions of the bubble, particle, and wall. These are illustrated in Fig. 19 for a cubic shape particle (selected to be simple enough without being a sphere, which would roll easier on the surface to be cleaned). The parameters in this case are: the spacing, \(d\), distance between the bubble and the dirt edges and the bubble standoff to the wall, \(X\).

(b) Relative size of the bubble and the particle.

(c) Relative sizes of bubble, particle, and shear layer thickness.

(d) Magnitudes of the bubble collapse loads, the shear force, and the frictions/adhesion forces.

For illustrative purposes and for brevity, we will consider point (a) only in the examples shown below. Further detail and analysis of the other parameters will be presented in a separate publication.

4.3. Effect of the bubble and particle spacing, \(d\)

The suction and repulsion pressures exerted by the bubble depend on the distance of each discrete point of the dirt particle from the bubble center. The resulting forces are the integral of these pressures over the particle. This implies that the spacing between the dirt and the bubble has a significant influence on the particle motion. When \(d\) is small, 5 \(\mu\)m in the example shown...
below, the bubble and the dirt particle are very close to each other and as illustrated in Figs. 20 and 21 the suction forces are predominant. The initial short repulsion force generated during initial bubble expansion (Figs. 18a, 20a, and 21a for \( t < 1 \mu s \)) is rapidly overtaken by a strong and long suction force (Figs. 18a, 20b–d, and 21a for \( t > 1 \mu s \)). Fig. 20 shows four time sequences of the bubble dynamics and the particle response. As the bubble grows, one could think incorrectly because of the velocity vectors pointing toward the particle that the particle will be pushed away from the bubble. Instead, as discussed earlier, the pressure field sucks the particle toward the bubble. During the period separating Fig. 20a from Fig. 20c (~5 \( \mu s \)) the particle moves upstream about 25 \( \mu m \) (almost twice its characteristic size). This brings the particle practically below the bubble at its maximum radius, then it collapses downstream of the particle. The reentrant jet ends up moving toward the wall (Fig. 20d) downstream of the dirt particle, therefore exerting further force to continue moving the particle upstream.

Fig. 21 shows the trajectory of the center of gravity of the dirt particle in the three directions. The left pane shows the long time history illustrating mostly significant upstream horizontal motion of the particle, while the particle is seen bobbling up and down in the vertical direction. The right pane shows a zoom on the initial bubble period phase. The figure also shows the temporal variation of the bubble equivalent radius, which illustrates initial short lived repulsion of the dirt particle followed by particle strong attraction (suction) toward the bubble. This suction also results in lifting the dirt particle with the Z-coordinate of the dirt particle increasing during bubble growth. The bubble then shrinks and finally collapses on top of the dirt particle. Here, the collapse on the dirt particle results in forcing the dirt back toward the substrate.

For a larger spacing \( d \) between the bubble and the particle, the opposite scenario occurs. This is because the negative pressure gradient (toward the bubble) is limited to distances from the bubble center closer than about one and a half bubble radius [96]. As shown in Fig. 22 for an initial bubble-particle spacing, \( d = 20 \mu m \), very little motion of the particle is seen in the X-direction during the first bubble period. Only lifting of the downstream edge of the particle can be seen. The particle moves only very slightly toward the bubble as shown in Fig. 22b and then it moves away from it once the reentrant jet has advanced after impacting the wall (Fig. 22d). The bubble grows and collapses upstream of the particle almost unaffected by it. As a result the bubble collapse forms a strong jet, which moves the particle significantly to far downstream. The overall movement of dirt particle is shown in Fig. 23a, with a zoom on the first period shown in Fig. 23b.

Finally, Fig. 24 compares the two components of the trajectory of the particle for the two values of the spacing, \( d \), shown above. Since the problem has a plane of symmetry there is no movement of the particle in the Y-direction. Both the X and Z-direction clearly show similar initial motions of the particles (\( t < 1 \mu s \)) followed by opposite motions for larger times.

### 4.4. Effect of the standoff distance between the bubble and the wall

This section illustrates the effects on the particle motion of the distance between the bubble and the wall for a fixed spacing between bubble and particle. We illustrate the effect here by considering two standoffs 25 \( \mu m \) and 20 \( \mu m \) and a spacing of 10 \( \mu m \). The first case with a standoff of 25 \( \mu m \) and a spacing of 10 \( \mu m \) generates flow and pressure fields and bubble contours and dynamics similar to what we observed earlier in Figs. 22 and 23 (standoff of 25 \( \mu m \) and spacing of 20 \( \mu m \)) and is not shown here for brevity. Suction forces in that case were not strong. However, when the standoff is decreased to 20 \( \mu m \), the relative position of the bubble
and the particle and the effects of the bubble image in the wall become such that the bubble grows while sucking the particle toward it as shown in Fig. 25. The bubble growth and beginning of collapse occur practically while the bubble is over the particle, while the collapse with reentrant jet formation develops downstream of the particle, pushing it strongly upstream as in the cases with small bubble spacing seen in the previous subsection.

A comparison of the two components of the trajectory of the particle for the two values of the standoff, \( X \), are shown in Fig. 26. Here too, both the \( X \) and \( Z \)-direction clearly show similar initial motions of the particles (\( t < 1 \mu s \)) followed by opposite motions for larger times for the two standoffs.

The above describes qualitatively two types of interactions between an inertial cavitation bubble and a dirt particle. A more extensive detailed parametric study is necessary to fully cover the space of variables and will be addressed elsewhere.

5. Material removal simulation

Another aspect of surface cleaning involves removal of a layer of deposited coating, an oxidized thickness of the substrate, or a layer of another dirty material from the surface to clean. Modeling such a cleaning process requires inclusion of strong fluid–material interaction effects and modeling of strongly coupled fluid dynamics (liquid and bubbles) and material deformation dynamics. The numerical procedures we have developed to address this problem were introduced in Sections 2.4.3 and 2.4.4. We illustrate results of the approach here using a few examples.

The finite element computations for the layer to remove are conducted using stretched grids with material and fluid domain characteristic dimensions a thousand times larger than the bubble characteristic radius. This is to avoid strong material stress wave reflections from the domain edges and resulting artificial accumulation of stresses in the domain during the computations. As described in references [32,33] we have extensively applied this approach to the study of cavitation pitting for metallic and rubber-like materials. Fig. 27 shows the time evolution of the equivalent stresses in an aluminum plate subjected to the pressures resulting from the very strong bubble collapse shown in Fig. 28. In this case the bubble grew to a maximum radius of 40 times its initial radius. The bubble started with an initial radius of 50 \( \mu m \), attained a maximum equivalent bubble radius of 2.0 mm, and collapsed due to a collapse driving pressure of 10 MPa when its initial standoff was 1.5 mm.
The first very high stress occurs when the reentrant jet impacts the aluminum center, then propagates and moves radially out in the material as illustrated in Fig. 27. A second stronger impact occurs later when the bubble ring formed by the reentrant jet break-through collapses (Fig. 28). All regions that have been exposed to the red stress contour levels shown in Fig. 27 experience permanent deformation due to either the reentrant jet impact or the bubble ring collapse.

Fig. 28 show the time histories of the liquid pressure and the vertical displacement of the material surface at the center of the impacted surface. The material starts by getting compressed as the high pressure loading due to the reentrant jet impact reaches it, and the plate surface center point starts to move in. The maximum deformation occurs when the highest pressure loading peak due to the bubble ring collapse reaches the center of the plate. Once the bubble pressure loading stops the deformed surface oscillates until damping occurs. A pit is left on the surface following permanent deformation of regions where the local stresses exceeded the material elastic limit.

The above example is for a strong resistant material and for high cavitation loads. For cleaning softer deposits with smaller material resistance much weaker loads are needed. To illustrate this, we consider a coating with a material such as polyurea or a 10 times "softer material as illustrated in the properties in Table 1. For these cases, we model the materials using the Johnson–Cook model for the material behavior presented in...
Section 2.4.3 and Eq. (31). The model constants were selected based on Hopkinson bar tests [89,94] and are shown in Table 1. A second fictitious material, with values of $A$, $B$, and $C$ ten times smaller was also chosen for numerical testing of a very soft deposit at the surface to clean. We will dub it VS (“very soft”) material in the following.

Fig. 29 shows a set of cases where the applied load to the material is large enough to strip out the layer of material off a much stronger substrate assumed to be not deformable. The permanent deformation for three thicknesses of polyurea is shown. As the thickness of the impacted layer is reduced, the maximum plastic strains responsible for permanent deformation and potential failure, is seen to move from the surface of the material (Fig. 29a and b) to the interface region connecting the layer to the rigid substrate. This is more clearly seen in Fig. 30, where both loads and layer thicknesses are lower, the deformations are more moderate, and it is easier to see the various levels of stresses and strains in the material.

The potential to clean a layer of deposited material on a substrate using a weak bubble is examined below. The imposed pressure, shown in Fig. 31a, is a pressure drop from 0.1 MPa to the liquid vapor pressure for a duration of 2.5 ms followed by a return to the 0.1 MPa pressure. The bubble grows to a maximum size of 2 mm then collapse violently with the formation of a reentrant jet when placed near a rigid wall at a normalized standoff distance of 0.75 (Fig. 31b). Concerning a layer to be removed, the properties of the fictitious weak material introduced in Table 1 as VS are used in the structure code DynaN. Since the loads do not become significant until the reentrant jet is formed [32], the solution from the BEM code shown in Fig. 31b right before the reentrant jet impacts the opposite side of the bubble, is used to initiate the FSI computations coupling 3DYNAS-Comp with DynaN as described in [32,33]. As the impact pressure from the reentrant jet impacting the opposite side of the bubble reaches the wall, the coating starts deforming as shown in Fig. 32a. This shows a crosscut of the toroidal bubble with the axis of symmetry being the left $Y$-axis and the white contour being the bubble ring outline. The deformation increases further as the bubble collapse proceeds as shown in Fig. 32b and c. The final pit shape with deformed mesh is shown in Fig. 33. Here also, the axis of symmetry is the left $Y$-axis and the material/liquid interface is the upper deformed line.

The evolution of the pit depth with time can be seen in Fig. 34. The figure also shows the effect of the initial thickness of the coating on the progress of the pit depth. We can see that no deformation occurs (~1 μs) until the effect of the reentrant jet is felt by the wall. From there on, the deformation evolves regularly and
increases as the coating thickness increases because more material thickness is available to absorb the strain. The final pit shapes for the different initial coating thicknesses can be seen in Fig. 35. As the thickness becomes smaller and smaller, the material becomes susceptible to removal as a result of cracking and failure, which is not taken into account in the present computations. However, indications of this effect have been seen in Figs. 29c and 30a and b, where very high strains develop at the interface between the coating and the substrate.

6. Summary

Surface cleaning is usually achieved by creating strong shear at the surface to be cleaned. However, as the requirements for better or more efficient cleaning become more demanding, cavitating bubbles become a good source for enhanced cleaning. Viscous effects prevent the velocities generated by conventional methods (i.e. both jet flow and acoustic ultrasonic or megasonic flows) to generate forces large enough to dislodge and lift microscopic particles.
Fig. 27. Time sequence of the equivalent stress contours in an aluminum Al 7075 plate from the collapse of a bubble with initial $R_0 = 50 \mu m$, maximum equivalent bubble radius $R_{max} = 2.0 \ mm$, and collapse pressure $P_{amb} = 10 \ MPa$ and normalized standoff $X = 0.75$.

Fig. 28. Time history (a) total simulation time (b) initial simulation time of pressure and vertical displacement monitored at the center location of the aluminum Al 7075 material for a bubble with initial $R_0 = 50 \mu m$, maximum equivalent bubble radius $R_{max} = 2.0 \ mm$, and collapse pressure $P_{amb} = 10 \ MPa$ and normalized standoff $X = 0.75$.

Table 1
Material coefficients of Johnson–Cook model for polyurea and a fictitious much softer material.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>$A$ (Pa)</th>
<th>$B$ (Pa)</th>
<th>$n$</th>
<th>$C$</th>
<th>$m$</th>
<th>$T_s$ (K)</th>
<th>$T_m$ (K)</th>
<th>$G$ (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyurea</td>
<td>$4.343 \times 10^5$</td>
<td>$1.447 \times 10^5$</td>
<td>0.613</td>
<td>1.61</td>
<td>1.5</td>
<td>298</td>
<td>750</td>
<td>$4.13 \times 10^7$</td>
</tr>
<tr>
<td>VS: very soft</td>
<td>$4.343 \times 10^4$</td>
<td>$1.447 \times 10^4$</td>
<td>0.613</td>
<td>1.61</td>
<td>1.5</td>
<td>298</td>
<td>750</td>
<td>$4.13 \times 10^6$</td>
</tr>
</tbody>
</table>

Fig. 29. Permanent deformation of Polyurea with plastic strain contours. The applied amplitude of the load for all cases is 500 MPa while the material layer thickness is (a) 250 $\mu m$, (b) 190 $\mu m$, and (c) 120 $\mu m$.

Fig. 30. Permanent deformation of Polyurea with plastic strain contours. The applied amplitude of the load for all three cases is 100 MPa while the material layer thickness is (a) 60 $\mu m$, (b) 40 $\mu m$, and (c) 25 $\mu m$.

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particles away from the surface to clean. Activating microscopic (or nanoscopic) bubble in the boundary layer very close to the wall and forcing them to behave in an inertial fashion (i.e. strong growth and collapse) offers a solution to the problem. The strong collapse of these bubbles results in the propagation of shock waves, which can interact with the dirt particle and break in into particles away from the surface to clean. Activating microscopic (or nanoscopic) bubble in the boundary layer very close to the wall and forcing them to behave in an inertial fashion (i.e. strong growth and collapse) offers a solution to the problem. The strong collapse of these bubbles results in the propagation of shock waves, which can interact with the dirt particle and break in into particles away from the surface to clean. Activating microscopic (or nanoscopic) bubble in the boundary layer very close to the wall and forcing them to behave in an inertial fashion (i.e. strong growth and collapse) offers a solution to the problem. The strong collapse of these bubbles results in the propagation of shock waves, which can interact with the dirt particle and break in into particles away from the surface to clean. Activating microscopic (or nanoscopic) bubble in the boundary layer very close to the wall and forcing them to behave in an inertial fashion (i.e. strong
finer particles. This aspect was not addressed in this contribution but will be addressed next.

In this contribution we have seen that the bubble dynamics can generate suction and repulsion forces and pressure gradients, which can move the small particles toward or away from the bubble depending on the original bubble/particle/wall geometric configurations. Bubble suction occurs mainly during the relatively slow bubble growth phase for particles very close to the bubble, while repulsion occurs during the highly inertial phases of initial bubble growth and rebound and the phase of collapse. In addition to the above, the formation and development of the bubble reentrant jet is a strong source of much localized high shear, which results in strong particle lifting from the surface, tumbling, and repulsion away for the jet impact region at the wall.

The formation and development of the reentrant jet, as well as the ensuing formation and collapse of a vortex ring bubble, can also be strong sources of surface cleaning through removal of coatings or thin layers of adhered material. The strong loads generated by the jet dynamics and the resulting shock waves from both jet impact and bubble ring collapse can impart permanent deformation or form pits on the coating. Further increases in the intensity can result in material failure and coating mass loss or coating removal. The cumulative effects of the multitude of bubbles and bubble cloud collapses can—similar to undesirable cavitation mass-erosion—remove unwanted deposits and be harnessed to clean material surfaces.

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References


