Nonsingular boundary integral method for deformable drops in viscous flows

Citation for published version (APA):

Bajlekov, I. B., Anderson, P. D., & Meijer, H. E. H. (2004). Nonsingular boundary integral method for deformable drops in viscous flows. *Physics of Fluids*, 16(4), 1064-1081. <https://doi.org/10.1063/1.1648639>

DOI:

[10.1063/1.1648639](https://doi.org/10.1063/1.1648639)

Document status and date:

Published: 01/01/2004

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

[Link to publication](#)

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license above, please follow below link for the End User Agreement:

www.tue.nl/taverne

Take down policy

If you believe that this document breaches copyright please contact us at:

openaccess@tue.nl

providing details and we will investigate your claim.

Nonsingular boundary integral method for deformable drops in viscous flows

Ivan B. Bazhlekov, Patrick D. Anderson, and Han E. H. Meijer

Materials Technology, Dutch Polymer Institute, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

(Received 25 March 2003; accepted 23 December 2003; published online 8 March 2004)

A three-dimensional boundary integral method for deformable drops in viscous flows at low Reynolds numbers is presented. The method is based on a new nonsingular contour-integral representation of the single and double layers of the free-space Green's function. The contour integration overcomes the main difficulty with boundary-integral calculations: the singularities of the kernels. It also improves the accuracy of the calculations as well as the numerical stability. A new element of the presented method is also a higher-order interface approximation, which improves the accuracy of the interface-to-interface distance calculations and in this way makes simulations of polydispersed foam dynamics possible. Moreover, a multiple time-step integration scheme, which improves the numerical stability and thus the performance of the method, is introduced. To demonstrate the advantages of the method presented here, a number of challenging flow problems is considered: drop deformation and breakup at high viscosity ratios for zero and finite surface tension; drop-to-drop interaction in close approach, including film formation and its drainage; and formation of a foam drop and its deformation in simple shear flow, including all structural and dynamic elements of polydispersed foams. © 2004 American Institute of Physics. [DOI: 10.1063/1.1648639]

I. INTRODUCTION

The main advantage of the boundary integral methods, compared with other methods (e.g., FDM, VOF, FEM), is that for a number of multiphase flow problems its implementation involves integration only on the interfaces. Thus, discretization of the interfaces only is required, which allows for a higher accuracy and performance, especially in three-dimensional (3D) simulations.

Boundary integral methods have been successfully used recently for simulations of complex multiphase flows: drop deformation and breakup;^{1–5} drop-to-drop interaction;^{6–8} suspension of liquid drops in viscous flow;^{9–11} deformation of a liquid drop adhering to a solid surface and free-surface viscoelastic flows.^{12–14}

The main disadvantage of the boundary integral method is the singularity of the free-space Green's kernels.¹⁵ In most of the studies special attention is paid to the accurate calculation of the boundary integrals around the singular point. The two most commonly used approaches are local mesh refinement and/or higher-order integration rules in the vicinity of the singular point,^{1,16} and near singularity subtraction, where for a closed interface, using volume conservation identities, the integrals over the singular point vicinity are represented via the integral over the residual of the interface.^{6,10,17,18} Both approaches, however, cannot give satisfactory results when the singular point is close to the residual of the interface.¹⁶ In our method, the recently proposed¹⁹ nonsingular contour-integral representation of the layer potentials is used for the calculation of the boundary integrals.

Another problem, related to a numerical simulation of transient interfaces, is the numerical instability due to the interfacial tension. The problem is typical for the case of small capillary numbers and small space steps and can lead to a prohibitively small time step.^{6,17} The situation is even worse in the case of thin films in the presence of long-range intermolecular van der Waals forces, which are typical for foam dynamics. In this case, numerical instabilities appear due to the strong dependence of the van der Waals forces on the film thickness. Here, we propose a multiple time-step approach which improves the stability of the method without increasing the computational time.

Other important elements of a boundary integral method for deformable drops are the curvature and normal vector calculations as well as mesh refinement. Curvature and normal vector calculations have been discussed by several authors.^{10,17,20,21} In these studies different approaches have been used: line (or also called contour) integration;¹⁰ local fitting with a smooth interface;^{17,20} and differentiation of the normal vector, which is defined as the area average, followed by linear interpolation of the normal vectors of the neighboring flat triangular elements.²¹ In the present method, due to the representation of the layer potentials via contour integrals, the normal vector does not take part in the boundary integral formulation. This eliminates any effect of the error due to the normal vector calculation on the velocity field. The mean curvature has in general a smaller variation than the normal vector and therefore introduces a smaller error in the velocity calculation. For the mean curvature calculation we use line integration.¹⁰

Adaptive algorithms for mesh refinement of deformable

interfaces have also been widely discussed.^{10,17,22–24} Two approaches are commonly used, as well as their combination. The first is mesh size optimization, also called mesh relaxation or mesh stabilization. In this approach, for a fixed mesh topology, the nodes are moved with a tangential field which is locally¹⁰ or globally¹⁷ defined by a dynamical system of massless springs with properly chosen tensions. The second approach includes topological transformations such as addition and subtraction of nodes as well as node reconnection.^{22–24} In the present study we use a combination of both. New elements in our method, regarding mesh refinement, are extra terms in the tangential velocity, which prevents mesh distortion due to the tangential hydrodynamic velocity, and a reconnection of the nodes, which maintains an optimal mesh topology.

In the case when the viscosity ratio is not equal to one, the interface velocity is given by a system of integral equations, usually solved by iterative methods.^{6,16,17} In these methods a significant improvement of the convergence is achieved by deflating the spectrum of the double-layer operator by removing the marginal unit eigenvalues, as described by Pozrikidis.¹⁵ The commonly used iteration method is the method of successive substitutions,^{6,16} which is also applied here. To improve the poor convergence of the successive iterations for extremely large or small viscosity ratios, and interfaces in very close approach, Zinchenko *et al.*¹⁷ proposed a combination of successive iterations and biconjugate gradient iterations.

Sections II and III are devoted to the mathematical model, the boundary integral formulation and the general elements of the numerical technique. In Sec. IV numerically challenging 3D problems for drops in linear viscous flows are presented: drop deformation at zero surface tension; drop deformation and breakup at finite surface tension; drop-to-drop interaction, including drainage of dimpled films; and foam-drop dynamics.

II. MATHEMATICAL FORMULATION

A. Mathematical model

We consider deformable drops of a Newtonian fluid with viscosity $\lambda\mu$ in another immiscible Newtonian fluid with viscosity μ , subjected to a linear flow. All fluids are considered incompressible and inertial forces are negligible. In dimensionless terms the governing equations are

$$-\nabla \cdot \Pi^i = 0, \quad \nabla \cdot \mathbf{u}^i = 0 \in \Omega_i, \quad i = 0, 1, 2, \dots; \quad (1)$$

where $\Pi^i = -p^i \mathbf{I} + \lambda_i (\nabla \mathbf{u}^i + (\nabla \mathbf{u}^i)^T)$ is the stress tensor, $\mathbf{I}$ is the unit tensor, p^i is the pressure, and $\mathbf{u}^i$ is the velocity in the i th phase Ω_i . The problem has only one viscosity ratio λ ($\lambda_0 = 1$ and $\lambda_i = \lambda$ for $i > 0$).

The boundary conditions at the interface $S^i = \Omega_i \cap \Omega_0$ are the stress balance boundary condition and continuity of the velocity across the interface,

$$(\Pi^0(\mathbf{x}) - \Pi^i(\mathbf{x})) \cdot \mathbf{n}(\mathbf{x}) = f(\mathbf{x}) \mathbf{n}(\mathbf{x}), \quad \mathbf{u}^0(\mathbf{x}) = \mathbf{u}^i(\mathbf{x}), \quad (2)$$

where $\mathbf{n}(\mathbf{x})$ is the unit vector normal to S^i . Thus, the present study is limited to interfacial forces that are normal to the

interfaces. The numerical results presented in Sec. IV involve the capillary and the disjoining pressure

$$f(\mathbf{x}) = 2k(\mathbf{x})/\text{Ca} - A/h^3(\mathbf{x}), \quad (3)$$

where $k(\mathbf{x}) = 0.5(1/R^1 + 1/R^2)$ is the mean curvature of the interface, R^1 and R^2 are the main radii of the curvature. The capillary number (in the case of simple shear flow) is defined as $\text{Ca} = R\dot{\gamma}\mu/\sigma$, where $\dot{\gamma}$ is the shear rate, σ is the interfacial tension and R is an equivalent radius of the drops. The second term in (3), called disjoining pressure, takes into account the repulsive van der Waals forces and is important only at extremely small interface-to-interface distances, $h(\mathbf{x}) \ll R$. The dimensionless parameter A is proportional to the Hamaker constant H , $A = H/(6\pi R^3 \dot{\gamma}\mu)$. In the present study the disjoining pressure is considered only in the case of foam-drop dynamics in Sec. IV D.

The velocity at infinity is prescribed via a boundary condition,

$$\mathbf{u}_\infty(\mathbf{x}) = \mathbf{L} \cdot \mathbf{x}, \quad \|\mathbf{x}\| = \infty, \quad (4)$$

where $\mathbf{L}$ specifies the type of linear flow.

The evolution of the interface $S(\mathbf{x}, t)$ is given by the kinematic condition

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) + \mathbf{w}(\mathbf{x}, t), \quad \mathbf{x} \in S, \quad (5)$$

where $\mathbf{w}$ can be an arbitrary velocity, tangential to S . In the present method $\mathbf{w}$ is chosen in a way similar to the approach of Loewenberg and Hinch.¹⁰

B. Boundary integral formulation

For a given position of the interfaces S^i the solution of the mathematical model (1)–(3) for the velocity $\mathbf{u}(\mathbf{x}_0)$ at a given point $\mathbf{x}_0$ can be obtained by means of the boundary integral formulation,^{6,15,17}

$$(\lambda + 1)\mathbf{u}(\mathbf{x}_0) = 2\mathbf{u}_\infty(\mathbf{x}_0) - \frac{1}{4\pi} \int_S f(\mathbf{x}) \mathbf{G}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) - \frac{\lambda - 1}{4\pi} \int_S \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}), \quad (6)$$

where the integration is over the total interfacial area $S = \cup_i S^i$. The tensors $\mathbf{G}$ and $\mathbf{T}$ are the Stokeslet and stresslet, respectively,

$$\mathbf{G}(\mathbf{x}_0, \mathbf{x}) = \mathbf{I}/r + \hat{\mathbf{x}}\hat{\mathbf{x}}/r^3, \quad \mathbf{T}(\mathbf{x}_0, \mathbf{x}) = -6\hat{\mathbf{x}}\hat{\mathbf{x}}\hat{\mathbf{x}}/r^5,$$

$$\text{where } \hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0, \quad r = |\hat{\mathbf{x}}|.$$

The main advantage of a boundary integral method is that it involves integration only on the interfaces. The main problem, however, regarding the numerical implementation of (6), is due to the singularities of the kernels $\mathbf{G}$ and $\mathbf{T}$ at $\mathbf{x} = \mathbf{x}_0$, which is discussed in the following section.

C. Nonsingular contour-integral representations of the single and double-layer potentials

Important properties of the Stokeslet and stresslet are the following identities:¹⁵

FIG. 1. Interface discretization by triangles with vortices $\circ$. The basic surface element S_j is defined by the centers of mass of the triangles ($\square$) and element sides ($\blacksquare$) to which the node $\mathbf{x}_j$ belongs.

$$\int_{S_c} \mathbf{G}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}_s(\mathbf{x}) ds(\mathbf{x}) = 0, \quad (7)$$

$$- \int_{S_c} \mathbf{T}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}_s(\mathbf{x}) ds(\mathbf{x}) = \mathbf{I} \begin{cases} 8\pi, & \text{if } \mathbf{x}_0 \text{ inside } S_c \\ 4\pi, & \text{if } \mathbf{x}_0 \text{ on } S_c \\ 0, & \text{if } \mathbf{x}_0 \text{ outside } S_c \end{cases}, \quad (8)$$

which hold for an arbitrary closed surface S_c , where $\mathbf{n}_s(\mathbf{x})$ is the unit normal to S_c directed outwards.

Based on (7) and (8), it was proven¹⁹ that the single- and double-layer potentials on a part D of the interface can be expressed as integrals over its contour ∂D ,

$$\int_D \mathbf{G}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}_D(\mathbf{x}) ds(\mathbf{x}) = \oint_{\partial D} \frac{d\mathbf{y} \times \mathbf{y}}{|\mathbf{y}|}; \quad (9)$$

$$\int_D \mathbf{T}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}_D(\mathbf{x}) ds(\mathbf{x}) = 2 \oint_{\partial D} \frac{\mathbf{y}(\mathbf{y} \times d\mathbf{y})}{|\mathbf{y}|^3} + 2\mathbf{I} \left(C + \oint_{\partial D} \frac{\mathbf{a} \cdot (d\mathbf{y} \times \mathbf{y})}{|\mathbf{y}|(|\mathbf{y}| + \mathbf{a} \cdot \mathbf{y})} \right), \quad (10)$$

where $\mathbf{y} = \hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0$; $\mathbf{x} \in \partial D$ and $\mathbf{a}$ is an arbitrary unit vector. In the above equations, $d\mathbf{y} = \mathbf{t} dl(\mathbf{y})$, where $\mathbf{t}$ is the unit vector tangential to the contour ∂D defined as $\mathbf{t} = \mathbf{b} \times \mathbf{n}$, see Fig. 1. The absolute value of the sum in the brackets of (10) has to be equal to the solid angle $\omega(\mathbf{x}_0, D)$, defined by the pole $\mathbf{x}_0$ and D , and its sign depends on the direction of the normal vector $\mathbf{n}_D(\mathbf{x})$. The last integral in (10) is a measure of the solid angle $\omega_a(\mathbf{x}_0, \partial D)$ defined by the pole $\mathbf{x}_0$ and the contour ∂D to which the ray $A_{\mathbf{x}_0}^{-a} = \{\mathbf{x}_0 - \alpha \mathbf{a}; \alpha > 0\}$ does not belong. In general, there are two solid angles defined by $\mathbf{x}_0$ and ∂D . Thus, the constant C accounts for the difference between $\omega(\mathbf{x}_0, D)$ and $\omega(\mathbf{x}_0, \partial D)$: if $\mathbf{x}_0 \in D$, then $C = -2\pi \text{sign}(\mathbf{a} \cdot \mathbf{n}(\mathbf{x}_0))$; if $A_{\mathbf{x}_0}^{-a}$ crosses D in a point $\mathbf{A}_D$, then $C = -4\pi \text{sign}(\mathbf{a} \cdot \mathbf{n}(\mathbf{A}_D))$.

The main advantage of the contour representations (9) and (10) is that they are nonsingular. This is obvious for the single-layer potential. For the double layer (10) this can be seen projecting the contour ∂D on the unit sphere centered at $\mathbf{x}_0$, see section 3.2 of Bazhlekov.¹⁹ The nonsingularity of the last integral in (10) is achieved by a proper choice of the vector $\mathbf{a}$ ($\mathbf{a} \neq -\mathbf{y}/|\mathbf{y}|, \mathbf{y} \in \partial D$). These steps are used in Sec. III D to improve the accuracy of the contour-integral calculation, see Eq. (20). A nontrivial situation can appear when $\mathbf{x}_0 \rightarrow \mathbf{x}_0' \in \partial D$. This is not related, however, to a singularity of the integrals, but to the uniqueness of the projection of $\mathbf{x}_0 \in \partial D$ on the unit sphere and can be easily overcome. In the present numerical method such situation ($\mathbf{x}_0 \in \partial D$) cannot happen and the unit-sphere projection of ∂D is always well defined.

Other advantages of the contour representations (9) and (10) are that their implementation for nonclosed interfaces is direct and they involve integration on a curve instead of on a surface. In addition, the precise knowledge of the normal vector $\mathbf{n}_D$ is not necessary for the calculation of the layer potentials. By applying the contour integration on the elements of a partitioning of a closed interface, the identities (7) and (8) are satisfied exactly, regardless of the accuracy of the calculation of the contour integrals.

III. NUMERICAL METHOD

The main elements of the numerical method such as the calculation of the velocity field given by the boundary integral formulation (6) and the evolution of the interfaces via a time integration scheme are discussed here.

A. Interface discretization and mesh refinement

The initially spherical interfaces are triangulated by flat triangles.¹⁰ Each triangular phase of an icosahedron inscribed in a sphere is subdivided into n^2 equal triangles, whose vertices are projected onto the sphere. This triangulation consists of $N = 20n^2$ flat triangles and is optimal for a closed interface topology: $N/2 - 10$ vortices have coordination number $N_c = 6$ and 12 vortices with $N_c = 5$. Based on this triangulation, the interface is discretized by surface elements S_j corresponding to the nodal points $\mathbf{x}_j$ of the mesh. Every element S_j is composed by 1/3 of the triangles to which $\mathbf{x}_j$ belongs, see Fig. 1; S_j are the basic surface elements where the curvature and the boundary integrals are calculated.

In addition, the mesh properties are optimized in three ways.

- (i) Element size optimization:¹⁰ for a fixed mesh topology the nodes are additionally moved with the extra tangential velocity $\mathbf{w}(\mathbf{x}, t)$, see (5). This velocity is determined on the base of the local characteristics of the mesh and the interfaces, such as element size, curvature k and the distance to the closest interface h ,

$$\mathbf{w}(\mathbf{x}_i) = (\mathbf{I} - \mathbf{nn}) \left(\sum_j [a + b(h(\mathbf{x}_j)) + c|k(\mathbf{x}_j)|^{3/2}] \times (\mathbf{x}_j - \mathbf{x}_i) \Delta S_j - \mathbf{u}(\mathbf{x}_i) + \mathbf{u}_s \right), \quad (11)$$

FIG. 2. Schematic sketch of subtraction (a) and addition (b) of edges (nodes and elements), and reconnection of nodes (c).

where the summation involves only the nodes $\mathbf{x}_j$ that are directly connected to $\mathbf{x}_i$; $\mathbf{u}_s$ is an average velocity of the interface to which $\mathbf{x}_i$ belongs. The term $-\mathbf{u}(\mathbf{x}_i) + \mathbf{u}_s$ in (11) eliminates a mesh distortion due to the tangential component of the hydrodynamic velocity $\mathbf{u}$. The constant c controls how fine the mesh is in the high curvature regions. The function b depends on the problem under consideration: in the case of drop-to-drop interaction the mesh is required to be finer in the film regions, thus $b(h) = \text{const } h^{-1}$; in the case of foam-drop dynamics $b(h) = \text{const } h$ and in this way the mesh is maintained finer in plateau borders and junctions, where the curvature and h have larger gradients. For these two types of problems we use only the mesh size optimization in the simulation. In the case of drop deformation good mesh properties cannot always be achieved only through element size optimization and a change in the topology is necessary.

- (ii) Subtraction and addition of edges according to a criterion for the proper edge length,^{4,24}

$$l_0^j = \max(\min(l_{\max}, \text{const } k_j^{-1}), l_{\min}), \quad (12)$$

where k_j is a local curvature,²⁴ $l_{\min}$ and $l_{\max}$ are given in advance and denote the global minimal and maximal edge lengths. Thus, if the length of an edge l_j is smaller than $l_0^j \cdot 3/4$, the edge is removed,²² as is shown in Fig. 2(a). The edge subtraction is followed by addition of edges:²⁵ if for a given edge, $l_j > l_0^j \cdot 3/2$, it is split into two by adding the middle point, marked by (○) in Fig. 2(b). Then every triangle with split edges is subdivided into two, three, or four triangles depending on the number of edges which are split, as shown in Fig. 2(b).

- (iii) Topology optimization: After edge subtraction and addition the coordination number of some nodes can deviate substantially from the optimal ($N_c = 6$). This leads

to unwanted large or small angles, see Figs. 2(c) or 3(e). An optimization of the coordination number can be easily achieved by reconnecting the nodes in two neighboring triangles. Such an example is shown in Fig. 2(c), where the dashed-dotted edge is replaced by the dashed one. From this figure is seen that this reconnection optimizes locally the coordination numbers from (8,4,7,5) to (7,5,6,6). For meshes used in the present study the coordination number N_c is always in the interval $5 \leq N_c \leq 7$.

The standard scheme for mesh refinement involving a change of the mesh topology is as follows, see also Figs. 3(a)–3(d): subtraction and addition of element edges followed by topological optimization and finally element size optimization in combination with a projection of the nodes on the initial interface.

A comparison between Figs. 3(d) and 3(e) demonstrates how useful the topological optimization can be. A disadvantage of the local element-size optimization (11) is the stability constrain, which can be much tighter than that of the passive stabilization algorithm.¹⁷ However, the present approach is more flexible for mesh refinement in high curvature regions or near contact zones. Moreover, it can be directly extended to take into account other important characteristics, such as high gradients of the surfactant concentration or the temperature. In addition, the time integration scheme, proposed in Sec. III E, overcomes the difficulties due to the poor numerical stability of the local element-size optimization (11).

B. Curvature calculation

The mean curvature $k(\mathbf{x})$ and the normal vector $\mathbf{n}(\mathbf{x})$ for the surface element S_j are computed by means of a commonly used formula, see for instance¹⁰

$$k(\mathbf{x}_j)\mathbf{n}(\mathbf{x}_j)\Delta S_j \approx \int_{S_j} k(\mathbf{x})\mathbf{n}(\mathbf{x})ds = - \oint_{\Gamma_j} \mathbf{b} dl, \quad (13)$$

where $\Gamma_j = \partial S_j$ is the contour of S_j and $\mathbf{b}$ is the unit outward normal to Γ_j vector lying in the plane tangential to S_j , see Fig. 1. Different possibilities for the choice of S_j exist.

- Loewenberg and Hinch¹⁰ defined Γ_j by the bisectors of the triangle edges surrounding the vertex $\mathbf{x}_j$.
- In the present study S_j is the basic element for the node $\mathbf{x}_j$, as defined in the preceding section, see also Fig. 1.

The most popular test for the accuracy of a curvature calculation is the following:¹⁷ for an analytically given interface shape the mesh nodes are projected on the interface and the numerically calculated curvature is compared with the analytical one. According to this test, the curvature calculated by (13), where S_j is chosen as in (b), does not converge even for uniform meshes on a sphere. In the nodes with $N_c = 5$ the error is about 14%, independently of the number of elements. It is our opinion, however, that according to (6) a spherical (nondeformed) interface is one which has constant curvature. Indeed, for a given mesh in the absence of

FIG. 3. An example of a mesh refinement that involves topological changes (a) the mesh before refinement; (b) after subtraction and addition of edges; (c) after topological optimization; (d) final mesh, after mesh size optimization (relaxation); (e) as (d), however, without topological optimization.

any external flows or forces, the drop would relax to a shape for which the curvature in all nodes will be equal, independently of the way of curvature calculation. Then, by comparing the relaxed interface with the equivalent sphere, a conclusion for the accuracy of the curvature calculation can be drawn. According to this test the present method of curvature calculation converges for a sphere and has a second-order accuracy, which is seen in Fig. 4. Similar tests can also be designed for nonspherical interfaces.¹⁷

Zinchenko *et al.*¹⁷ have proposed an approach for the calculation of the curvature and normal vector, which is based on a local paraboloid fitting. We find their approach very efficient and more accurate than the contour integration (13). An advantage of the present method, however, is that it provides an average curvature in S_j , which is consistent with the calculation of the boundary integrals on S_j . In other methods^{10,17} the calculation of the boundary integrals has a second-order accuracy only for uniform meshes. For nonuni-

FIG. 4. The maximal deviation of relaxed [according to (6)] drop with equivalent radius 1 from unit sphere for different meshes. N is the number of mesh nodes.

FIG. 5. Schematic 2D version of the higher-order approximation of the interface (thicker curve). It is constructed based on the initial discretization (thinner lines) and the circles $C_j(\mathbf{O}_j, R_j)$ (dashed lines).

form meshes the integration deviates from the trapezoidal rule and loses the second-order accuracy.

In the case of drop-to-drop interaction we compared the two approaches for curvature calculation (13), based on the choices (a) and (b). The results were identical for relatively uniform meshes, however, for nonuniform meshes approach (a) led to numerical instabilities, while approach (b) still supplied stable results.

It is worth to mention that the contour integration (9) and (10) of the layer potentials does not include the normal vector. Thus, in the present method the normal vector appears only in the element size optimization (11) and the higher-order interface approximation, presented in the following section. This makes our method less sensitive to errors in the normal vector calculation.

C. Higher-order approximation of the interfaces

The reason for the construction of a higher-order interface approximation arose from the simulations of foam-drop dynamics, see Sec. IV D. A typical feature of a foam structure is the presence of film regions, where the interface-to-interface distance h can be a few orders of magnitude smaller than the drop size. The main problem arises from the disjoining pressure in (3), where small disturbances in the value of h can introduce a significant inaccuracy to the calculation of the interfacial forces and lead to continuously growing numerical instabilities. In the case of monodispersed foams, because of the flat film regions, the initial interface approximation can provide sufficient accuracy. For polydispersed foams the film regions have, in general, nonzero curvature and a better approximation of the interfaces is necessary. To improve the accuracy of the calculation of $h(\mathbf{x})$ we propose a higher-order approximation of the interfaces. It is based on the initial triangulation by linear triangles and information about the curvature and the normal vector in the nodal points. It is constructed following the next scheme, for illustration see the two-dimensional example in Fig. 5.

- (1) A sphere $C_j(\mathbf{O}_j, R_j)$ is associated with every nodal point $\mathbf{x}_j$,

$$R_j = |k(\mathbf{x}_j)|^{-1}, \quad \mathbf{O}_j = \mathbf{x}_j - \mathbf{n}(\mathbf{x}_j)/k(\mathbf{x}_j). \quad (14)$$

- (2) Node $\mathbf{x}$ of the triangle with vertices $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ is projected radially on the sphere C_l ; $l = 1, 2, 3$, see Fig. 5,

$$\mathbf{x}_l^p = R_l(\mathbf{x} - \mathbf{O}_l)/|\mathbf{x} - \mathbf{O}_l|, \quad l = 1, 2, 3. \quad (15)$$

- (3) The projection of the node $\mathbf{x}$ on the higher-order interface approximation S^p is defined by means of the linear combination,

$$\mathbf{x}^p = \sum_{l=1}^3 w_l \cdot \mathbf{x}_l^p. \quad (16)$$

The coefficients w_l are functions of the distances from $\mathbf{x}$ to the vertices and edges of the triangle and can be defined to be continuous across the edges,

$$w_l = \sum_{k=l-1}^l w_l^k w^{k+1} w^{k-1}/w,$$

where k and l correspond to the local numeration of the sides and the nodes in the triangle [the l th node belongs to the $(l-1)$ th and l th sides]; w^k is the distance $|\mathbf{x} - \mathbf{y}_k|$, where $\mathbf{y}_k$ is a projection of $\mathbf{x}$ on the k th side ($w^0 = w^3$; $w^4 = w^1$); and $w_l^k = |\mathbf{x}_j - \mathbf{y}_k|/|\mathbf{x}_l - \mathbf{x}_j|$ correspond to the linear description of $\mathbf{y}_k$ on the k th side (the j th and l th nodes are the vertices of the k th side). Finally, w is defined as

$$w = \sum_{k=1}^3 w^k w^{k+1},$$

which automatically leads to

$$\sum_{l=1}^3 w_l = 1.$$

Different possibilities exist for the projection $\mathbf{y}_k$ of $\mathbf{x}$ on the edges. In the present study we use the orthogonal one.

Apparently, when $\mathbf{x}$ is on an edge of the mesh, the coefficients w_l are those from the linear description of $\mathbf{x}$ on the edge. Thus, the approximation S^p of the interface S is globally smooth and its curvature is globally continuous. The interface-to-interface distance $h^p(\mathbf{x})$ calculated on the base of the higher-order interface approximation is also globally smooth and is directly related with the curvature via (14).

A disadvantage of the approximation S^p is that it is based on a local fitting with spheres, which is not appropriate in the general case of a nonspherical surface. Zinchenko *et al.*¹⁷ developed an efficient method for local paraboloid fitting for the curvature and normal vector calculation. We expect that a significant improvement of the interface approximation can be achieved simply by replacement of the projection on the sphere in step (2) above with that on a paraboloid. We found, however, that the approximation presented here is sufficient for the simulation in Sec. IV D, where the interfaces in the film regions are well approximated locally by spheres, see Fig. 6.

D. Boundary integral calculation

One of the most important aspects of a boundary integral method is the calculation of the integrals in (6). Applying the mean value theorem on the surface elements S_j , the boundary integrals can be approximated as

FIG. 6. Comparison of the initial interface approximation by flat triangles (solid line) with the higher-order one (dashed lines). Zoomed film region from Fig. 18(c) is shown.

$$\int_S f(\mathbf{x}) \mathbf{G}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) = \sum_j f(\mathbf{x}_j) \int_{S_j} \mathbf{G}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) + O(\Delta x^2), \quad (17)$$

$$\int_S \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) = \sum_j \mathbf{u}(\mathbf{x}_j) \cdot \int_{S_j} \mathbf{T}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) + O(\Delta x^2), \quad (18)$$

where $f(\mathbf{x}_j)$ and $\mathbf{u}(\mathbf{x}_j)$ are average values on S_j . The integrals on the right-hand side of (17) and (18) are calculated by means of the contour integrations (9) and (10). In the present method the contour Γ_j is a polygon, $\Gamma_j = \cup_i \Gamma_j^i = \cup_i [\mathbf{y}^i, \mathbf{y}^{i+1}]$, see Fig. 1, and (9) and (10) read¹⁹

$$\begin{aligned} I_G^j(\mathbf{x}_0) &= \int_{S_j} \mathbf{G}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) \\ &= \int_{\Gamma_j} \frac{d\mathbf{y} \times \mathbf{y}}{|\mathbf{y}|} = \sum_i |\mathbf{y}^i| \sin(\beta_i) \\ &\quad \times \log \left| \frac{(1 + \cos(\beta_i)) \cdot (1 + \cos(\gamma_i))}{\sin(\beta_i) \cdot \sin(\gamma_i)} \right| \cdot \frac{\mathbf{y}^i \times \mathbf{y}^{i+1}}{|\mathbf{y}^i \times \mathbf{y}^{i+1}|} \end{aligned} \quad (19)$$

and

$$\begin{aligned} I_T^j(\mathbf{x}_0) &= \int_{S_j} \mathbf{T}(\mathbf{x}_0, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds(\mathbf{x}) \\ &= 2 \oint_{\Gamma_j} \frac{\mathbf{y}(\mathbf{y} \times d\mathbf{y})}{|\mathbf{y}|^3} + 2\mathbf{I} \left(C_j + \oint_{\Gamma_j} \frac{\mathbf{a} \cdot (d\mathbf{y} \times \mathbf{y})}{|\mathbf{y}| \cdot (|\mathbf{y}| + \mathbf{a} \cdot \mathbf{y})} \right) \\ &= 2 \sum_i \frac{(\mathbf{z}^i + \mathbf{z}^{i+1})(\mathbf{z}^i \times \mathbf{z}^{i+1})}{1 + \mathbf{z}^i \cdot \mathbf{z}^{i+1}} \\ &\quad + 2\mathbf{I} \left[C_j + \sum_i \frac{2\mathbf{a} \cdot (\mathbf{z}^i \times \mathbf{z}^{i+1})}{g_i |\mathbf{z}^i \times \mathbf{z}^{i+1}|} \right. \\ &\quad \left. \times \left[\arctan \left[\frac{(1 - f_i) \cdot \tan(\alpha_i/2) + e_i}{g_i} \right] - \arctan \left[\frac{e_i}{g_i} \right] \right] \right], \end{aligned} \quad (20)$$

where $\mathbf{z}^i = \mathbf{y}^i/|\mathbf{y}^i|$; $e_i = [\cos(\theta_{i+1}) - \cos(\theta_i) \cdot \cos(\alpha_i)]/\sin(\alpha_i)$; $f_i = \cos(\theta_i)$ and $g_i = \sqrt{1 - e_i^2 - f_i^2}$. The constant C_j depends on the position of the pole $\mathbf{x}_0$ and the direction of the vector $\mathbf{a}$ with respect to the surface element S_j as described in Sec. II C. The angle α_i is determined by the vectors $\mathbf{z}^i$ and $\mathbf{z}^{i+1}$, and θ_i by $\mathbf{a}$ and $\mathbf{z}^i$.

FIG. 7. The relative error $\|I_Q - I_Q^{\text{ex}}\|/\|I_Q^{\text{ex}}\|$, where I_Q is calculated by three different methods. Q stands for (a) G and (b) T . The norm of the exact solution $\|I_Q^{\text{ex}}\|$ (thicker lines) is not given in %.

In order to check the validity of the contour-integral representations (19) and (20) we performed the following numerical test. Consider a surface element S_j , see Fig. 1, from a discretization ($\Delta x \approx 0.025$) of the unit sphere centered at the origin. The integrals I_Q^j (Q stands for G or T) are calculated both by (19) and (20), and as surface integrals. The surface integration (dashed lines in Fig. 7) is based on

- a commonly used^{6,17} one-point integration rule, $I_Q^j = \Delta S_j \mathbf{Q}(\mathbf{x}_0, \mathbf{x}_j) \cdot \mathbf{n}(\mathbf{x}_j)$, where the exact value for the normal vector, $\mathbf{n}(\mathbf{x}_j) = \mathbf{x}_j$, is taken,
- subdivision of every triangle $(\mathbf{x}_j, \mathbf{y}^i, \mathbf{x}^{i+1})$, see Fig. 7, into N_t^2 equal triangles. Then the above one-point integration rule is applied to every subtriangle after its vertices and mass center (the integration point) have been projected on the unit sphere and for the normal vector the exact value is taken.

The results are compared in Fig. 7 with the exact solution I_Q^{ex} , obtained by the contour integration (9) and (10) applied for the projection Γ_j^p of Γ_j on the unit sphere. In the present test the pole $\mathbf{x}_0$ moves radially towards the point $\mathbf{y}^1 = (\mathbf{x}_j + \mathbf{x}_l)/2$, where $\mathbf{x}_l$ is a node directly connected to $\mathbf{x}_j$, see Fig. 1. Thus, the horizontal axis, $|\mathbf{x}_0| - 1$, in Fig. 7 corresponds to the distance pole interface.

Figure 7 shows that when the number of the integration

points N_t^2 increases, then the surface integrals converge to the exact values I_Q^{ex} , which indicates the validity of the contour-integral representations (9) and (10). It is also seen that for a distance pole interface of about 0.01, the one-point integration has more than 10% error. In contrast, when the contour integration is used the error is less than 0.1%, independently of the distance pole interface (the error did not increase even at $|\mathbf{x}_0| - 1 = |\mathbf{x}_0 - \mathbf{y}^1| = 10^{-7}$). This also indicates the nonsingularity of the contour integration (note that $\mathbf{y}^1 \in \partial S_j$). For relatively large distance pole-interface (for instance $|\mathbf{x}_0| - 1 > 0.2$) both, surface and contour, integrations have comparable accuracy.

The main disadvantage of the contour integration (19) and (20) is that it involves intrinsic functions that slow down the performance of the method. Compared with the one-point surface integration, the contour integration is an order of magnitude slower. To improve the performance of the method, the exact formulas (19) and (20) are used only for S_j that are close (two layers of elements) to $\mathbf{x}_0$. For the rest of the interface the contour integrals are calculated by means of two-point integration rule applied to every segment of the contour Γ_j . This procedure improves the performance about twice, but it is still 5–6 times slower than the surface integration. We think, that a significant improvement could be achieved if the contour integration in a vicinity of $\mathbf{x}_0$ is combined with the surface integration on the rest of the interfaces.

E. Multiple step time-integration scheme

A well-known difficulty during the simulation of free boundary problems is the numerical instability due to the surface tension. Such instabilities limit the time step and thus slow down the performance, especially for small capillary numbers and small element size. An estimate for the time step required for a stable solution is^{6,17}

$$\Delta t < O(\text{Ca} \min(\Delta \mathbf{x})), \quad (21)$$

where $\min(\Delta \mathbf{x})$ is the minimal element size. In addition, the disjoining pressure A/h^3 as well as the element-size optimization (11) can further limit the time step. To overcome this difficulty an idea is used here, which is based on the following two facts. First, the above-mentioned numerical instabilities are local, i.e., the instabilities in a node $\mathbf{x}_j$ from the interface are mainly due to the time discretization of $f(\mathbf{x})$ in the nodes that are in a close vicinity of $\mathbf{x}_j$ (denote the set of these nodes by N_j). Second, the calculation of $f(\mathbf{x})$ and $\mathbf{w}(\mathbf{x})$ requires $O(N)$ operations, while for the boundary integrals they are $O(N^2)$. The idea is when the velocity at $\mathbf{x}_j$ is calculated, we refresh the values corresponding to nodes in N_j at every time step Δt and all other values—after M such time steps. The extra tangential velocity $\mathbf{w}(\mathbf{x})$ is also calculated at every time step.

To illustrate this idea, the boundary integral formulation (6) (after discretization) is rearranged as follows:

$$\begin{aligned} (\lambda + 1) \mathbf{u}(\mathbf{x}_j) = & -\frac{\lambda - 1}{4\pi} \sum_{i \in N} \mathbf{u}(\mathbf{x}_i) \cdot \mathbf{I}_T^i(\mathbf{x}_j) \\ & -\frac{1}{4\pi} \sum_{i \in \bar{N}_j} f(\mathbf{x}_i) \mathbf{I}_G^i(\mathbf{x}_j) + \left(2\mathbf{u}_\infty(\mathbf{x}_j) \right. \\ & \left. -\frac{1}{4\pi} \sum_{i \in \bar{N}_j} f(\mathbf{x}_i) \mathbf{I}_G^i(\mathbf{x}_j) \right), \end{aligned} \quad (22)$$

where N denotes the set of all nodes and $\bar{N}_j = N/N_j$.

In the present method only the terms $f(\mathbf{x}_i)$ and $\mathbf{u}_\infty(\mathbf{x}_j)$ in the brackets in (22), are calculated at every time step Δt , which requires $O(N)$ operations. The other terms on the right-hand side of (22) are kept unchanged for M time steps. Their calculation requires $O(N^2)$ operations and is performed once within every time interval $\Delta T = M\Delta t$. Thus, the total number of operations for a time interval of length ΔT is $O(N^2 + M \cdot N)$. For the standard iteration scheme,^{6,17,18} where all terms on the right-hand side of (22) are calculated at every time step Δt , the corresponding number of operations is $O(M \cdot N^2)$. Thus, for $M \ll N$ the proposed time integration scheme is about M times faster than the standard one.

An estimate for an optimal value of M can be obtained comparing the contribution to the total error of that due to the time integration with that due to the spatial discretization. The total error can be estimated as $O((M \cdot \Delta t)^2) + O(\max(\Delta x)^2)$. Taking into account (21), a comparison between the two terms in the total error leads to $M \approx O(\max(\Delta x)/(\text{Ca} \min(\Delta x)))$. For a number of problems, for instance at small Ca and highly nonuniform meshes, M can have a significant value. Other examples are steady-state problems as well as those with small time gradients, where the total error is dominated by the error due to the spatial discretization. In such cases the time step usually is limited by a condition for numerical stability, e.g., (21), and can be much smaller than that necessary for an accurate solution.

To demonstrate how the performance and the accuracy depend on the value of M (ΔT), we consider the following test problem: deformation of an initially spherical drop of radius R and viscosity μ in a planar extensional flow ($u_1 = Gx_1$; $u_2 = -Gx_2$; $u_3 = 0$) in the time interval $[0; 0.2]$ at $\text{Ca} = \mu GR/\sigma = 0.05$, the case $\lambda = 1$ is considered for simplicity. The drop deformation in the considered time interval is shown in Fig. 8. A relatively large gradient of the deformation is observed, which is an indication of the relevance of the test (for steady problems the present scheme would not introduce any additional error, independently of the value of M). A mesh of 10 580 triangular elements was used at time step $\Delta t = 2.5 \times 10^{-4}$, which is an order of magnitude smaller than the stability limit (21). The simulations for different values of $M = 2^l$; $l = 1, 2, \dots, 10$ were performed and compared with the standard scheme ($M = 1$). The relative extra (due to the proposed scheme) error in % for the drop deformation at $t = 0.2$ is shown in Fig. 9. A linear dependence of the performance on M is also seen (○). For instance, at $M = 256$ the performance of the present scheme corresponds to that of the standard time integration at time step about 0.064, which is 10 times larger than the stability limit. Thus, for the test problem considered here, the present time integration

FIG. 8. Drop deformation in a planar extensional flow. $B < W < L$ are the three lengths of the drop—along x_1 , x_3 , and x_2 axes, respectively.

scheme at $\Delta T = 0.064$ is an order of magnitude faster than the standard one, and introduces an extra error less than 0.5%. The performance and the error are determined by the large time step ΔT and are almost insensitive to the values of Δt and $M = \Delta T / \Delta t$, provided $M \ll N$. The present scheme is stable even at $\Delta T = 0.25$ ($M = 1000$), however, the accuracy is unacceptable.

For the simulations in the present study, time steps Δt several times smaller than the stability limit were used with M of the order 100. Thus, in most of the cases the CPU time determining time step ΔT was about an order of magnitude larger than the stability limit (21). The set N_j consists of the node $\mathbf{x}_j$, the node $\mathbf{x}_l$ closest to $\mathbf{x}_j$ that belongs to another interface and the nodes directly connected to $\mathbf{x}_l$ as well.

The algebraic system (22) is solved by the method of successive substitutions.^{6,16} To demonstrate how this is done in combination with the multiple step time-integration scheme, the system is written in the form

$$\mathbf{u}^{k+1}(t) = \mathbf{u}^k(t) \cdot A_T(t) + b_G(t), \quad (23)$$

FIG. 9. Comparisons for the accuracy and performance between the multiple step time-integration scheme and the standard scheme for different value of the parameter M . The extra relative error in % for D (Δ) and C ($\square$); the relative CPU time is given by ($\circ$).

where the matrix A_T corresponds to the double layer operator, after it has been deflated.¹⁵ The vector b_G takes into account the single-layer potentials and the external flow as well. At every big time step $M \cdot \Delta t$ all elements of A_T and b_G are calculated and then successive iterations $k=0,1,2,\dots$ are performed. At the small time steps $m \cdot \Delta t$, $m=1,2,\dots,M$ only a part of b_G is recalculated and iterations are performed if b_G differs significantly from the corresponding value when the last iteration process has been performed. Thus, if the previous iterations of (23) have been performed at small time step $m_1 < M$ and if

$$\max_j \left[\sum_{m=m_1}^{m_2} |b_G(\mathbf{x}_j, t + m \cdot \Delta t) - b_G(\mathbf{x}_j, t + (m+1) \cdot \Delta t)| \right] > \epsilon,$$

then successive iterations are performed at time step $m_2 - 1$ as well. Otherwise the solution at time step m_2 is obtained based on the previous step and the difference in b_G , i.e.,

$$\mathbf{u}(\mathbf{x}_j, t + m_2 \cdot \Delta t) = \mathbf{u}(\mathbf{x}_j, t + (m_2 - 1) \cdot \Delta t) + b_G(\mathbf{x}_j, t + m_2 \cdot \Delta t) - b_G(\mathbf{x}_j, t + (m_2 - 1) \cdot \Delta t).$$

As a criterion for convergence the standard one is used, $\|\mathbf{u}^k(t) - \mathbf{u}^{k-1}(t)\| < \epsilon$, with a typical value $\epsilon = 10^{-3}$.

Zinchenko *et al.*¹⁷ have used a combination of biconjugate gradient iterations and simple iterations, which could be a better alternative. For the problems considered in the following section we found the method of successive substitutions sufficiently efficient: for most of the simulations only 2–3 iterations per big step ΔT were necessary for convergence.

IV. NUMERICAL RESULTS

To demonstrate the accuracy and stability of the method different problems for deformable interfaces are considered in this section, including challenging problems that involve large curvature or interfaces at very close approach.

A. Drop deformation at zero interfacial tension

Drop deformation in simple shear and planar extensional flows at zero surface tension $Ca = \infty$ is considered below. This problem was chosen mainly as a test for the calculation of the boundary integrals I_T^i and the iterative method (22) at $\lambda \neq 1$, as well as a shape-stabilizing procedure given in this section.

Recently, Wetzel and Tucker²⁶ presented an analytical model for the deformation of an ellipsoidal drop of zero interfacial tension in a linear velocity field. Comparisons with some of their results are performed here to validate our model for the case of zero interfacial tension. The main difficulty for a direct numerical simulation of such an extreme situation is the loss of the smooth shape of the interface. Indeed, initially small errors due to the discretization of the interface grow continuously because of the velocity gradient.

FIG. 10. Comparisons with the results of Wetzel and Tucker (Ref. 26) (thick lines) and Toose (1998) (○). The present results are given by (*): (a) Drop deformation in simple shear flow for $\lambda=3$, the angle between the major axis of the drop and the flow direction is also shown (dashed line); (b) drop deformation in planar extensional flow for $\lambda=18.6$.

To overcome this, we propose a shape-stabilizing procedure. It is, in fact, an addition of an extra interfacial velocity based on the local gradient of the curvature,

$$\mathbf{w}_s(\mathbf{x}_j) = \text{const} \Delta S_j \sum_i (k(\mathbf{x}_i) - k(\mathbf{x}_j)) I_G^{ij}(\mathbf{x}_j), \quad (24)$$

where $I_G^{ij}(\mathbf{x}_j)$ are the contour integrals (19) for the segment $\Gamma_{ij} = \partial S_i \cap \partial S_j$ when $\mathbf{x}_0 = \mathbf{x}_j$. In fact, the summation in (24) involves only the nodes i directly connected with j (for every other node $\Gamma_{ij} = \emptyset$). Thus, the extra velocity $\mathbf{w}_s(\mathbf{x}_j)$ in the node $\mathbf{x}_j$ depends only on the curvature in $\mathbf{x}_j$ and the neighboring nodes. It is easy to see that if the curvature k is a linear function on the interface around $\mathbf{x}_j$, the velocity $\mathbf{w}_s(\mathbf{x}_j)$ would be negligible. In the cases when the curvature has a local minimum or maximum in $\mathbf{x}_j$, the extra velocity $\mathbf{w}_s(\mathbf{x}_j)$ can be significant and will smooth the interfaces. The constant in (24) determines the strength of the smoothing and in the present simulation is set to $N \times 10^{-3}$, at which value $\mathbf{w}_s$ is small enough to influence the hydrodynamic velocity, but is capable to keep the interface smooth.

Figure 10 shows comparisons of our results with Wetzel and Tucker²⁶ and also with the boundary integral method simulations of Toose (1998), as referred in Wetzel and Tucker.²⁶ In Fig. 10(b) our results for a finite capillary number $Ca=1$ are also given. They illustrate the applicability of the results of Wetzel and Tucker²⁶ to the case of small but nonzero interfacial tension. Similar agreement was obtained

FIG. 11. Steady shape of a bubble, $\lambda=0$, in simple shear flow, $u=y$, at $Ca=1.25$: (a) Side view, in (x,y) plane; (b) top view, in (x,z) plane.

with the results of Wetzel and Tucker,²⁶ presented in their Fig. 3, regarding drop tumbling for $\lambda=10$ and $\lambda=20$, and drop widening for $\lambda=0.1$.

The good agreement with the results of Wetzel and Tucker²⁶ indicates the ability of the present method for simulation of deformable interfaces at zero interfacial tension. The comparisons also show that the shape-stabilizing procedure (24) does not influence the results. Thus, this procedure can be successfully used in the case of nonzero interfacial tension (finite capillary numbers), where the shape stabilization (24) is expected to have less influence on the solution. In the simulations presented in the following sections, however, the interfaces were sufficiently smooth and the procedure was not used. It was used only in some cases as a local shape relaxation procedure, applied after mesh refinement which involves topological changes.

B. Drop deformation and breakup at finite interfacial tension

A number of simulations were performed in the case of drop deformation at finite interfacial tension. The first group of simulations concerns steady drop shape in simple shear flow. The comparisons with the steady drop shapes presented by Cristini *et al.*²⁴ (see their Fig. 3) for $Ca=1.43$; $\lambda=3$ and $Ca=0.8$; $\lambda=0.01$ showed good agreement in the second case: less than 2% relative difference regarding the drop axis ratios. In the first case ($Ca=1.43$; $\lambda=3$), however, our results showed about 20% smaller deformation than that of Cristini *et al.*,²⁴ but are in good agreement with the results of Zinchenko (private communication, 2003). Figure 11 shows the steady shape of a bubble, $\lambda=0$ and $Ca=1.25$. Sharp drop edges can be seen in the figure, the situation typical for small drop viscosity with respect to the continuous phase viscosity, $\lambda \ll 1$. These results prove the applicability of the presented numerical method for the simulation of bubble deformation that involves high curvature regions (the curvature at the drop ends is about 50) as well as the effectiveness of the mesh adaptation.

The other group of simulations concerns transient drop

FIG. 12. Drop breakup in simple shear flow $[u=0.5(x+y); v=-0.5(x+y)]$ at $Ca=0.25$, $\lambda=10$ —frames (b)–(d). Initially, for $t=0-13.65$, the drop is elongated in planar extensional flow ($u=x$; $v=-y$)—frames (a).

deformation in different kinds of flows that leads to drop breakup. Good agreement is obtained with the results of Cristini *et al.*²⁴ for $\lambda=1$ presented in their Sec. IV C. Drop deformation and breakup at $Ca=0.25$ and high viscosity ratio, $\lambda=10$, is shown in Fig. 12. It is known that at $\lambda=10$ the drop will not breakup in simple shear flow unless it has not

undergone a substantial initial deformation.²⁷ Thus, for the simulation presented in Fig. 12 the following protocol for the external flow was used. Starting from spherical shape at $t=0$ the drop is elongated in planar extensional flow ($u=x$; $v=-y$), frames (a). At time $t=13.65$, when the drop length is about 5.8 from the equivalent drop radius, the flow is

FIG. 13. The evolution of the neck radius, R_{neck} around $t=21$ from the simulation presented in Fig. 12.

switched to a simple shear flow [$u=0.5(x+y)$; $v=-0.5(x+y)$], frames (b). The orientation of the chosen simple shear flow is essential. If, for instance, the standard shear flow, $u=y$, is applied, the drop will retract without breakup. After the flow is switched to simple shear flow, the drop elongation continues mainly due to the chosen flow direction, see the left frame (b) ($t=16.05$). At this time the drop is already aligned with the flow direction, which is followed by retraction of the drop combined with a necking, see the last frames (b) for ($t=20.8$ and $t=21.44$). Around $t=21$ the thinning of the neck becomes dominant due to the increasing effect of the surface tension, which indicates that the breakup is imminent, see also Fig. 13. At the end of the simulation, $t=21.44$, the neck radius is about 2% of the equivalent drop radius.

To maintain a sufficient accuracy, the mesh in the neck region is about two orders of magnitude smaller than the maximal element size, see the left frame (c). Following an idea of Cristini *et al.*,²⁴ the neck is pinched off by splicing of the mesh, the middle frame (c), followed by mesh relaxation (24), the right frame (c). Finally, the two newly formed drops relax towards a steady shape in simple shear flow, see frame (d). The results presented in Fig. 12 demonstrate the possibility of drop breakup in simple shear flow at $\lambda=10$, see also Stegeman.²⁷ At $\lambda=1$ our simulations always indicate formation of satellite drops during breakup.^{24,27} For the simulation presented in Fig. 11 our result, however, cannot predict whether a satellite drop will be formed during the breakup. Any further refinement of the mesh in the neck region introduced irregularities on the interface, which (due to the large curvature) led to inaccurate results.

C. Drop-to-drop interaction

As an essential part of the coalescence process the drop-to-drop interaction is widely investigated.²⁸ One of the main difficulties in the numerical simulation of the process is the presence of a relatively stable liquid film region where the distance between the interfaces is several orders of magnitude smaller than the drop size.

In contrast to the neck thinning during the drop breakup, the film drainage between interacting drops can be relatively slow. This means that numerical errors can more easily influence the results for drop coalescence than that for breakup.

For instance, a neck radius of 10% of the drop size already can predict imminent breakup⁸ (see also Fig. 13), while two orders of magnitude thinner film (0.1%) could be insufficient for prediction of film rupture and, subsequently, coalescence. In addition, the small capillary numbers typical for coalescing systems make the numerical simulations of the coalescence process even more difficult and challenging.

In order to predict coalescence during drop interaction, the evolution of the film thickness has to be traced to values of the order of the critical film thickness, when the attractive van der Waals forces become dominant leading to film rupture. Most of the existing 3D simulations of drop-to-drop interaction, obtained without restriction on the drop deformation, face significant difficulties to resolve films of thickness less than 1% of the drop radius. The results of Zinchenko *et al.*¹⁷ are the first simulations of films thinner than 1% of the drop radius.

Numerical results for much thinner films were obtained^{28–31} based on so-called asymptotic theory. In this approach axisymmetric iterations of slightly deformable drops (film radius much smaller than drop radius) are considered, where the film flow is governed by the lubrication equations. Recently, Rother and Davis³² have extended the asymptotic theory to the case of drop-to-drop interaction in linear flows. Here, we compare our results with the predictions of the asymptotic theory, regarding film drainage between drops interacting in simple shear flow.

The time step for the numerical simulations of drop-to-drop interaction is chosen, as in Zinchenko *et al.*,¹⁷ to depend on the minimal film thickness, $\Delta T = \Delta T_0 h_{\text{min}}^{1/2}$. Here, however, the optimal initial time step ΔT_0 is taken to guarantee numerical accuracy, while in the standard time integration scheme^{10,17} it is limited by a stability constrain. This is especially important for the present simulations (at small capillary numbers), where time steps an order of magnitude larger than the stability limit are used.

The first group of simulations is for axisymmetric interactions of two equal drops in compressional flow at $\text{Ca}=0.05$, see Fig. 14(a). The 3D simulations were performed using nonuniform meshes, see Fig. 14(b). The time step $\Delta T_0=0.1$ (the stability limit is about 0.01) was used with $M=100$. For $\lambda=1$ three different meshes were used, in order to check the convergence with respect to the space discretization. The results for the evolution of the center and minimal film thickness are shown in Fig. 14(c). The mesh of 2000 elements per drop was insufficient to supply accurate results for the minimal film thickness below 0.003 of the drop radius, while the other two meshes give almost identical results. They are also in agreement with the predictions of a version of the present code for axisymmetric problems. In Fig. 14(d) the film profiles are compared at minimal film thickness $h_{\text{min}}=0.0025$. A comparison with the asymptotic theory for the results presented in Fig. 14 was not possible due to the large film radius (0.4) and externally driven recirculation within the drops, which influences the film drainage. In this case the recirculation flow inside the drop completely stops the film drainage leading to stationary long-time configuration. This phenomenon has been observed for the first time by Cristini *et al.*²⁴

FIG. 14. Drop-to-drop interaction in axisymmetric compressional flow ($u = 0.5x$; $v = -y$; $w = 0.5z$) at $Ca = 0.05$. The drops are initially spherical and centered at $(0; 0; \pm 1.5)$: (a) side view and (b) view from the film side of one of the drops at $t = 20$ for mesh of 3920 elements per drop; (c) the evolution of the film thickness in the center and the minimal film thickness for three different meshes; (d) film profiles (cross section with plane $z = 0$) at equal minimal film thickness, $h_{min} = 2.5 \times 10^{-3}$.

In an attempt to extend the simulations presented above to the case of small viscosity ratio ($\lambda = 0.1$ and $\lambda = 0$) we faced serious difficulties. The results were in good agreement with the predictions of the axisymmetric code for film thickness of about 0.01, however, deviated significantly for smaller h_{min} . Thus, the results for $\lambda \ll 1$ in Figs. 5.7–8 of Bazhlekov¹⁹ are not correct for $h_{min} < 0.01$. After we checked different sources for the inaccurate results at $\lambda \ll 1$, we concluded, that a possible reason could be the combination of the coarse mesh in the rear part of the drops [see Fig. 14(a)] and Wielandt's deflation. The elimination of the eigenvalues from the spectrum of the double layer operator leads to ad-

ditional (uniform expansion and rigid-body motion) terms in the boundary integral formulation, see for instance Eqs. (9)–(15) of Zinchenko *et al.*¹⁷ The uniform expansion and the rigid-body motion, being integral characteristics of an interface, are influenced by the global error, and thus, transfer it to the interface velocity. In other words, the global error, which is dictated by the error in the coarsest part of the mesh, could effect the interface velocity everywhere. In the case of single drop or drops at relatively large distance, this would have an insignificant effect on the relative position of the interfaces. However, in the presence of interfaces at close approach, it could have a crucial influence on the accuracy of

the calculation of the film thickness. Thus, the simulations of drops in close approach at small or large viscosity ratio require mesh refinement not only in the gap region, which makes them computationally very expensive.

To the end of this section the predictions of the present method are compared with that of the asymptotic theory. We consider the formation and drainage of a film between drops interacting in simple shear flow. The drops are equal, initially spherical and centered at $(\mp 1.5; \pm 0.25; 0)$. Each drop interface is triangulated by a mesh of 5120 triangles, and the time step $\Delta T_0 = 0.05$ is chosen (the stability limit is again an order of magnitude smaller, about 0.005). The parameter M is set to a relatively large value, $M = 200$ ($\Delta t_0 = 0.00025$), in order to maintain sufficiently smooth and fast redistribution of the nodes in the gap region. The viscosity ratio is $\lambda = 1$ and the capillary number is relatively small, $Ca = 0.025$, in order to guarantee the validity of the asymptotic theory. In the asymptotic theory the evolution of the film is given by the solution of simplified axisymmetric film-drainage equations^{29–32} in the gap between the drops. The drop interaction enters as a boundary condition for the film drainage model,³¹ to take into account the external flow or force. In the present comparison the formula of Hadamar and Rybczynski³³ for the force between two spherical drops in simple shear flow is used:

$$F = 4.34 \frac{2/3 + \lambda}{1 + \lambda} \pi \mu R^2 \dot{\gamma} \sin 2\beta, \quad (25)$$

where β is the angle between the line through the drop centers and the flow direction and has to be given.

More general and accurate expressions for the interaction force and angles can be obtained.^{32,34} However, for the present case (equal drops at $\lambda = 1$) we found expression (25) sufficiently accurate. A larger error, at $Ca = 0.025$, can be accumulated during the time integration for the angle β and also due to the choice of its initial value. The main goal of the present comparison is to verify the accuracy of the boundary integral solution in the gap, which corresponds to the film drainage part of the asymptotic theory. Because of that, in order to reduce the influence of the errors from the outer solution, the angle β in (25) is taken from the boundary integral calculation, starting at a drop-to-drop distance which is an order of magnitude larger than that for the film formation.

Except for a shift of about 0.2 in time, the agreement between both results presented in Fig. 15 is good, bearing in mind the extremely small interface separation. The agreement between the predictions for the film radius is also good. A more detailed investigation shows that the film profile obtained by the boundary-integral calculations is very close to axisymmetric; deviation less than 1%, even though the interaction is essentially 3D. This agrees with the analyses,^{30,32} that during 3D drop interactions at small capillary numbers, the film drainage remains axisymmetric. Another quantification of the validity of the inner solution of the asymptotic theory, regarding the assumption for small deformation, follows from the comparison discussed. This comparison indicates that, for a moderate viscosity ratio, the film drainage

FIG. 15. Drop-to-drop interaction in simple shear flow ($u = -y$) at $Ca = 0.025$ and $\lambda = 1$. The drops are initially spherical and centered at $(\mp 1.5; \pm 0.25; 0)$. The fluctuations of the present results for $h_{\min}$ and R_{film} are due to their discrete evaluation—in the nodes of the mesh.

model is valid even when the film radius is about 20% of the drop radius. The local film thickness minimum, at t about 5.8, is due to the disappearance of the dimple during drop separation, predicted also by the boundary-integral calculation.³² Finally, the shift in the time between both simulations presented in Fig. 15 is due to the assumption of small deformation in the asymptotic theory. The drop deformation outside the gap region in the 3D simulation initially accumulates part of the interaction leading to more gentle collision and a delay of the film formation and, subsequently, the whole process.

D. Foam-drop formation and its dynamics in simple shear flow

Liquid foams have a highly structured geometry: liquid films, plateau borders and junctions, see Fig. 16. The presence of relatively large interfacial areas and liquids films of several orders of magnitude thinner than the particle size, determines their complex rheological behavior and, consequently, their practical importance. This, however, introduces the main difficulties during the experimental and theoretical investigations of foam dynamics. Thus, most of the numerical investigations are limited to 2D foams or 3D dry-film foams.^{35,36} In the dry-film models, films with zero thickness are considered and modelled as mathematical surfaces, neglecting the film drainage and interfacial effects. To our knowledge, the simulations of Loewenberg, de Cunha, Blazwdziewich, and Cristini (1999), as referred by Kraynik and Reinelt,³⁵ are the first for 3D wet foams. They are restricted, however, to the monodisperse case and then only to the formation of the foam during uniform expansion in the absence of external flows.

In the present section we consider a foam-drop: a compound drop that consists of several inner drops at high volume fraction completely covered by another immiscible liquid. Such a drop has all structural elements of a polydispersed foam: liquid films bounded by interfaces of significant curvature, plateau borders and junctions, see Fig.

FIG. 16. Foam-drop structure, four inner drops at 95% volume fraction. The film regions (made transparent) are connected via plateau borders, joined in junctions.

16. Simple shear flow is considered here as an example of external flow. For simplicity, the surface tension coefficients for all of the interfaces are assumed equal, σ , and the viscosities of all liquids equal to μ . Thus, the problem has two dimensionless hydrodynamic parameters: the capillary number $Ca = \dot{\gamma} \cdot R \cdot \mu / \sigma$ (R is the equivalent radius of the foam-drop) and the dimensionless Hamaker constant, A , see the discussion after Eq. (3). The disjoining pressure in (3) is very important for the film and thus for the foam stability. Here it is modelled, following Kraynik and Reinelt,³⁵ as $-A/h^3(x)$.

In Fig. 17 a foam-drop formation is shown, the first three pairs of frames (a)–(c). The first column shows the outer interface and the second, the inner-drop interfaces. Initially the drops are spherical, the outer drop has radius R , the eight equal-size inner drops of radius $0.3R$, frames (a) of Fig. 17. The inner drops are then subjected to a nonuniform expansion, where the expansion rate depends on the distance to the closest interface $\mathbf{u}_{\text{exp}}(\mathbf{x}_j) = \text{const } \mathbf{n}(\mathbf{x}_j) \cdot \mathbf{h}(\mathbf{x}_j)$. When the relative volume of the inner drops reaches 95%, the expansion stops and the interfaces relax. Thus, at time $t = 12.4$, frames (c), the foam-drop with 95% volume fraction (four inner drops of 13.5% and four of 10.25% relative volume) is at equilibrium. After $t = 12.4$ the drop is sheared at $Ca = 0.2$, frames (c)–(e), during which the foam-drop deforms in a tumbling-like way.³⁷ Such dynamics is due to the repositioning of the inner drops inside the foam-drop, which is a typical process of the dynamics of foams: the particles change their neighbors, which is related with topological transitions between films, plateau borders and junctions.

It is known that a configuration is stable when the films are connected 3×3 in plateau borders, and the plateau borders are connected 4×4 in junctions, which is the case in Fig. 16. Let us follow the evolution of the four front (upper) inner drops in frames (c)–(e) of Fig. 17. Initially, the left and right drops are separated by the other two drops, which are in

contact—there is a liquid film between them, see frames (c). During the shearing, however, this film disappears leading to a plateau border (connecting four films) between the four drops under consideration, see frames (d). A junction connecting five plateau borders [four of which are seen on left frame (d) and the fifth is that between the four drops] is also formed. Thus, this metastable configuration changes to a stable one, where the initially separated drops are now in contact, forming film between them, and the other two drops separate, see frame (e). The process of drop repositioning can be also seen in Fig. 18, where cross sections in a plane, fitted with the centers of the four drops, are shown at different time instances. Thus, the discussed simulation has not only the main structural, but also the dynamic elements of polydispersed foams.

The simulation presented here was performed using 8820 triangular elements on the outer interface and 3380 elements per every inner drop—35 860 elements in total. The mesh is kept finer ($\Delta \mathbf{x} \approx 0.01$) in the plateau border and junction regions, where the gradients of the curvature and interface-to-interface distance are larger. In the film regions, of almost constant thickness, the edge size is an order of magnitude larger ($\Delta \mathbf{x} \approx 0.1$). To maintain such mesh properties during the whole dynamics, only mesh-size optimization was used, without topological changes. The minimal film thickness is about 2.5×10^{-3} , and as it was mentioned above, the interfaces in the film regions are discretized by elements with two orders in magnitude larger size. In addition, some of the film regions have a significant curvature ($k \approx 3$). Thus, the use of the higher-order interface approximation presented in Sec. III is essential, see Fig. 6. For comparison, when the initial approximation of the interfaces by flat triangles was used, we managed to expand the inner drops only to about 60% volume fraction [slightly before frame (b)].

The results presented in Fig. 17 were obtained for about three days on Risc 10K 225 MHz single processor. The time step was $\Delta t = 10^{-5}$, which was sufficient to obtain numerically stable solution. The limitation on the time step is mainly due to the disjoining pressure term, proportional to $h^{-3}(\mathbf{x})$ [$h(\mathbf{x}) \approx 2.5 \times 10^{-3}$ in the film regions]. The parameter M in the multiple step time-integration scheme was taken $M = 1000$. For this value the most CPU time consuming single layer potential was calculated only once at every time interval $\Delta T = 10^{-2}$. Finally, the higher accuracy due to the contour integration is also very important for the presented simulation of the foam-drop dynamics, mainly due to the presence of interfaces in an extremely close approach and the high gradient of the normal vector in the plateau border regions.

The main goal of the simulation presented here was to demonstrate the numerical stability of the method in the presence of disjoining pressure in film regions with significant curvature. A direct and practically important extension of the present simulation can be made by an incorporation of triply boundary conditions.^{9,10} Recently, Zinchenko and Davis¹¹ made significant improvement in this direction, considering up to 200 drops per periodic box at 55% volume fraction.

FIG. 17. Expansion of the inner drops at constant volume of the whole foam-drop at $A = 2.5 \times 10^{-6}$ (a)–(c). The relative volume of the inner drops is (a) 22%; (b) 77%; (c) 95%. Foam-drop deformation in shear flow at $Ca = 0.2$ and $A = 2.5 \times 10^{-6}$ (c)–(e).

FIG. 18. Cross sections of the foam drop at different time instances.

V. CONCLUDING REMARKS

A three-dimensional boundary-integral method is presented for deformable drops in viscous flows at low Reynolds numbers. The main advantage of the method is the calculation of the boundary integrals, based on a contour-integral representation of the single and double-layer potentials. Due to the nonsingular formulation, the contour integration offer a higher accuracy in the vicinity of the singular point, compared with the standard surface integration. Far from the singular point both integrations show comparable accuracy. The main disadvantage of the contour integration is that its performance is about an order of magnitude slower. Thus, an improvement could be achieved, combining the

contour integration around the singular point with surface integration in the rest of the interfaces. Another advantage is that the contour integration, in contrast with the commonly used near singularity subtraction, can be directly applied for nonclosed interfaces. Typical examples in this case are the problems involving three-phase contact lines, which will be a direction of our future efforts.¹⁹ In addition, the normal vector is automatically accounted in the contour-integral representation, which makes the results less sensitive to the errors due to the normal vector calculation.

The time integration in the present method is stabilized by the proposed multiple step scheme. The scheme offers a solution of the well-known problem of numerical instabilities due to the surface tension. The stabilizing effect of the multiple time-step integration is also important for simulations that involve repulsive van der Waals forces, mainly because of their strong dependence of the film thickness. In addition, the proposed time integration overcomes the numerical instabilities due to the mesh-size optimization technique based on the local grid tension method.

The higher-order interface approximation plays an essential role in the accurate calculation of the interface-to-interface distance, especially in film regions with significant curvature. It is important not only for an accurate calculation of the disjoining pressure, but also for a numerical stability during the simulation of polydispersed foam dynamics. An improvement of the present variant of the interface approximation can be easily achieved by making use of the local paraboloid fitting procedure.³⁰

In Sec. IV we present simulations of multiphase problems that involve regions of a high interface curvature and small interface-to-interface distance as well as a strong influence of the capillary and disjoining pressure. The simulations of drop-to-drop interaction show a good accuracy for film thickness of about 0.2% of the drop radius in the case of matching viscosities, $\lambda = 1$. However, at small viscosity ratio, $\lambda \ll 0.1$, the results were inaccurate for film thickness below 1% of the drop radius. We think, that in the case of contrast viscosities, $\lambda \ll 1$ or $\lambda \gg 1$, the error due to the space discretization becomes global, and is dominated by the error in the coarsest part of the mesh. Thus, the idea of a local mesh refinement in the film region is less attractive in these cases.

An important and direct extension of the present method can be made by an incorporation of the effect of an insoluble surfactant.^{38,39} This, together with an extension applying periodic boundary conditions can make the method an useful tool for a better understanding of the physics within complex multiphase flows.

ACKNOWLEDGMENT

This work is sponsored by the Dutch Polymer Institute (Project No. 161).

¹C. Pozrikidis, "Three-dimensional oscillations of inviscid drops induced by surface tension," *Comput. Fluids* **30**, 417 (2001).

²H. Stone and L. Leal, "Relaxation and breakup of initially extended drop in an otherwise quiescent fluid," *J. Fluid Mech.* **198**, 399 (1989).

³S. Kwak, M. Fyrrillas, and C. Pozrikidis, "Effect of surfactants on the

- instability of a liquid thread. Part II: Extensional flow," *Int. J. Multiphase Flow* **27**, 39 (2001).
- ⁴V. Cristini, J. Blawdziewicz, and M. Loewenberg, "Drop breakup in three-dimensional viscous flows," *Phys. Fluids* **10**, 1781 (1998).
- ⁵V. Cristini, R. Hooper, C. Macosko, M. Simeone, and S. Guido, "A numerical and experimental investigation of lamellar blend morphologies," *Ind. Eng. Chem. Res.* **41**, 6305 (2002).
- ⁶M. Loewenberg and E. Hinch, "Collision of two deformable drops in shear flow," *J. Fluid Mech.* **338**, 299 (1997).
- ⁷A. Zinchenko, M. Rother, and R. Davis, "Cusping, capture, and breakup of interacting drops by a curvatureless boundary-integral algorithm," *J. Fluid Mech.* **391**, 249 (1999).
- ⁸R. Davis, "Buoyancy-driven viscous interaction of a rising drop with a smaller trailing drop," *Phys. Fluids* **11**, 1016 (1999).
- ⁹C. Pozrikidis, "On the transient motion of ordered suspensions of liquid drops," *J. Fluid Mech.* **246**, 301 (1993).
- ¹⁰M. Loewenberg and E. Hinch, "Numerical simulation of concentrated emulsion in shear flow," *J. Fluid Mech.* **321**, 395 (1996).
- ¹¹A. Zinchenko and R. Davis, "Shear flow of highly concentrated emulsions of deformable drops by numerical simulations," *J. Fluid Mech.* **455**, 21 (2002).
- ¹²R. Khayat, "Three-dimensional boundary element analysis of drop deformation in confined flow for Newtonian and viscoelastic systems," *Int. J. Numer. Methods Fluids* **34**, 241 (2000).
- ¹³R. Khayat and N. Ashrafi, "A boundary-element analysis of transient viscoelastic blade coating flow," *Eng. Anal. Boundary Elem.* **24**, 363 (2000).
- ¹⁴M. Toose, "Simulation of the deformation of non-Newtonian drop in a viscous flow," Ph.D. thesis, University of Twente, The Netherlands, 1997.
- ¹⁵C. Pozrikidis, *Boundary-Integral and Singularity Methods for Linearized Viscous Flow* (Cambridge University Press, Cambridge, UK, 1992).
- ¹⁶S. Yon and C. Pozrikidis, "Deformation of a liquid drop adhering to a plane wall: Significance of the drop viscosity and the effect of an insoluble surfactant," *Phys. Fluids* **11**, 1297 (1999).
- ¹⁷A. Zinchenko, M. Rother, and R. Davis, "A novel boundary-integral algorithm for viscous interaction of deformable drops," *Phys. Fluids* **9**, 1493 (1997).
- ¹⁸X. Li and C. Pozrikidis, "Shear flow over a liquid drop adhering to a solid surface," *J. Fluid Mech.* **307**, 167 (1996).
- ¹⁹I. Bazhlekoy, "Non-singular boundary-integral method for deformable drops in viscous flows," Ph.D. thesis, Eindhoven University of Technology, The Netherlands, 2003.
- ²⁰J. Rallison, "A numerical study of the deformation and burst of a viscous drop in general shear flow," *J. Fluid Mech.* **109**, 465 (1981).
- ²¹R. Khayat and K. Marek, "An adaptive boundary-element approach to 3D transient free-surface flow of viscous fluids," *Eng. Anal. Boundary Elem.* **23**, 111 (1999).
- ²²S. Unverdi and G. Tryggvason, "A front-tracking method for viscous, incompressible, multi-fluid flows," *J. Comput. Phys.* **100**, 25 (1992).
- ²³D. Mavriplis, "Unstructured grid techniques," *Annu. Rev. Fluid Mech.* **129**, 473 (1997).
- ²⁴V. Cristini, J. Blawdziewicz, and M. Loewenberg, "An adaptive mesh algorithm for evolving surfaces: Simulation of drop breakup and coalescence," *J. Comput. Phys.* **168**, 445 (2001).
- ²⁵O. Galaktionov, P. Anderson, G. Peters, and F. van de Vosse, "An adaptive front-tracking technique for three-dimensional transient flows," *Int. J. Numer. Methods Fluids* **32**, 201 (2000).
- ²⁶E. Wetzel and C. Tucker III, "Drop deformation in dispersions with unequal viscosities and zero interfacial tension," *J. Fluid Mech.* **426**, 199 (2001).
- ²⁷Y. Stegeman, "Time dependent behaviour of drops in elongational flows," Ph.D. thesis, Eindhoven University of Technology, The Netherlands, 2002.
- ²⁸A. Chesters, "The modelling of coalescence of fluid-liquid dispersions: A review of current understanding," *Trans. Inst. Chem. Eng., Part A* **69**, 259 (1991).
- ²⁹S. Yantsios and R. Davis, "Close approach and deformation of two viscous drops due to gravity and van der Waals forces," *J. Colloid Interface Sci.* **144**, 412 (1991).
- ³⁰M. Rother, A. Zinchenko, and R. Davis, "Buoyancy-driven coalescence of slightly deformable drops," *J. Fluid Mech.* **346**, 117 (1997).
- ³¹I. Bazhlekoy, A. Chesters, and F. van de Vosse, "The effect of the dispersed to continuous-phase viscosity ratio on film drainage between interacting drops," *Int. J. Multiphase Flow* **26**, 445 (2000).
- ³²M. Rother and R. Davis, "The effect of slight deformation on drop coalescence in linear flows," *Phys. Fluids* **13**, 1178 (2001).
- ³³Ph. T. Jaeger, J. J. M. Janssen, F. Groeneweg, and W. G. M. Agterof, "Coalescence in emulsions containing inviscid drops with high interfacial mobility," *Colloids Surf., A* **85**, 255 (1994).
- ³⁴H. Wang, A. Zinchenko, and R. Davis, "The collision rate of small drops in linear flow fields," *J. Fluid Mech.* **256**, 161 (1994).
- ³⁵A. Kraynik and D. Reinelt, "Foam microrheology: From honeycombs to random foams," *Proceedings of the PPS-15 (CDrom)* ('s Hertogenbosch, The Netherlands, 1999).
- ³⁶A. Kraynik and D. Reinelt, "Linear elastic behaviour of dry soap foams," *J. Colloid Interface Sci.* **181**, 511 (1996).
- ³⁷I. Bazhlekoy, F. van de Vosse, and H. Meijer, "Boundary integral method for 3D simulation of foam dynamics," *Lect. Notes Comput. Sci.* **2179**, 401 (2001).
- ³⁸X. Li and C. Pozrikidis, "The effect of surfactants on drop deformation and on the rheology of dilute emulsions in Stokes flow," *J. Fluid Mech.* **341**, 165 (1997).
- ³⁹I. Bazhlekoy, P. Anderson, and H. Meijer, "Boundary integral method for deformable interfaces in the presence of insoluble surfactants," *Lect. Notes Comput. Sci.* **2907**, 355 (2004).