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Evolution of the volumetric interfacial area in two-phase mixtures

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Abstract

We investigate the time evolution of the density of interfaces in a two-phase mixture, with particular emphasis on the role of compressibility, dilatability and phase transitions. Two different and complementary routes are considered: a rather intuitive one based on exact results for dilute mixtures which are then interpolated to all concentrations, and a more systematic approach based on the statistical average of the exact transport equation for elementary pieces of interfaces. ***To cite this article: D. Lhuillier, C. R. Mecanique 332 (2004).***

Résumé

Evolution de l'aire interfaciale volumique dans les mélanges diphasiques. Nous cherchons à décrire l'évolution temporelle de la densité d'interfaces dans un mélange diphasique. L'accent est mis sur les effets de la compressibilité, de la dilatabilité et des changements de phase. Deux chemins complémentaires sont suivis : le premier, assez intuitif, est basé sur des résultats concernant les mélanges dilués, résultats qui sont ensuite interpolés à toute concentration ; le second, plus systématique, est basé sur la moyenne statistique de l'équation qui régit l'évolution temporelle d'un élément d'interface. ***Pour citer cet article : D. Lhuillier, C. R. Mecanique 332 (2004).***

Version française abrégée

Dans la description des suspensions de particules ou des mélanges diphasiques à l'aide du modèle à deux fluides, l'une des difficultés est de modéliser correctement les échanges entre constituants. Ces échanges font intervenir de façon cruciale l'aire totale des interfaces présentes et pour les suspensions de particules déformables (gouttes, bulles) on conçoit bien que la fraction volumique des particules n'est pas suffisante à elle seule pour quantifier ces échanges. Il faut en plus lui adjoindre la densité volumique des interfaces et trouver la façon dont celle-ci évolue dans le temps. Pour établir la forme générale de cette équation de transport, on se propose d'utiliser deux démarches

complémentaires. La première, à caractère intuitif, est basée sur des résultats connus (mais concernant uniquement les suspensions diluées) reliant la densité d'interface à la fraction volumique du milieu dilué et au nombre des particules par unité de volume. Une procédure d'interpolation permet de généraliser ces résultats à toutes les concentrations et aboutit à l'Éq. (3). La seconde est basée sur la moyenne statistique de l'équation d'évolution (5) d'un élément d'interface, et elle aboutit à l'Éq. (7) dans le plus simple des cas, c'est-à-dire quand on néglige toutes les fluctuations. La comparaison des résultats (3) et (7) permet de se faire une idée sur leur complémentarité. Dans l'approche intuitive la coalescence est bien modélisée, mais la fragmentation l'est de façon très sommaire. Dans l'approche rigoureuse (mais qui ne tient pas compte des fluctuations) la coalescence est absente mais la fragmentation est bien mieux modélisée puisque vue comme le résultat d'un étirement sous l'action du champ de vitesse et d'un retour vers une distribution isotrope des interfaces. La synthèse des deux approches apparaît dans le résultat (10).

1. Introduction

When describing the flow of two-phase mixtures or particulate suspensions, one of the main issues is the modelling of interphase exchanges. The intensity of these exchanges depends on the total area of the interfaces and, when the particles are likely to deform like drops or bubbles, their volume fraction is not enough to quantify their exchanges with the surrounding fluid. In addition, one must consider the interfacial area per unit volume and deduce the way it evolves with time. Almost thirty years ago, Ishii [1] proposed a very simple transport equation with a convective flux and a source term. Since that time, a lot of efforts were devoted to close that equation, i.e. to express the flux and the source terms as explicit functions of the volumetric interfacial area, the particles volume fraction, and the main variables (velocities, temperatures and pressures) entering the two-fluid model. At present this closure issue is far from being settled, as witnessed by a recent review on the subject [2]. It is noteworthy that the same type of problems is encountered in combustion science, whenever combustion occurs over relatively thin flame sheets. The so-called coherent flame model initiated by Marble and Broadwell [3], is based on a transport equation for the flame surface density. Their phenomenological approach was made rigorous by Candel and Poinsot [4] who derived the exact transport equation for what they called the "flame surface to volume ratio". It was realized only recently [5] that the same quantity was used under the name "function of presence of the interfaces" or "Dirac function on interfaces" by the two-phase community [6,7].

Our purpose here is to gain insight into the transport of interfacial area, following two different routes: firstly, a rather intuitive approach based on exact results for dilute suspensions and some extrapolation procedure to cover the whole volume fraction range and secondly, a more systematic approach based on the averaging of the exact small-scale transport equation. We will focus not only on deformable particles, but also on liquid–vapour mixtures in which the mass-exchange bears some resemblance with the chemical reactions in the coherent flame model.

2. Poor man's derivation

To get an intuitive insight into the evolution equation for the interface concentration, let us consider a superheated liquid. Soon after the boiling process is initiated, the mixture appears as a dispersion of spherical vapour bubbles moving through the liquid, while at the end of the process, it is a dispersion of spherical drops moving through the vapour. The evolution equation we are looking for must acknowledge the presence of spherical particles whenever one of the two volume fractions is decreasing to zero. For these two special cases (and for them only) one expects the interfacial density Q to be related to the volume fraction ϕ_d and to the number density n_d of the dispersed phase. When the size distribution of the dispersed phase is narrow, this relation can be formulated as $Q^3 \approx n_d \phi_d^2$ which implies

$$\partial Q/\partial t + \nabla \cdot Q\mathbf{V}_d = (2Q/3\phi_d)(\partial\phi_d/\partial t + \nabla \cdot \phi_d\mathbf{V}_d) + (Q/3n_d)(\partial n_d/\partial t + \nabla \cdot n_d\mathbf{V}_d) \qquad (1)$$

where $\mathbf{V}_d$ is the mean velocity of the dispersed phase. The evolution equation of the volume fraction can be presented in different (yet equivalent) ways. It was shown in [8] that one can benefit from writing them in the following "symmetric" form

$$\partial\phi_1/\partial t + \nabla \cdot \phi_1\mathbf{V}_1 = \phi_1\nabla \cdot \mathbf{U} - A - \Gamma\rho/\rho_1^\circ\rho_2^\circ$$
$$\partial\phi_2/\partial t + \nabla \cdot \phi_2\mathbf{V}_2 = \phi_2\nabla \cdot \mathbf{U} + A + \Gamma\rho/\rho_1^\circ\rho_2^\circ$$

In these evolution equations $\mathbf{U}$ is the volume-averaged velocity of the mixture ($\mathbf{U} = \phi_1\mathbf{V}_1 + \phi_2\mathbf{V}_2$), Γ is the mass production rate of component 2 ($\Gamma = \Gamma_2 = -\Gamma_1$), ρ is the mass density of the mixture ($\rho = \phi_1\rho_1^\circ + \phi_2\rho_2^\circ$) and A represents the difference of compressibility and dilatability between the two phases

$$A = \phi_1\phi_2\big[\big(1/\rho_1^\circ\big)\,d_1\rho_1^\circ/\,dt - \big(1/\rho_2^\circ\big)\,d_2\rho_2^\circ/\,dt\big] \tag{2}$$

where d_1/dt (respectively d_2/dt) is the convective time-derivative associated with $\mathbf{V}_1$ (respectively $\mathbf{V}_2$). Concerning the number density, its evolution in time is not that of a conserved quantity because of break-up and coalescence phenomena on the one hand, and because of nucleation and collapse phenomena on the other hand. In what follows we delete nucleation and collapse, with the risk of being wrong at the very beginning and at the very end of the phase change process. Since break-up is mainly a one-particle process and coalescence is mainly a two-particles process, one can write on purely dimensional grounds

$$\partial n_d/\partial t + \nabla \cdot n_d\mathbf{V}_d = 3n_d/T_{BR} - 3n_d V_{COA}Q$$

where T_{BR} is a characteristic time for break-up and V_{COA} is a characteristic velocity for coalescence. The factor 3 is for convenience only.

The above results suggest that a general evolution equation for Q which encompasses all phenomena *except nucleation and collapse* and which reduces to (1) in the limit of a dilute mixture is

$$\partial Q/\partial t + \nabla \cdot \big[(\phi_1\mathbf{V}_2 + \phi_2\mathbf{V}_1)Q\big] = (2Q/3)\nabla \cdot \mathbf{U} + (2Q/3)(1/\phi_2 - 1/\phi_1)\big(A + \Gamma\rho/\rho_1^\circ\rho_2^\circ\big)$$
$$+ Q/T_{BR} - V_{COA}Q^2 \tag{3}$$

The first two terms on the right-hand side represents the effects of compressibility and dilatability (present in A and $\nabla \cdot \mathbf{U}$) and phase transitions (present in Γ and $\nabla \cdot \mathbf{U}$). The quantity $(2Q/3)\nabla \cdot \mathbf{U}$ already appeared in [9]. A more general expression could be written for the term involving A and Γ with, instead of $1/\phi_2 - 1/\phi_1$, two different factors multiplying A and $\Gamma\rho/\rho_1^\circ\rho_2^\circ$. These two different factors must behave like $1/\phi_2$ when ϕ_2 is small and like $-1/\phi_1$ when ϕ_1 is small. Hence, the above common factor $1/\phi_2 - 1/\phi_1$ must be understood as the *simplest* function which interpolates correctly between these two extreme values. The third and fourth terms on the right-hand side represents the effects of break-up and coalescence respectively. The main difficulty is to give explicit expressions for both T_{BR} and V_{COA} in terms of the volume fractions and the physical quantities involved in the break-up and coalescence processes. As an example, for slow shear flows where viscous effects are dominant, one expects $V_{COA} = \phi_1\phi_2\sigma/\eta$ where σ is the surface tension and η is some effective viscosity of the mixture (η is noted $1/G_0$ in [5]).

3. Derivation from the local dynamics of interfaces

The small-scale description of interfacial phenomena requires each elementary portion of interface to be given its position, its orientation and its velocity, respectively represented by a two-dimensional Dirac function $\delta_I(\mathbf{x}, t)$, a unit normal $\mathbf{n}(\mathbf{x}, t)$ and a velocity field $\mathbf{V}^I(\mathbf{x}, t)$. The main relevant quantity is the symmetric tensor $\mathbf{nn}\delta_I$ and its statistical (ensemble) average $Q_{ij} = \langle n_i n_j \delta_I \rangle$ [10,11]. The trace Q of this tensor gives the mean interfacial area per

unit volume $Q = \langle \delta_I \rangle$, while its traceless part $q_{ij} = \langle (n_i n_j - \delta_{ij}/3)\delta_I \rangle$ describes the anisotropy of the interfacial orientation. The balance equation for Q_{ij} appears as [5]

$$\partial Q_{ij}/\partial t + \nabla \cdot \langle n_i n_j \mathbf{V}^I \delta_I \rangle = \langle (n_i n_j n_k n_l + n_i n_j \delta_{kl} - n_i n_k \delta_{jl} - n_j n_k \delta_{il}) \partial V_k^I / \partial x_l \delta_I \rangle \tag{4}$$

from which one deduces the evolution of the area concentration [4]

$$\partial Q/\partial t + \nabla \cdot \langle \mathbf{V}^I \delta_I \rangle = \langle (\mathbf{I} - \mathbf{nn}) : \nabla \mathbf{V}^I \delta_I \rangle \tag{5}$$

where $\mathbf{I}$ is the unit tensor. The interfacial velocity is linked to the local velocities of the two phases in the immediate vicinity of the interfaces [12]. Without phase transitions one has simply $\mathbf{V}^I = \mathbf{u}_1 = \mathbf{u}_2$. More generally, one can write $\mathbf{V}^I = \mathbf{u}_1 + (\mathbf{V}^I - \mathbf{u}_1) \cdot \mathbf{n}_1 \mathbf{n}_1$ or $\mathbf{V}^I = \mathbf{u}_2 + (\mathbf{V}^I - \mathbf{u}_2) \cdot \mathbf{n}_2 \mathbf{n}_2$ so that the tangential component of $\mathbf{V}^I$ is equal to the common tangential velocity of the two phases on each side of the interface, while the normal component is possibly different in case of phase changes between the liquid and the vapour. The issue is to choose some "symmetric" form of (5) in which the two phases will appear on an equal footing. Defining the local speeds of phase change $S_1 = (\mathbf{V}^I - \mathbf{u}_1) \cdot \mathbf{n}_1$ and $S_2 = (\mathbf{V}^I - \mathbf{u}_2) \cdot \mathbf{n}_2$, we propose a definition which looks "symmetric" regarding the two phases

$$\mathbf{V}^I = \phi_2(\mathbf{u}_1 + S_1 \mathbf{n}_1) + \phi_1(\mathbf{u}_2 + S_2 \mathbf{n}_2) \tag{6}$$

This special choice mixes averaged quantities (the volume fractions) with nonaveraged ones in such a way that $\mathbf{V}^I$ is linked preferentially to the velocities of the dispersed phase in case of a dilute mixture. As a consequence of this choice

$$\langle (\mathbf{I} - \mathbf{nn}) : \nabla \mathbf{V}^I \delta_I \rangle = 2/3 \langle (\phi_1 \nabla \cdot \mathbf{u}_1 + \phi_2 \nabla \cdot \mathbf{u}_2)\delta_I \rangle + 2/3(\phi_1 - \phi_2)\langle (\nabla \cdot \mathbf{u}_2 - \nabla \cdot \mathbf{u}_1)\delta_I \rangle$$
$$- \langle (\phi_2 \nabla \mathbf{u}_1 + \phi_1 \nabla \mathbf{u}_2) : (\mathbf{nn} - \mathbf{I}/3)\delta_I \rangle + \langle (\phi_2 S_1 \nabla \cdot \mathbf{n}_1 + \phi_1 S_2 \nabla \cdot \mathbf{n}_2)\delta_I \rangle$$

In this expression pure deformations were distinguished from dilatations. The four contributions on the right-hand side will now be given approximate expressions. If the true densities ρ_1° and ρ_2° do not display large differences between their values in the bulk and at the interfaces, one can write $\langle S_1 \delta_I \rangle \approx \Gamma_1/\rho_1^\circ$ and $\langle S_2 \delta_I \rangle \approx \Gamma_2/\rho_2^\circ$. The same assumption also means that the difference is not large between the divergence of $\mathbf{u}_k$ in the bulk of phase k and its divergence close to the interfaces. As a consequence

$$\langle (\phi_1 \nabla \cdot \mathbf{u}_1 + \phi_2 \nabla \cdot \mathbf{u}_2)\delta_I \rangle \approx Q(\phi_1 \langle \nabla \cdot \mathbf{u}_1 \rangle_1 + \phi_2 \langle \nabla \cdot \mathbf{u}_2 \rangle_2)$$
$$\langle (\nabla \cdot \mathbf{u}_2 - \nabla \cdot \mathbf{u}_1)\delta_I \rangle \approx Q(\langle \nabla \cdot \mathbf{u}_2 \rangle_2 - \langle \nabla \cdot \mathbf{u}_1 \rangle_1)$$

and

$$\langle (\phi_2 S_1 \nabla \cdot \mathbf{n}_1 + \phi_1 S_2 \nabla \cdot \mathbf{n}_2)\delta_I \rangle \approx \Gamma \langle \nabla \cdot \mathbf{n}_2 \rangle \rho/\rho_1^\circ \rho_2^\circ$$

where $\langle \nabla \cdot \mathbf{n}_2 \rangle$ is the average radius of curvature while $\langle \nabla \cdot \mathbf{u}_k \rangle_k$ is the average value of $\nabla \cdot \mathbf{u}_k$ in phase k. Since the divergence of $\mathbf{U}$ is the average of the divergence of the small-scale velocity, one deduces $\nabla \cdot \mathbf{U} = \phi_1 \langle \nabla \cdot \mathbf{u}_1 \rangle_1 + \phi_2 \langle \nabla \cdot \mathbf{u}_2 \rangle_2 + \langle (S_1 + S_2)\delta_I \rangle$ so that the balance equation for the interfacial area density becomes

$$\partial Q/\partial t + \nabla \cdot \left[(\phi_2 \mathbf{V}_1 + \phi_1 \mathbf{V}_2)Q \right] + \nabla \cdot \langle (\phi_2 S_1 \mathbf{n}_1 + \phi_1 S_2 \mathbf{n}_2)\delta_I \rangle$$
$$= (2Q/3)\nabla \cdot \mathbf{U} + (2Q/3)(\phi_1 - \phi_2)(\langle \nabla \cdot \mathbf{u}_2 \rangle_2 - \langle \nabla \cdot \mathbf{u}_1 \rangle_1) - \mathbf{q} : (\phi_2 \langle \nabla \mathbf{u}_1 \rangle_1 + \phi_1 \langle \nabla \mathbf{u}_2 \rangle_2)$$
$$+ \Gamma \left[(2Q/3)(1/\rho_1^\circ - 1/\rho_2^\circ) + \langle \nabla \cdot \mathbf{n}_2 \rangle \rho/\rho_1^\circ \rho_2^\circ \right] \tag{7}$$

As it stands, result (7) bears some resemblance with the intuitive result (3). Let us compare the two right-hand sides first. The terms involving $\nabla \cdot \mathbf{U}$ are identical. The term involving A in (3) is identical with the second term on the right-hand side of (7) provided $A \equiv \phi_1 \phi_2 (\langle \nabla \cdot \mathbf{u}_2 \rangle_2 - \langle \nabla \cdot \mathbf{u}_1 \rangle_1)$ which is quite compatible with the previous definition (2). The terms involving the mass exchange rate Γ are identical provided the mean radius of curvature can be written as

$$\langle \nabla \cdot \mathbf{n}_2 \rangle = (2Q/3\phi_1 \phi_2)(\phi_1^2 \rho_1^\circ - \phi_2^2 \rho_2^\circ)/\rho \tag{8}$$

The expected results $\langle \nabla \cdot \mathbf{n}_2 \rangle = 2Q/3\phi_2$ when $\phi_2 \ll 1$ and $\langle \nabla \cdot \mathbf{n}_2 \rangle = -2Q/3\phi_1$ when $\phi_1 \ll 1$ are recovered as special cases. Interestingly, the average radius of curvature vanishes for $\phi_1^2 \rho_1^\circ = \phi_2^2 \rho_2^\circ$ which is not unreasonable but needs some confirmation in the case of liquid–vapour mixtures which have a density ratio close to one thousand. Conversely, if one obtains a different modelling for $\langle \nabla \cdot \mathbf{n}_2 \rangle$ and introduces it into (7), the resulting coefficient in front of Γ will be different from the one appearing in (3). But the main difference between (7) and (3) is certainly the presence of the anisotropy tensor $\mathbf{q} = \langle (\mathbf{nn} - \mathbf{I}/3)\delta_I \rangle$ in (7). This means that the evolution equation for Q generally depends on $\mathbf{q}$ which itself obeys an evolution equation that can be deduced from (4) and (5). The point is that the evolution of $\mathbf{q}$ depends on $\langle \mathbf{nnnn}\delta_I \rangle$ and a closure problem arises. This situation is reminiscent of the closure problem for the turbulent kinetic energy $\langle v'^2 \rangle$ and there is in fact a certain analogy between the ways Q and $\langle v'^2 \rangle$ are evolving. In the example of emulsions of two immiscible liquids [5,13] it was shown that the phasic mean strain rates $\langle \nabla \mathbf{u}_1 \rangle_1$ and $\langle \nabla \mathbf{u}_2 \rangle_2$ can be expressed in terms of $\mathbf{q}$ and the symmetric and traceless strain rate $(\nabla \mathbf{U})^{S0}$ with the result,

$$\mathbf{q} : \left(\phi_2 \langle \nabla \mathbf{u}_1 \rangle_1 + \phi_1 \langle \nabla \mathbf{u}_2 \rangle_2 \right) = \alpha \mathbf{q} : (\nabla \mathbf{U})^{S0} + V_{ISO}\mathbf{q} : \mathbf{q} \tag{9}$$

where α is a scalar and V_{ISO} is a characteristic speed for return to isotropy. These two parameters are respectively associated with the stretch due to the average motion and with the relaxation towards an isotropic distribution of interfaces. When writing the Q/T_{BR} term of (3), it was implicitly assumed that the interfacial distribution was always close to isotropic and this term is, so to say, the ghost form of (9). Hence, break-up can be thought of as resulting from the combined action of stretch and relaxation towards isotropy. In the example of a slowly sheared suspension [5] one obtains $\alpha = 1 + (\phi_1 - \phi_2)(\eta_1 - \eta_2)/\eta$ and $V_{ISO} = \sigma/2\phi_1\phi_2\eta$. Note that V_{ISO} displays the same scaling as V_{COA} but a different dependence on the volume fractions. Concerning coalescence, it can be thought of as a relaxation process towards a state with a minimum density of interfaces. This process is missing from (7) but it is clear that we selected only the main contributions when writing (7), in particular we neglected all types of fluctuations. Hence, a coalescence term must be added to (7) similar to the $V_{COA}Q^2$ term in (3). So far we dealt with the sink and source terms of the right-hand side of (7). What about the convection terms appearing in the left-hand side? Obviously, there is no term in (3) which corresponds to $\langle (\phi_2 S_1 \mathbf{n}_1 + \phi_1 S_2 \mathbf{n}_2)\delta_I \rangle$ in (7). In fact this term is null when the volume fractions are uniform. In all other cases one must write $\langle (\phi_2 S_1 \mathbf{n}_1 + \phi_1 S_2 \mathbf{n}_2)\delta_I \rangle \approx -(\Gamma/Q)(\rho/\rho_1^\circ \rho_2^\circ)\nabla\phi_2$. This diffusion-like flux is usually negligible when compared to the convection flux $(\phi_1 \mathbf{V}_2 + \phi_2 \mathbf{V}_1)Q$.

4. Conclusion

When the role of nucleation and collapse can be neglected, the general form of the transport equation for the volumetric interface area can be presented as

$$\partial Q/\partial t + \nabla \cdot \left[(\phi_1 \mathbf{V}_2 + \phi_2 \mathbf{V}_1)Q \right]$$
$$= (2Q/3)\nabla \cdot \mathbf{U} - \alpha \mathbf{q} : (\nabla \mathbf{U})^{S0} + (2Q/3)(1/\phi_2 - 1/\phi_1)\left(A + \Gamma\rho/\rho_1^\circ \rho_2^\circ \right) - V_{ISO}\mathbf{q} : \mathbf{q} - V_{COA}Q^2 \tag{10}$$

In this expression, A and Γ must be given expressions compatible with a positive entropy production [8]. It is clear that the evolution of Q is connected to the anisotropy tensor $\mathbf{q}$ and one must solve the transport equation for $\mathbf{q}$ before closing the above equation. Each different type of flow will give different results for $\mathbf{q}$, so that a universal closure is not likely to appear. The similarity of the link between Q and $\mathbf{q}$, and the link between the fluctuational kinetic energy and the deviatoric part of the Reynolds stress is noteworthy. Moreover, if the mixture is in turbulent motion, one can imagine a coupling (due to the Curie symmetry principle of irreversible thermodynamics) between the area tensor $\langle \mathbf{nn}\delta_I \rangle$ and the Reynolds stress tensor. One can wonder whether such a coupling can provide a phenomenological interpretation of the modifications of turbulence close to moving and deformable boundaries.

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