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Derivation of a two-phase flow model with two-scale kinematics and surface tension by means of variational calculus

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Abstract

The present paper proposes a definition of a two-phase interface that relies on a probability density function. This definition enables to introduce a scale separation in the definition this interface and to define fields that characterize the geometry of the interface. Relying on these fields, we propose a two-phase flow model that is able to account for small and large scale separation of the interface description by means of supplementary convected geometric variables. The model accounts for two-scale kinematics and two-scale surface tension. At large scale, the flow and the full geometry of the interface may be retrieved thanks to the bulk variables and the volume fraction, while at small scale the interface dynamics is accurately recovered through the interfacial area density fluctuation and the mean curvature.

Introduction

Two-phase flow occur in many industrial processes and can display multiple flow topologies. For example a jet atomization involves separated phases close to the injector and dispersed phase downstream with in between a mixed region where complex elements such as ligaments and rings detach from the liquid core. These multi-scale phenomena are out-of-reach for direct numerical simulations in realistic configurations due to computational costs. This leads to the derivation of reduced-order models that are used for numerical simulations.

Two approaches are found in the literature to build reduced-order models for two-phase flows:

1. coupling two models, a first one for the dispersed flow by employing an element derived from the Kinetic Based Moment Method [1] which treats polydispersed droplets in size, velocity and temperature, and a second one dealing with the separated phase and the mixed region with either an hierarchy of diffuse interface models [2, 3], front tracking methods [4] or some level of LES on the interface dynamics [5].
2. employing a unified model that encompasses any flow topology. Works in this direction are found in [3, 6] where a unified model accounting for micro-inertia and micro-viscosity associated to bubble pulsation is proposed.

In the present work, the second approach is retained. In [3, 6], a model was designed to account for two-scale kinemat-

ics in the case of a mono-disperse flow with spherical gas inclusions by means of the Least Action Principle. Our contribution involves mainly three matters: first we propose a definition of the interface using a Probability Density Function, second we propose to drop some restricting hypotheses on the topology of the bubbly flow used in [2, 3], third we aim at not only accounting for two-scale kinematics but also for two-scale surface tension effects.

1 Description of a surface by means of a PDF

Our analysis relies on the key idea that the two-phase interface is not a geometric locus. Instead, we propose to use a probability density function (PDF) f that will characterize the properties of the interface \mathcal{S} . We will use this probabilistic description to distinguish small and large scales of the interface.

We suppose given a probability density function (PDF) $f : (t, \mathbf{x}, \varphi, H) \in \Omega \mapsto [0, 1]$, with $\Omega \subset [0, +\infty) \times \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}$. The quantity $f(t, \mathbf{x}, \varphi, H) d\mathbf{x}d\varphi dH$ represents the probability that at a position \mathbf{x} and the instant t the interface can be described by a level set function that takes the value φ and the field of interface mean curvature takes the value H .

In the following we shall note $\xi = (\varphi, H)$ and for the sake of simplicity we shall omit the time dependency of f in the notations.

Remark 1 *It is possible to consider different or additional interface features like the Gaussian curvature G , or the unit*

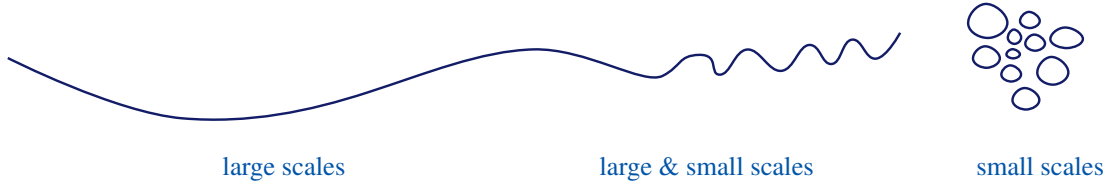


Figure 1: Large and small scale interface dynamics

normal \mathbf{n} as variables of f .

Thanks to zero-th moments of f we can then define fields over the whole space that characterize the interface as follows:

$$\varphi(\mathbf{x}) = \int \varphi' f(\mathbf{x}, \xi') d\xi', \quad (1a)$$

$$H(\mathbf{x}) = \int H' f(\mathbf{x}, \xi') d\xi'. \quad (1b)$$

The set $\varphi^{-1}(\{0\})$ defines a surface that we consider to be a probable geometrical locus for the interface \mathcal{S} . Similarly, the $H(\mathbf{x})$ will provide a probable value of the mean curvature of \mathcal{S} when \mathbf{x} lies in the vicinity of $\varphi^{-1}(\{0\})$. Let us note that thanks to (1a) it is possible to define a unit normal field $\mathbf{x} \in \mathbb{R}^d \mapsto \mathbf{n} \in \mathbb{R}^d$ by setting $\mathbf{n}(\mathbf{x}) = \nabla\varphi(\mathbf{x})/\|\nabla\varphi(\mathbf{x})\|$. Definition (1a) also provides an alternate definition H^{alt} for the mean curvature with $H^{\text{alt}}(\mathbf{x}) = \text{div}(\mathbf{n})$. In the following we shall consider that both definition are equivalent, *i.e.* $H^{\text{alt}} = H$.

We note $\mathbb{1}_A$ the characteristic function of a set $A \subset \mathbb{R}^d$ and $\mathbb{R}^+ = [0, +\infty)$. Considering that the interface \mathcal{S} separates two different fluid, we can define α the volume fraction of the fluid 1 as

$$\alpha(\mathbf{x}) = \int \mathbb{1}_{\mathbb{R}^+}(\varphi') f(\mathbf{x}, \xi') d\xi'. \quad (2)$$

Let us underline that the approach that is described above allows to retrieve the classic definition of an interface by a surface. Indeed, given a surface defined by a level set function $\mathbf{x} \mapsto \bar{\varphi}$, defining the measure

$$f(\mathbf{x}', \xi') d\mathbf{x}' d\xi' = \delta(\varphi' - \bar{\varphi}(\mathbf{x}')) \delta\left(H' - \text{div}\left(\frac{\nabla\bar{\varphi}(\mathbf{x}')}{\|\nabla\bar{\varphi}(\mathbf{x}')\|}\right)\right)$$

allows to retrieve $\varphi = \bar{\varphi}$ and $H = \text{div}(\nabla\bar{\varphi}/\|\nabla\bar{\varphi}\|)$. Nevertheless, we emphasize that there is no physical reason to consider such case. Indeed, a sharp interface is just a model for finitely fine transition zone.

The PDF f is supposed to be able to encompass all the scales l of \mathcal{S} , $l \in]0, +\infty[$. If obtained by a DNS, it would be then limited to the mesh minimum size, such that $l \in]l_{DNS}, +\infty[$.

2 Two-scale description of a surface

Filtering of the PDF

We now want to introduce a separation between large and small scales of the interface \mathcal{S} . Let $l_c > l$ be the cutoff

characteristic length scale, such that $l \in]l, l_c]$ (resp. $l \in]l_c, +\infty[$) corresponds to the small (resp. large) scales of \mathcal{S} .

We introduce a new PDF f_c characterizing all the scales of \mathcal{S} up to the cutoff length scale l_c , $l \in]l_c, +\infty[$. Let us note $\mathcal{B}_c(\mathbf{x}) = \{\mathbf{x}' / \|\mathbf{x} - \mathbf{x}'\| < l_c/2\}$. Since f_c does not account for any scale below l_c , we propose to operate a spatial averaging over $\mathcal{B}_c(\mathbf{x})$ by considering the distribution defined by

$$\frac{1}{|\mathcal{B}_c(\mathbf{x})|} \int \mathbb{1}_{\mathcal{B}_c(\mathbf{x})}(\mathbf{x}') f(\mathbf{x}', \xi) d\mathbf{x}'.$$

In order to define f_c we propose further filter the values of f : since f_c has undergone a spatial averaging, it seems reasonable to upper-bound the possible mean curvature H described by f_c with a value H^{max} . Consequently we choose to set

$$f_c(\mathbf{x}, \xi) = \frac{1}{|\mathcal{B}_c(\mathbf{x})|} \int_{\mathcal{B}_c(\mathbf{x})} \mathbb{1}_{\mathbb{R}^+}(H^{\text{max}} - H') f(\mathbf{x}', \xi) d\mathbf{x}'. \quad (3)$$

For the sake of consistency, we assume in the following that when $l_c \rightarrow 0$ and $H^{\text{max}} \rightarrow +\infty$ we have $f_c \rightarrow f$ in some sense. Furthermore, we propose to define H^{max} by the curvature of the ball of radius $l_c/2$, *i.e.* $H^{\text{max}} = 2/l_c$.

Using the moments of f_c , we can define a filtered level set φ_c , filtered mean curvature H_c and a filtered volume fraction, α_c by setting

$$\varphi_c(\mathbf{x}) = \int \varphi' f_c(\mathbf{x}, \xi') d\xi', \quad (4a)$$

$$H_c(\mathbf{x}) = \int H' f_c(\mathbf{x}, \xi') d\xi' \quad (4b)$$

$$\alpha_c(\mathbf{x}) = \int \mathbb{1}_{\mathbb{R}^+}(\varphi') f_c(\mathbf{x}, \xi') d\xi'. \quad (4c)$$

We now notice that $\alpha = \int \mathbb{1}_{\mathbb{R}^+}(\varphi')(f - f_c + f_c) d\xi'$, which yields a natural decomposition of α as

$$\alpha = \tilde{\alpha} + \alpha_c, \quad \text{with} \quad \tilde{\alpha} = \int \mathbb{1}_{\mathbb{R}^+}(\varphi')(f - f_c) d\xi' / \quad (5)$$

Thus α is the superposition of a contribution coming from f_c and a fluctuating part $\tilde{\alpha}$. Let us emphasize that $\tilde{\alpha} \in [-1, 1]$ while $\alpha \in [0, 1]$ and $\alpha_c \in [0, 1]$. Figure 2 illustrates this remark by showing the effect of the spatial averaging on the ball $\mathcal{B}_c(\mathbf{x})$. In such example, α equals either 1 or 0, $\alpha_c \in [0, 1]$ but $\tilde{\alpha}(\mathbf{x}) < 0$ when $\alpha(\mathbf{x}) = 0$.

We can now also define the interfacial density area inside the ball \mathcal{B}_c by integrating the local mean curvature, H over $\mathcal{B}_c(\mathbf{x})$, more precisely we set

$$\Sigma(\mathbf{x}) = \frac{1}{|\mathcal{B}_c(\mathbf{x})|} \int_{\varphi'=0} H' f(\mathbf{x}', \xi') \mathbb{1}_{\mathcal{B}_c(\mathbf{x})}(\mathbf{x}') d\mathbf{x}' d\xi'. \quad (6)$$

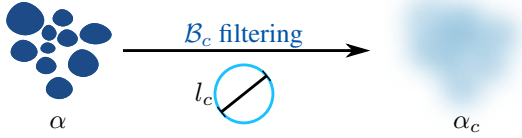



Figure 2: Filtering of the volume fraction using the spatial averaging on the ball \mathcal{B}_c , $\alpha = 0$  $\alpha = 1$.

In a similar manner, we define Σ_c the filtered interfacial area density, Σ_c , as

$$\Sigma_c(\mathbf{x}) = \frac{1}{|\mathcal{B}_c(\mathbf{x})|} \int_{\varphi'=0} H' f_c(\mathbf{x}', \xi') \mathbb{1}_{\mathcal{B}_c(\mathbf{x})}(\mathbf{x}') d\mathbf{x}' d\xi'. \quad (7)$$

Consequently, using similar lines as for the volume fraction, Σ can be split into two contributions, Σ_c and a fluctuating part $\tilde{\Sigma}$ defined by

$$\tilde{\Sigma} = \Sigma - \Sigma_c. \quad (8)$$

As opposed to the volume fraction, the interfacial area density, being defined with respect to the \mathcal{B}_c , is not affected by the spatial averaging on \mathcal{B}_c . Therefore, we have

$$0 \leq \Sigma_c \leq \Sigma \quad 0 \leq \tilde{\Sigma} \leq \Sigma. \quad (9)$$

In the same lines, we define the filtered mean curvature H_c and decompose the mean curvature into two contributions,

$$H = H_c + \tilde{H}. \quad (10)$$

As a result of the filtering proposed in Equation (3) on the mean curvature maximum value, we have

$$H_c < H^{max} = 2/l_c \quad (11)$$

It is possible to characterize the difference between α and α_c . Indeed, we have

$$f(\mathbf{x}) - f_c(\mathbf{x}) = \frac{1}{|\mathcal{B}_c|} \int_{\mathcal{B}_c(\mathbf{x})} (f(\mathbf{x}) - f_c(\mathbf{x}')) d\mathbf{x}'. \quad (12)$$

Since $\mathbf{x}' \in \mathcal{B}_c(\mathbf{x})$, if we suppose that f is smooth with respect to the space variable, a Taylor expansion yields

$$f(\mathbf{x}) - f_c(\mathbf{x}') = \frac{\partial f}{\partial \mathbf{x}} l_c \mathbf{r} + \mathcal{O}(l_c^2) \quad (13)$$

where $\mathbf{x} - \mathbf{x}' = l_c \mathbf{r}$, $\mathbf{r} \in \mathcal{B}_c(\mathbf{0})$. Thus

$$f(\mathbf{x}) - f_c(\mathbf{x}) = \mathcal{O}(l_c^2), \quad (14)$$

and finally we obtain

$$\alpha(\mathbf{x}) = \alpha_c(\mathbf{x}) + \mathcal{O}(l_c^2) \quad (15)$$

Two-scale two-phase flow interface

We now turn to the derivation of a two-phase flow model using our two-scale interface description. We assume that the pressure and velocity of each component are at equilibrium. We consider a set of bulk variables: the total density ρ , the mass fraction of fluid 1 Y and the velocity \mathbf{v} , then we consider variables that characterize the position geometry of the interface. In classic approaches like [7] this characterization is achieved by using the volume fraction which can only capture large scale interface features: small scales are lost. Such model cannot account accurately for complex two-phase flow topology variations across several scales.

Our goal is two-fold: first we aim at enriching the description of the interface by solving supplementary geometric variables such as the interfacial density area, Σ and the mean curvature H . Second, we propose to account for a two-scale kinematic evolution.

We suppose the two-phase flow interface to be defined by a PDF f that describes all the scales of the interface. Let us consider a cut-off length scale l_c . We can now express variables that characterize the interface in terms of f and f_c .

The Lagrangian energy L of the system is the difference between the kinetic energy, \mathcal{K} and the potential energy, \mathcal{U} , of the system. We separate bulk and interfacial contribution of the potential energy, denoting the bulk potential \mathcal{U}_b and the interfacial energy \mathcal{U}_i . The bulk kinetic energy contribution \mathcal{K} is defined through the bulk variables only, and therefore no distinction between small and large scales are needed.

$$\mathcal{K} = \frac{1}{2} \rho \|\mathbf{v}\|^2 \quad (16)$$

We suppose that the bulk potential energy takes the form

$$\mathcal{U}_b = \rho e(\rho, Y, \alpha).$$

Let us note that \mathcal{U}_b depends on bulk variables but also on α .

In order to account for surface tensions effects we also add a potential interfacial energy \mathcal{U}_i . If we have access to all scales of the interface, we can express the potential interfacial energy by

$$\mathcal{U}_i = \frac{1}{2} \sigma \|\nabla \alpha\| \quad (17)$$

where σ is the surface tension coefficient of the mixture and α , defined in Equation (2), is accounting for small and large scales. After filtering small scales, $\nabla \alpha_c$ cannot describe small scale surface tension. By (4c) and (5), we have

$$\nabla \alpha = \nabla \alpha_c + \nabla \tilde{\alpha}. \quad (18)$$

This suggests that the interfacial energy, accounting for scale separation can be expressed as

$$\mathcal{U}_i = \frac{1}{2} \sigma \|\nabla \alpha_c\| + W, \quad (19)$$

where W is a subscale interfacial energy W that we intend to model using the geometric characterization of the interface.

We suppose that small scale interfacial energy variations are involved when there is a variation of the fluctuation of interfacial density area $\tilde{\Sigma}$. Under such variations we suppose that surface tension forces are oriented along the normal \mathbf{n} to the interface and proportional to the local mean curvature. We also assume that for small scales the interface can only undergo displacement $\delta h \mathbf{n}$ that are oriented along the normal to the interface. The infinitesimal energy variation involved with the infinitesimal work of such forces read the interface $\delta h \mathbf{n}$, reads

$$\delta W = \gamma H \delta h, \quad (20)$$

where γ is a constant characterizing the surface tension properties of the mixture. In [6], relationships related to geometric variables describing the interface have been derived when the interface is subjected to a small displacement $\delta h \mathbf{n}$. These relations can be expressed as follows

$$\delta \tilde{\Sigma} = -2H \tilde{\Sigma} \delta h, \quad \delta \alpha = \tilde{\Sigma} \delta h, \quad (21)$$

where δ characterizes an infinitesimal variation. Let us emphasize that (21) involves α , and not $\tilde{\alpha}$. This is due to the fact that the small scale interface is only accurately described by α as shown in Figure 2. Therefore the infinitesimal variation of small scale interfacial energy takes the form

$$\delta W = \frac{1}{2} \gamma \frac{\delta \tilde{\Sigma}}{\tilde{\Sigma}}. \quad (22)$$

This suggests that

$$W = \frac{1}{2} \gamma \ln \left(\frac{\tilde{\Sigma}}{\Sigma^0} \right) \quad (23)$$

where Σ^0 is defined as the interfacial density area of $\mathcal{B}_c(\mathbf{0})$, $\Sigma^0 = 6/l_c$, *i.e.* the interfacial density area associated to the maximal curvature that can be capture at any point \mathbf{x} by α_c . The limit case $\tilde{\Sigma}(\mathbf{x}) \rightarrow 0$ in (23) has to be discarded as in this case there is no interface in the vicinity of \mathbf{x} . We propose to detect such situations using the values of H . This suggests to adopt an alternate definition for W by considering

$$W = \frac{\hat{\gamma}(H)}{2} \ln \left[\frac{\tilde{\Sigma}}{\Sigma^0} \right], \quad (24)$$

$$\hat{\gamma}(H) = \begin{cases} \gamma & \text{if } H \geq H^{\max}, \\ 0 & \text{otherwise.} \end{cases} \quad (25)$$

We now turn to the definition of the small scale kinetic energy \mathcal{K}_i by setting

$$\mathcal{K}_i = \frac{1}{2} m (D_t h)^2. \quad (26)$$

The coefficient m has the dimension of a mass. Injecting the Equation (21), it yields

$$\mathcal{K}_i = \frac{1}{2} m \frac{(D_t \alpha)^2}{\tilde{\Sigma}^2}. \quad (27)$$

We thus propose to define the interfacial energy as

$$\begin{aligned} \mathcal{K}_i + \mathcal{U}_i &= \frac{1}{2} \sigma \|\nabla \alpha\| \quad (28) \\ &= \frac{1}{2} m \frac{(D_t \alpha)^2}{\tilde{\Sigma}^2} + \frac{1}{2} \sigma \|\nabla \alpha_c\| - \hat{\gamma}(H) \ln \left(\frac{\tilde{\Sigma}}{\Sigma^0} \right) \quad (29) \end{aligned}$$

where Equation (28) gives the form of the interfacial energy in terms of geometric variables that cover the whole range of scales whereas Equation (29) shows the decomposition of the interfacial energy induced by the introduction of a cutoff length scale and therefore is defined with respect to filtered and fluctuating geometric quantities.

Relation (15) suggests that we can substitute α by α_c in the bulk potential energy. Therefore when accounting for a scale separation between small and large scale, the Lagrangian of the system is now a function of $(\rho, Y, \mathbf{v}, \alpha_c, \tilde{\Sigma})$ and can be written as

$$\begin{aligned} L(\rho, Y, \mathbf{v}, \alpha_c, \tilde{\Sigma}) &= \frac{1}{2} \rho \mathbf{v}^2 + \frac{1}{2} m \frac{(D_t \alpha_c)^2}{\tilde{\Sigma}^2} \\ &+ \frac{1}{2} \sigma \|\nabla \alpha_c\| - \hat{\gamma}(H) \ln \left(\frac{\tilde{\Sigma}}{\Sigma^0} \right) \\ &- \rho e(\rho, Y, \alpha_c). \quad (30) \end{aligned}$$

From now on, we shall assume the mean curvature $\mathbf{x} \mapsto H$ to be a fixed given field. Discarding this restriction will be the matter of future works. To simplify notation, we will now drop the notations for fluctuating and filtered quantities on the volume fraction and the interfacial density area and suppose m , σ and γ to be constant.

3 Extremization of the Action

We now follow classic lines of the Least Action Principle. Consider $\mathcal{B}(t) \subset \mathbb{R}^3$ the volume occupied by the fluid for $t \in [t_0, t_1]$. Let $\mathbf{X} \in \mathcal{B}(t_0)$ be the Lagrangian coordinates associated with the reference frame at instant $t = t_0$, then we note $(t, \mathbf{X}) \mapsto \varphi^L$ the position of the fluid particle whose position is \mathbf{x} at $t = t_0$. If $(t, \mathbf{x}) \mapsto b$ is any Eulerian field it can be associated with the Lagrangian field $(t, \mathbf{X}) \mapsto b^L$ by setting $b(\varphi^L(\mathbf{X}, t), t) = b^L(\mathbf{X}, t)$. The flow can be fully characterized by $(t, \mathbf{x}) \mapsto (\rho, \mathbf{v}, Y, \alpha, \Sigma)$ or equivalently by $\mathbf{x} \mapsto (Y, \alpha, \Sigma)$ and $(t, \mathbf{X}) \mapsto \varphi^L$ if φ^L complies with the mass conservation equation.

For a given transformation of the medium $\mathbf{x} \mapsto (Y, \alpha, \Sigma)$ and $(t, \mathbf{X}) \mapsto \varphi^L$, let $(t, \mathbf{x}, \lambda) \mapsto (Y_\lambda, \alpha_\lambda, \Sigma_\lambda)$ and $(t, \mathbf{X}, \lambda) \mapsto \tilde{\varphi}^L$ be a family of medium transformations parametrized by $\lambda \in [0, 1]$. We note $\tilde{\Omega}(\lambda) = \{(t, \tilde{\varphi}^L(t, \mathbf{X}, \lambda)) | \mathbf{X} \in \mathcal{B}(t_0), t \in [t_0, t_1]\}$ and we require these fields to satisfy constraints pertaining to mass conservation

$$\frac{\partial \rho_\lambda}{\partial t} + \nabla \cdot (\rho_\lambda \mathbf{v}_\lambda) = 0, \quad \frac{\partial \rho_\lambda Y_\lambda}{\partial t} + \nabla \cdot (\rho_\lambda Y_\lambda \mathbf{v}_\lambda) = 0 \quad (31)$$

supplemented by constraints regarding the topology evolution

$$D_t \Sigma_\lambda + 2H \Sigma_\lambda D_t h_\lambda = 0, \quad D_t \alpha_\lambda - \Sigma_\lambda D_t h_\lambda = 0, \quad (32)$$

and finally classic boundary constraints

$$(Y_\lambda, \alpha_\lambda, \Sigma_\lambda)(t, \mathbf{x}, \lambda = 0, 1) = (Y, \alpha, \Sigma)(t, \mathbf{x}), \quad (33a)$$

$$\widetilde{\varphi}^L(\mathbf{X}, t, \lambda = 0, 1) = \varphi^L(\mathbf{X}, t), \quad (33b)$$

$$(Y_\lambda, \alpha_\lambda, \Sigma_\lambda)(t, \mathbf{x}, \lambda)|_{(t, \mathbf{x}) \in \partial \widetilde{\Omega}(\lambda)} = g(Y, \alpha, \Sigma)(t, \mathbf{x}), \quad (33c)$$

$$\widetilde{\varphi}^L(\mathbf{X}, t, \lambda)|_{(t, \mathbf{X}) \in \partial([t_0, t_1] \times \mathcal{B}(t_0))} = \varphi^L(\mathbf{X}, t). \quad (33d)$$

Following standard lines, this family of transformation yields a family of infinitesimal transformations defined as follows

$$\delta_\lambda \varphi(t, \varphi^L(t, \mathbf{X})) = \left(\frac{\partial \widetilde{\varphi}^L}{\partial \lambda} \right)_{t, \mathbf{X}} (t, \mathbf{X}, \lambda = 0), \quad (34a)$$

$$\delta_\lambda b(t, \mathbf{x}) = \left(\frac{\partial \widetilde{b}}{\partial \lambda} \right)_{t, \mathbf{x}} (t, \mathbf{x}, \lambda = 0), \quad (34b)$$

for $b \in \{\rho, Y, \mathbf{v}, \alpha, \Sigma\}$. Let us now define the Hamiltonian action \mathcal{A} associated with Ω for the family of transformations $(t, \mathbf{x}, \lambda) \mapsto (Y_\lambda, \alpha_\lambda, \Sigma_\lambda)$ and $(t, \mathbf{X}, \lambda) \mapsto \widetilde{\varphi}^L$

$$\mathcal{A}(\lambda) = \int_{\widetilde{\Omega}(\lambda)} L(\rho_\lambda, Y_\lambda, \mathbf{v}_\lambda, D_t h_\lambda, \alpha_\lambda, \Sigma_\lambda, \nabla \alpha_\lambda) d\mathbf{x} dt. \quad (35)$$

The Least Action Principle states that a physical transformation of the system verifies

$$\frac{d\mathcal{A}}{d\lambda}(0) = 0. \quad (36)$$

Relation (36) will provide the motion equations of the flow. In order to obtain a set of partial differential equations, we need to express $d\mathcal{A}/d\lambda$. Using definition (34b) we can write

$$\begin{aligned} \frac{d\mathcal{A}}{d\lambda}(0) = \int_{\Omega(0)} & \left[\frac{\partial L}{\partial \rho} \delta_\lambda \rho + \frac{\partial L}{\partial Y} \delta_\lambda Y + \frac{\partial L}{\partial \mathbf{v}} \delta_\lambda \mathbf{v} \right. \\ & + \frac{\partial L}{\partial (D_t h)} \delta_\lambda (D_t h) + \frac{\partial L}{\partial \alpha} \delta_\lambda \alpha + \frac{\partial L}{\partial \Sigma} \delta_\lambda \Sigma \\ & \left. + \frac{\partial L}{\partial (\nabla \alpha)} \delta_\lambda (\nabla \alpha) \right] d\mathbf{x} dt. \quad (37) \end{aligned}$$

Applying (34b) with the constraints (31) allows to express following relations between the infinitesimal variations

$$\delta_\lambda \rho = -\nabla \cdot (\rho \delta_\lambda \varphi), \quad (38a)$$

$$\delta_\lambda Y = -\nabla Y^T \delta_\lambda \varphi, \quad (38b)$$

$$\delta_\lambda \mathbf{v} = D_t (\delta_\lambda \varphi) - (\delta_\lambda \varphi^T \nabla) \mathbf{v}, \quad (38c)$$

$$\delta_\lambda (D_t h) = \frac{1}{\Sigma} \delta_\lambda (D_t \alpha) - \frac{D_t h}{\Sigma} \delta_\lambda \Sigma. \quad (38d)$$

Recasting relations (38) into (37) provides

$$\int_{\Omega(0)} [\mathbf{A}^T \delta \varphi + \mathbf{B} \delta \alpha + \mathbf{C} \delta \Sigma] d\mathbf{x} dt = 0, \quad (39)$$

$$\begin{aligned} \mathbf{A}^T = \partial_t & \left(\frac{\partial L}{\partial \mathbf{v}} \right) + \nabla \cdot [(\frac{\partial L}{\partial \mathbf{v}})^T \mathbf{v}^T] + (\nabla \mathbf{v})^T \left(\frac{\partial L}{\partial \mathbf{v}} \right)^T \\ & + \partial_t \left(\frac{1}{\Sigma} \frac{\partial L}{\partial D_t h} \nabla \alpha \right) + \nabla \cdot \left[\frac{1}{\Sigma} \frac{\partial L}{\partial D_t h} (\nabla \alpha)^T \mathbf{v} \right] \\ & + \frac{1}{\Sigma} \frac{\partial L}{\partial D_t h} (\nabla \mathbf{v})^T \nabla \alpha - \rho \left(\nabla \left[\frac{\partial L}{\partial \rho} \right] \right)^T + \frac{\partial L}{\partial Y} \nabla Y, \quad (40a) \end{aligned}$$

$$\begin{aligned} \mathbf{B} = \frac{\partial L}{\partial \alpha} - \nabla \cdot & \left[\frac{\partial L}{\partial \nabla \alpha} \right] - \partial_t \left(\frac{1}{\Sigma} \frac{\partial L}{\partial D_t h} \right) \\ & - \nabla \cdot \left[\frac{1}{\Sigma} \frac{\partial L}{\partial D_t h} \mathbf{v} \right], \quad (40b) \end{aligned}$$

$$\mathbf{C} = \frac{\partial L}{\partial \Sigma} - \frac{1}{\Sigma} \frac{\partial L}{\partial D_t h} D_t h. \quad (40c)$$

We can conclude that the Least Action Principles applied to the Lagrangian energy defined by (30) yields the following equations of motion

$$\mathbf{A} = 0, \quad \mathbf{B} = 0, \quad \mathbf{C} = 0. \quad (41)$$

Let us further express the equations of motions into a more familiar form. With the definition (30) of L one then has

$$\partial_\rho L = \frac{|\mathbf{v}|^2}{2} - e - \rho \partial_\rho e, \quad \partial_Y L = -\rho \partial_Y e, \quad (42a)$$

$$\partial_{\mathbf{v}} L = \rho \mathbf{v}, \quad \partial_{(D_t h)} L = m D_t h, \quad (42b)$$

$$\partial_\Sigma L = -\frac{\hat{\gamma}}{\Sigma}, \quad \partial_\alpha L = -\rho \partial_\alpha e, \quad (42c)$$

$$\partial_{(\nabla \alpha)} L = \sigma \frac{\nabla \alpha}{\|\nabla \alpha\|}. \quad (42d)$$

We obtain

$$\begin{aligned} \mathbf{A} = \partial_t & (\rho \mathbf{v}) + \nabla \cdot [\rho \mathbf{v} \mathbf{v}^T] + \rho \nabla \mathbf{v} \cdot \mathbf{v} + \partial_t \left(\frac{m}{\Sigma} D_t h \nabla \alpha \right) \\ & + \nabla \cdot \left[\frac{m}{\Sigma} D_t h (\nabla \alpha)^T \mathbf{v} \right] + \frac{m}{\Sigma} D_t h (\nabla \mathbf{v})^T \nabla \alpha \\ & - \rho \nabla [1/2 |\mathbf{v}|^2 - e - \rho \partial_\rho e] - \rho \partial_Y e \nabla Y, \quad (43a) \end{aligned}$$

$$\begin{aligned} \mathbf{B} = \partial_t & \left(\frac{m}{\Sigma} D_t h \right) + \nabla \cdot \left[\frac{m}{\Sigma} D_t h \mathbf{v} \right] \\ & + \rho \partial_\alpha e + \nabla \cdot \left[\sigma \frac{\nabla \alpha}{\|\nabla \alpha\|} \right], \quad (43b) \end{aligned}$$

$$\mathbf{C} = -\frac{\hat{\gamma}}{\Sigma} - \frac{m}{\Sigma} (D_t h)^2. \quad (43c)$$

4 Final form of the system

We define the pressure p of the two-phase medium and the partial pressures p_k of each phase by

$$p = \rho^2 \frac{\partial e}{\partial \rho}, \quad p_k = \rho_k^2 \frac{\partial e}{\partial \rho_k}, \quad (44)$$

where ρ is the mixture density defined as $\rho = \alpha_1\rho_1 + \alpha_2\rho_2$, α_k is the volume fraction of phase $k = 1, 2$, ρ_k the partial density. Then by injecting relations (42a) into (41) one obtains the system

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho \mathbf{v}] = 0, \quad (45a)$$

$$\frac{\partial \rho Y}{\partial t} + \nabla \cdot [\rho Y \mathbf{v}] = 0, \quad (45b)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[(\rho \mathbf{v} \mathbf{v}^T) + \left(p + \frac{\hat{\gamma}}{2} \right) I_d \right] \quad (45c)$$

$$+ \nabla \cdot \left[\sigma \frac{\nabla \alpha \nabla \alpha^T}{\|\nabla \alpha\|} - \frac{1}{2} \sigma \|\nabla \alpha\| I_d + \frac{\hat{\gamma}}{\Sigma} I_d \right] = 0,$$

$$D_t \alpha - \sqrt{-\frac{\hat{\gamma}}{m} \Sigma} = 0, \quad (45d)$$

$$D_t \left(\frac{1}{\Sigma} \right) + \frac{1}{\sqrt{-m\hat{\gamma}}} \left(p_2 - p_1 + \nabla \cdot \left[\sigma \frac{\nabla \alpha}{\|\nabla \alpha\|} \right] \right) = 0. \quad (45e)$$

System (45) is a generalization of the system found in [2, 3] and degenerates towards it when considering the interfacial area density as a function of the volume fraction only. In the momentum equation (45d), the terms function of the volume fraction gradient are common terms found in the literature [8]. Equation (45e) is the transport equation of the fluctuating interfacial density area. In a steady state regime, Equation (45e) yields the classic Poisson equation

$$p_2 - p_1 + \nabla \cdot \left[\sigma \frac{\nabla \alpha}{\|\nabla \alpha\|} \right] = 0 \quad (46)$$

It is important to notice that System (45) is valid for any flow topology as opposed to the system found in [2, 3] only valid for dispersed flow.

Conclusions

In the present work, we presented a definition of a two-phase interface by means of a PDF that departs from the classic geometrical definition. Then we derived two-phase flow model accounting for small and large scale separation of the interface description by means of supplementary convected geometric variables.

The Least Action Principle yields a model that accounts for two-scale kinematics and two-scale surface tension through the introduction of density area fluctuations. This is an extension of previous work that was able to account for a mono-disperse spherical bubbly flow at the small scale [3, 6].

In future works, we will try to encompass new effects of the interface dynamics such as stretching through the evolution of the mean curvature that was assumed constant in the present work.

References

- [1] Sibra, A., Dupays, J., Murrone, A., Laurent, F., and Massot, M., *Simulation of reactive polydisperse sprays strongly coupled to unsteady flows in solid rocket motors: Efficient strategy using Eulerian Multi-Fluid methods*, J. Comput. Phys. 339:210–246, 2017.
- [2] Drui, F., Larat, A., Kokh, S., and Massot, M. “A hierarchy of simple hyperbolic two-fluid models for bubbly flows”. in revision for JFM. 2019.
- [3] Drui, F., *Eulerian modeling and simulations of separated and disperse two-phase flows : development of a unified modeling approach and associated numerical methods for highly parallel computations*, PhD Thesis, 2017.
- [4] Vaudor, G., Ménard, T., Aniszewski, W., Doring, M., and Berlemont, A., *A consistent mass and momentum flux computation method for two phase flows. Application to atomization process*, Computers & Fluids, 152, 2017.
- [5] Herrmann, M., *A sub-grid surface dynamics model for sub-filter surface tension induced interface dynamics*, Computers & Fluids, 87:92–101, 2013.
- [6] Cordesse, P., Kokh, S., Di Battista, R., and Massot, M., *Derivation of a two-phase flow model with two-scale kinematics and surface tension by means of variational calculus*, NASA Technical Memorandum, Summer Program 2018, NASA Ames Research Center, 2018.
- [7] Kapila, A. K., Menikoff, R., Bdzil, J. B., Son, S. F., and Stewart, D. S., *Two-phase modeling of deflagration-to-detonation transition in granular materials: Reduced equations*, Phys. Fluids, 13(10):3002–3024, 2001.
- [8] Blanchard, G., Zuzio, D., and Villedieu, P., *A large scale multi-fluid/dispersed phase approach for spray generation in aeronautical fuel injectors*, proceeding, ICMF, Florence, Italy, 2016.