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Modélisation stochastique d'écoulements diphasiques avec changement de phase

Stochastic modelling of two-phase flows including phase change

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RÉSUMÉ

La modélisation stochastique avec point de vue lagrangien a déjà été développée et appliquée au cadre des écoulements monophasiques et des écoulements diphasiques incompressibles. Cet article propose une extension de ce formalisme aux écoulements diphasiques compressibles avec changement de phase (de type eau-vapeur par exemple). L'accent est mis sur deux aspects essentiels, dont la formulation est nouvelle en modélisation stochastique : un modèle de changement de phase et l'expression d'une contrainte portant sur la conservation du volume. Enfin, à titre d'exemple, des éléments de réflexion sont présentés pour deux modèles bifluides.

ABSTRACT

Stochastic modelling has already been developed and applied for single-phase flows and incompressible two-phase flows. In this article, we propose an extension of this modelling approach to two-phase flows including phase change (e.g. for steam-water flows). Two aspects are emphasised: a stochastic model accounting for phase transition and a modelling constraint which arises from volume conservation. To illustrate the whole approach, some remarks are eventually proposed for two-fluid models.

Abridged English version

Over the last decades, modelling of compressible two-phase flows has been tackled using approaches based on sets of Partial Differential Equations (PDEs), whose unknowns are Eulerian mean fields [1,2]. Therefore, the derivation of constitutive laws, even those describing highly non-linear local phenomena (e.g. the phase change), is directly done using mean fields, which represent a restricted statistical information. These Eulerian models are satisfactory for a certain range of industrial situations. Nonetheless, when the governing phenomena are highly non-linear (e.g. when dealing with cavitation, polydispersed bubbles, nucleate boiling, ...), such approaches can lead to descriptions that are not accurate enough. In these situations, one can benefit of the stochastic modelling approach using a Lagrangian point of view [3,4] (or Lagrangian stochastic modelling). This approach has already been applied to different configurations: incompressible single-phase flows have been widely addressed, see [3] among others for a complete presentation, whereas the effect of compressibility in

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single-phase flows has been less investigated [5]. Modelling of two-phase flows introduces new aspects, some of which have been addressed in [4] for incompressible flows. In the present paper, we propose an extension to compressible two-phase flows. It is worth recalling that the Lagrangian stochastic approach amounts to closing the Probabiliy Density Function (PDF) of the variables chosen to describe the flow, from which classical PDEs for the corresponding mean fields may be obtained.

Flows are described using particles, where each particle represents a sufficient number of molecules so that the classical notions of the continuum mechanics still make sense. Each particle of phase k (with $k = 1, 2$) is associated with a mass m_k, a position in the physical space x_k, a velocity u_k, a volume v_k and an internal energy e_k. This set of variables is one possible minimal set of variables necessary to describe non-uniform transient compressible flows (in the compressible single-phase case depicted in [5], the pressure has been chosen instead of the volume). All other quantities are functions of these five variables: for example pressures $p_k = \mathcal{P}_k(v_k, e_k)$ and the densities $\rho_k = m_k/v_k$. An important point to be put forward is that, since the position in space x_k and the velocity u_k (and thus the trajectory) are variable, we are dealing with a Lagrangian description. The time evolution of the variables is governed by stochastic differential equations, each one involving two modelling terms: one term that describes the evolution of the expectation, and one term defining the behaviour of the dispersion around the expectation. These terms are not detailed in the sequel, except those for the volumes v_k.

Phase change is modelled using two ingredients: a condition to fulfill for each particle to change phase and an instantaneous "transformation" applied to the variables $(m_k, x_k, u_k, v_k, e_k)$ when the transition occurs. The choice for the latter is straightforward: the value of the variables does not change. Despite its simplicity, this choice obviously guarantees conservation of the variables $(m_k, x_k, u_k, v_k, e_k)$ and of the total local number of particles. Phase transition is assumed to be instantaneous. In order to account for the non-zero characteristic time scale τ for the phase change of a set of identical particles, we add a variable $\mathcal{D}$ to each particle. This variable follows an exponential law with a parameter $1/\tau$. It represents the lifetime of the particle before the phase transition. Finally, phase change occurs if and only if it is followed by a decrease of the chemical potential and if the realisation D of $\mathcal{D}$ is less than δt, where the latter stands for the physical time represented by the phase transition (i.e. for example, δt is a time step when considering a numerical scheme).

Once the model has been defined, it is possible to write a Chapmann–Kolmogorov equation (2) which governs the time evolution of the PDF $f^L(t; Z_1^L, Z_2^L)$ of the process in the phase-space, where $Z_k^L = (x_k^*, u_k^*, m_k^*, v_k^*, e_k^*)$ for $k = 1, 2$. This PDF is the basis of the definition of the volumic fraction for the phase k:

$$\alpha_k(t,x) \stackrel{\text{def}}{=} \int v_k^* \delta\big(x - x_k^*\big) f^L\big(t; Z_1^L, Z_2^L\big)\, \mathrm{d}Z_1^L\, \mathrm{d}Z_2^L$$

This Eulerian field represents the fraction of volume per unit of volume occupied by the phase k. In order to ensure the consistency of our model with the physics, the sum of the volumic fractions must always be equal to one. This is related to the so-called volume conservation property. The Chapmann–Kolmogorov equation for f^L leads to PDEs (3) on the expectation of any function of Z_k^L. Using the PDEs (3) for the expectation of the inverse of the densities, two PDEs for α_k may be found. Then, it can be shown that the constraint $\alpha_1(t,x) + \alpha_2(t,x) = 1$ is equivalent to the constraint (5) on the modelling terms A_k^v for the volumes of the particles. When this constraint is fulfilled, it appears that all the PDE systems on the mean fields that can be derived from the stochastic model contain the two equations (6).

It is interesting to focus on the two equations (6) for dispersed spherical bubbles in a liquid. On the one hand, a simplified Rayleigh–Plesset equation (8) for the pulsation of the bubbles can be used to define A_1^v. Then the modelling term A_2^v is chosen according to (5), to ensure the property of volume conservation. The resulting equation for α_1 is close to the equation of the models of [7–10]. On the other hand, a modelling term for the bubble volume that allows to retrieve the standard two-fluid model can be exhibited (12). It is very intricate and its exact physical content remains an open question.

The modelling approach proposed herein suggests some forthcoming works. First, systems of PDEs can be derived from a physical description of compressible two-phase flows, carried out by a Lagrangian stochastic model. In this approach, the physical hypotheses underlying PDE systems appear more clearly. At last, numerical simulations of two-phase flows involving phase transition could be improved by applying hybrid schemes, following the ideas developed in [12,13]. The latter requires to have a stochastic model and a PDE system derived from this model.

1. Introduction

La physique des écoulements diphasiques compressibles est complexe et, à ce jour, certains de ses aspects restent encore mal compris. C'est notamment le cas des échanges de masse, de quantité de mouvement ou d'énergie entre les phases qui constituent des éléments clefs dans la phénoménologie des applications industrielles.

Depuis plusieurs dizaines d'années la modélisation mathématique de tels écoulements repose essentiellement sur des approches basées sur des champs eulériens moyens. Les systèmes d'équations aux dérivées partielles (EDP) associés à ces modèles sont obtenus en appliquant des opérateurs de moyenne sur des « poches de fluide » monophasiques [1,2]. D'un point de vue formel, une fonction indicatrice définit la répartition spatio-temporelle des phases et dans chacune des zones ainsi décrites un système d'EDP monophasique (Euler par exemple en compressible) régit l'évolution instantanée des champs du fluide. Les systèmes d'EDP pour les champs moyens sont ensuite obtenus par application d'un opérateur de moyenne. Finalement, la modélisation des échanges entre les phases est réalisée *a posteriori* sur les champs moyens obtenus.

Les approches basées sur une description particulaire avec modélisation stochastique permettent d'établir les modèles sur les grandeurs instantanées et non sur les champs moyens [3,4]. Ensuite, une fois le modèle instantané établi, il est