International Journal of Multiphase Flow 66 (2014) 62–78

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmulflow

Towards the direct numerical simulation of nucleate boiling flows

S. Le Martelot [a,*], R. Saurel [a,b,c], B. Nkonga [d]

[a] RS2N, Bastidon de la Caou, 13360 Roquevaire, France
[b] University Institute of France, CNRS, IUSTI, 5 rue E. Fermi, 13453 Marseille Cedex 13, France
[c] Aix-Marseille University, CNRS, IUSTI, 5 rue E. Fermi, 13453 Marseille Cedex 13, France
[d] University of Nice, LJAD UMR CNRS 7351, Parc Valrose, 06108 Nice Cedex, France

ARTICLE INFO

Article history:
Received 19 September 2013
Received in revised form 27 June 2014
Accepted 29 June 2014
Available online 17 July 2014

Keywords:
Hyperbolic systems
Multifluid
Multiphase
Phase change
DNS
Preconditioning
HLLC

ABSTRACT

A flow model is built to capture evaporating interfaces separating liquid and vapour. Surface tension, heat conduction, Gibbs free energy relaxation and compressibility effects are considered. The corresponding flow model is hyperbolic, conservative and in agreement with the second law of thermodynamics. Phase transition is considered through Gibbs energy relaxation, in the same mind as in Saurel et al. (2008). Surface tension effects are modelled following the lines of Brackbill et al. (1992). There is thus no need to resolve the interface structure as jump conditions are inherent features of the model formulation. With the present approach, the same set of partial differential equations is solved everywhere, in pure fluids as well as in the captured diffuse interface. There is thus a unique hyperbolic flow solver that handles flow dynamics, interface motion and eventually acoustic wave dynamics. To make distinction between "pure" fluids and liquid–vapour mixture treatment, different sets of algebraic equations are considered in the relaxation solver. To guarantee accurate computation of the liquid and gas dynamics the preconditioned implicit scheme of LeMartelot et al. (2013) is adapted to the present boiling flow model. The model and method are validated against a one-dimensional test problem having exact solution. Multidimensional computations are then shown to illustrate method capabilities.

Introduction

This paper deals with the numerical simulation of boiling flows with a DNS-like approach (Direct Numerical Simulation). This research topic has important applications in nuclear and space engineering, for example, and many other technical and environmental areas. Existing heat and mass exchange correlations (widely used in averaged multiphase flow models and codes) have important limitations. The error bar covers several orders of magnitude. Flow topology changes, from bubbly to separated flows with vapour film at walls, have dramatic consequences on heat exchanges. The main issue relies on the fact that averaged two-phase flow models are unable to account for flow topology changes. Therefore, DNS-like of boiling flows may help for the derivation of sub-scale models. However, this research area is difficult as liquid–gas interfaces are present, in conjunction with heat conduction, phase transition and surface tension effects. Only a few numerical approaches deal with such flows, the most natural being due to Tryggvason et al. (2001) and Juric and Tryggvason (1998), where the interface is considered as a sharp discontinuity, solved with a front tracking algorithm. The other approaches consider the interface as a diffuse zone.

With diffuse interface models, two different kinds of approaches have to be mentioned.

The first one takes essence in chemical–physics with the pioneer work of Cahn and Hilliard (1958), also called in the literature "second gradient theory" and "theory of Korteweg-type fluids". This theory works quite well in the vicinity of the thermodynamic critical point where liquid and vapour density become very close. The fluid density is considered as the order parameter and the fluid internal energy is considered as a function of the density and the density gradient. Considerable efforts have been done in this modelling direction (see Anderson et al. (1998) for example). Examples of computational works in this frame are reported in this last reference and in (Jamet et al., 2001). In addition to the very limited density ratio at interfaces, another limitation appears. Indeed, the interface capillary structure has to be resolved, which results in very fine meshes and associated computational limitations.

The second diffuse interface approach takes essence in discontinuity capturing methods and particularly Godunov contributions. In this frame, discontinuities are captured as a consequence of the conservative formulation of the equations. There is no need

* Corresponding author.
E-mail addresses: sebastien.lemartelot@gmail.com (S. Le Martelot), richard.saurel@univ-amu.fr (R. Saurel), boniface.nkonga@unice.fr (B. Nkonga).

http://dx.doi.org/10.1016/j.ijmultiphaseflow.2014.06.010
0301-9322/

to resolve the internal structure of discontinuities as jump conditions are present in the formulation. This approach has been competing with front tracking methods during the 70s, with artificial viscosity methods during the 80s, and is now used in nearly all computational codes dealing with gas dynamics equations and more generally with hyperbolic systems of conservation laws. The present work belongs to this class of approaches.

The diffuse interface approach based on multiphase descriptions of mixture cells with the help of hyperbolic systems with relaxation is due to (Saurel and Abgrall, 1999). This approach has shown its efficiency for the computation of flows in severe conditions, with arbitrarily high pressure and density ratios, with applications ranging from detonation physics (Petitpas et al., 2009; Saad, 1992; Saurel and Abgrall, 1999; Saurel et al., 2007; Saurel et al., 2008; Saurel et al., 2009; Schoch et al., 2013), shock waves in heterogeneous media, cavitating flows (Petitpas et al., 2009) to solid mechanics (Favrie et al., 2009). The difficulties are related to the models and numerical schemes building, especially when non-conservative equations are present. In this paper, low speed boiling flows are considered through a specific diffuse interfaces formulation.

To deal with interface zones in local mechanical and thermal equilibrium, a reduction of the Kapila et al. (2001) model is done. The model considered in the present paper is a temperature equilibrium version of the model derived in (Saurel et al., 2008). Mechanical and thermal equilibrium reduction is justified as, to model phase change, conductive heat transfer is needed. As a consequence there is no temperature discontinuity (in the frame of DNS like approach) at the interface and a single temperature model is appropriate. To be more precise, Kapila et al. (2001) model involves two temperatures and is well suited for interfaces computations as temperature and entropy discontinuities are present when the interface separates two non-miscible fluids, such as for example liquid water and air. When heat conduction is present, the temperature becomes continuous and a single temperature model is more appropriate. Indeed, the conduction layer has to be solved in the present context of boiling flows, as in flame computations. The temperature equilibrium model involves four partial differential equations only, is hyperbolic and conservative. Gibbs free energy relaxation terms are considered to model phase change. The flow model is in agreement with the second law of thermodynamics. It is reminiscent of the reactive Euler equations, widely used in combustion modelling. The main difference appears in the fact that each phase occupies its own volume, contrarily to gas mixtures, where each gas component occupies the entire volume. This difference has serious consequences regarding the thermodynamic closure. For gas mixtures, the mixture equation of state derives from the Dalton law. Here, it is derived from the mixture energy definition and temperature and pressure equilibrium conditions.

From the basic temperature equilibrium flow model with four partial differential equations, extra physics is added to deal with boiling flows. Surface tension effects are modelled with Brackbill et al. (1992) method, already considered in the context of compressible fluids (Perigaud and Saurel, 2005). Heat conduction and gravity effects are also added.

The second issue addressed in the paper is related to the numerical approximation of the flow model, especially hyperbolic and elliptic parts, capillary terms and thermochemical relaxation.

The hyperbolic step is solved with a variant of the preconditioned implicit hyperbolic solver detailed in (LeMartelot et al., 2013). It is an extension of Guillard and Viozat (1999) method for low Mach number flows, this method being itself a conservative and time accurate extension of Turkel (1987) preconditioning algorithm.

The relaxation solver used to fulfil interface conditions of evaporating interfaces is detailed with particular attention paid to the single phase limit. The hyperbolic and relaxation solvers are then combined to solve the flow model in 1D, obviously in absence of capillary effects, to check model and method convergence against an exact solution of sharp evaporating interface. Convergence being reached in 1D, computational boiling flows examples are shown in 2D with the various needed physical effects. A 2D configuration with several bubbles is considered and computed. From this first computation, a new physical feature appears, never reported before in the authors knowledge. Starting from an initial situation where some nucleation sites are present, bubbles appear dynamically from the sites location, but also from other locations where perfect wall conditions are used. The bubbles appearance and size selection thus appear as a self sustained process independent of nucleation sites. Dynamic interfaces appearance was a feature already observed in the context of cavitating flows, using the temperature non-equilibrium model shown in section 'Out of equilibrium model'.

Model building

The starting point of the analysis relies on the mechanical equilibrium, temperatures non-equilibrium flow model of Kapila et al. (2001), where heat and mass exchanges have been inserted (Saurel et al., 2008).

Out of equilibrium model

The model given in the last reference reads:

$$\frac{\partial \alpha_1}{\partial t} + \mathbf{u} \bullet \mathbf{grad}(\alpha_1) = \frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}} \mathrm{div}(\mathbf{u}) + \rho v (g_2 - g_1) \frac{\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}} + \frac{\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}} H(T_2 - T_1),$$

$$\begin{aligned}
&\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \mathbf{u}) = \rho v (g_2 - g_1), \\
&\frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \mathbf{u}) = -\rho v (g_2 - g_1), \\
&\frac{\partial \rho \mathbf{u}}{\partial t} + \mathrm{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + P \underline{I}\right) = 0, \\
&\frac{\partial \rho E}{\partial t} + \mathrm{div}((\rho E + P)\mathbf{u}) = 0.
\end{aligned} \tag{1}$$

The total energy is defined as $E = Y_1 e_1 + Y_2 e_2 + \frac{1}{2}\mathbf{u} \bullet \mathbf{u}$ where $Y_k = \frac{\alpha_k \rho_k}{\rho}$ represent the mass fractions and $\rho = \sum_k (\alpha_k \rho_k)$ the mixture density. This model is hyperbolic with the same wave speeds as the gas dynamics equations but with Wood (1930) sound speed, c_w, which presents a non monotonic behaviour with respect to the volume fractions (α_k),

$$\frac{1}{\rho c_w^2} = \sum_k \frac{\alpha_k}{\rho_k c_k^2}, \tag{2}$$

where c_k represents the sound speed associated to phase k.

It is worth to mention that the sound speed is always defined, provided that each phase has a convex equation of state. This feature is not satisfied by mixture flow based on cubic equations of state, like the Van der Waals one. The present equation of state providing the thermodynamic closure is obtained from the mixture energy definition and the pressure equilibrium condition. This equation of states involves at least three argument: $P = P(\rho, e, \alpha_1)$. For example, when each phase obeys the stiffened gas equation of state (see Le Métayer et al. (2004) for parameters determination),

$$p_k = (\gamma_k - 1)\rho_k (e_k - q_k) - \gamma_k P_{\infty,k}, \tag{3}$$