Modeling droplet phase change in the presence of a multi-component gas mixture

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A B S T R A C T

Dispersed liquid droplet flows with evaporation and condensation in multi-component gas mixture made of vapor and other gas phase chemical species such as air occur in many engineering applications dealing with two-phase flows. However, existing models are essentially derived for vaporization occurring in sprays combustion. It means that the energy is transferred from a hot gas to the liquid to produce its phase change. This is thus a non-symmetric approach as in some situations the energy is already stored in the liquid phase and flashing occurs as a consequence of pressure drop.

   In the present paper a droplet mass transfer model is derived and is valid in any situation: evaporation, flashing and condensation. It accounts for:

- coupled heat and mass diffusion in the gas phase,
- thermodynamics of the multi-component gas mixture,
- heat diffusion inside the liquid droplet, enabling consideration of both droplet heating and cooling. These effects are important in evaporating and flashing situations respectively.

   The resulting model consists in an algebraic non-linear system of three equations giving the interface temperature, the mass flow rate and vapor species concentration at the interface. These interfacial variables enable computation of the mass species, momentum and energy transfer rates appearing in volume averaged two-phase flow models.

   Computational examples are shown with this mass transfer model embedded in a compressible two-phase flow model of Baer and Nunziato (1986) type.

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1. Introduction

Dispersed droplet flows with phase change appear in many fundamental and applied science situations such as for example combustion in automotive and spacecraft engines, cryogenic combustion and atmospheric liquid dispersion to cite a few. In most situations phase change occurs between liquid drops and corresponding vapor mixed with other gas phase chemical species, such as for example air. In such instances, phase change involves both heat diffusion in the liquid and gas phases as well as mass diffusion of the chemical species in the gas phase.

Main difficulties related to such modeling are related to multidimensional effects that have to be summarized by ODEs and algebraic systems, i.e. in 0D. Many efforts have been carried out in this direction, mainly in the frame of two-phase spray combustion (see [19,20,10,2,1,18], and references therein). In the last reference arrays of droplets were considered while in former ones isolated droplets only were studied.

The present work considers the behavior of a single droplet, cumulative effects to the mean flow being accounted for through the specific interfacial area of the droplets cloud, under the assumption of absence of interaction between drops. Moreover, the liquid phase is described with a single size of drops, space and time varying.

The present contribution follows the lines of Abramzon and Sirignano [2] (AS89) in the sense that:

- Gas phase boundary layer effects around the droplet are considered through Nusselt and Sherwood numbers correlations. This method enables computation of heat and mass diffusion fluxes through the gas to the interface without spatial resolution of the surrounding gas. Also, this approach considers velocity slip between the liquid and gas phases as Sherwood and Nusselt numbers correlations account for it through the particle Reynolds number.
- Local thermodynamic equilibrium is considered at the interface.
- Droplet heating is considered through a heat exchange coefficient between the liquid–gas interface and the droplet core. In AS89 two-dimensional flow internal to the droplet was considered to this respect.

However, the AS89 model was derived in the aim of spray combustion modeling. In such a situation phase change occurs as a result of heat exchange from the (hot) gas to the (initially cold) droplet. The internal heat exchange to the droplet is needed to compute:

- droplet heating before reaching the saturation temperature,
- heat losses from the interface to the cold droplet core that lower the mass transfer rate through the interface energy balance.

In AS89 the energy exchange internal to the droplet is thus a corrective term to the main heat flux that comes from the gas to the interface.

In situations different to spray combustion the mass transfer rate may be a result of the energy already stored in the liquid droplet. Such situations occur for instance when the surrounding gas is suddenly depressurized, as for example in nozzle flows or in the whole sequence of spherical explosions. In these situations the liquid core temperature is higher than the saturation temperature at local pressure. Consequently droplet flashing occurs as a limit case.

In the present work a phase transition model valid in any situation is built as a generalization and non-linear extension of the AS89 model. Both liquid and gas diffusion effects are considered without giving priority to the gas transfer heat exchange to the interface. In this sense, the model becomes symmetric and as a consequence, highly non-linear.

Rather than having weakly coupled relations for the mass and heat transfers terms such as in the AS89 model a fully coupled non-linear system of three algebraic equations is obtained. This is the first main difference. These algebraic equations are clearly established from local jump conditions of mass and energy at the interface, the closure being realized by the assumption of local thermodynamic equilibrium at the interface.

A second important difference is made for the computation of the liquid heat transfer flux. In AS89 multi-D motion inside the droplet was considered through a reduction method to compute the interfacial heat flux. In the present work, the temperature inside the drop is assumed to obey a specific profile, corresponding to a boundary layer near the interface and a core zone at uniform temperature. The boundary layer thickness is determined from the assumed temperature profile and knowledge of the liquid average temperature. The average liquid temperature is a direct consequence of the two-phase average flow model resolution.

With this method, no parameter is present. Moreover:

- The interfacial heat flux is in perfect agreement with the direct resolution of the heat equation inside the drop at any time.
- The only constraint used is energy conservation through the explicit use of the average liquid temperature.

Therefore, whatever the flow complexity is inside the drop, the present approach provides accurate interfacial heat flux provided that a core zone with uniform temperature is present and connected to the interface through a boundary layer profile. No internal mesh to the liquid droplet is used.

The mass transfer model thus consists in a set of three non-linear algebraic equations. There is no parameter in the model except physical properties of fluids in presence. The solution of this system is reached numerically in each computational cell and at each time step of the two-phase average equations resolution. It results in the computation of the mass flow rate from liquid to gas, positive in evaporation conditions and negative in condensation. It also provides mass, momentum and energy transfer terms to embed in volume average two-phase flow models.

The paper is organized as follows. The two-phase flow model under examination, with heat and mass transfers added as source terms is presented in Section 2. The conventional closure relations of this model are addressed in Section 3. The local and symmetric heat and mass transfer model for a single liquid droplet is built as follows: mass and energy interface conditions are addressed in Section 4 while the local thermodynamic equilibrium interface condition is derived in Section 5. The