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Towards a unified treatment of fully flashing sprays

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ABSTRACT

This paper presents a systematic study on flashing atomisation, which includes both standards and retrograde fluids. A novel data reduction method is proposed in terms of the controlling parameters for (bubble) nucleation. The analysis indicates that bubble nucleation is the rate-controlling process for both the transition to fully flashing and for the spray lateral spreading. Specifically, the onset condition coincides with the surmount of the energy barrier to nucleation. The spray lateral spreading, instead, is directly linked to the population of bubble clusters: the larger the population the wider the spray angle. Theoretical aspects of bubble nucleation theory are also reviewed. An interesting conclusion of the analysis is that the experimental trends observed in fully flashing jets are compliant with recent advances in nucleation theory. At very high initial superheat, a complex shock wave structure appears around the flashing jets. The novel aspect of this work is that such shock-systems are observed consistently in both standard and retrograde substances. This similarity indirectly confirms that, far from the critical temperature, the phase transition mechanism is the same for all substances, independently from their degree of retrogradicity.

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1. Introduction

Flash-atomisation occurs when a liquid is discharged into a gaseous environment at an ambient pressure lower than the saturation pressure of the fuel. Although flash-boiling is considered to be detrimental in many technical applications (e.g. the accidental release of flammable and toxic pressure-liquefied gases in the nuclear and chemical industry), it can have some potential benefits in propulsion systems. In fact, it is known to produce a fine spray with enhanced atomisation, to increase the effective spray angle and to decrease the spray penetration. These significant changes in the spray characteristics have an important impact on the fuel oxidant mixing and hence on the combustion efficiency, leading to reduced pollutants' emissions (Senda et al., 2007). From a heuristic point of view, the process of flash-atomisation and vaporisation is clearly described as the subsequent progression of homogeneous (or heterogeneous) nucleation, bubble growth (Brown and York, 1962), breakup through bubble disruption, and (superheated) droplet evaporation. Due to its relevance for automotive, aerospace and industrial applications, considerable progress has been made in the modelling (e.g., Kawano et al., 2006; Schmehl and Steelant, 2009) and experimental (e.g., Vieira and

Simoes-Moreira, 2007; Desnous et al., 2011) investigation of a flash-atomising liquid spray. In general, the quality of a flashing spray is evaluated in terms of empirical correlations for droplet sizes, velocity distributions, jet spreading angle, and penetration lengths. The reader is referred to the works of Witlox et al. (2005), Cleary et al. (2007), and Yildiz et al. (2004, 2006) for studies at atmospheric conditions and to Lecourt et al. (2009) for near vacuum conditions, just to cite a few. The above mentioned studies had the merit to provide significant insights into the physics of superheated atomisation. Still, this improved understanding could not be conveyed towards the development of a predictive tool for engineering applications, mainly due to the following factors:

- Most experimental data are collected in the dilute region of the spray, where the superheated liquid has almost relaxed towards thermodynamic equilibrium. Hence they can provide only limited information on the mechanism of flash-atomisation.
- The range of applicability of the proposed correlations is rather limited, being restricted to the particular fluids (namely water and ethanol) and operating conditions tested. Cleary et al. (2007) tried to extrapolate these empirical models to other fluids through similarity scaling laws, expressed in terms of non-dimensional numbers. Despite the noteworthy attempt, considerable research is still required to corroborate the proposed extrapolation technique.

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This concise summary on the state-of-the art of superheated atomisation modelling shows that, in order to predict these phenomena and create a proper engineering tool, two conditions have to be satisfied. First of all, experimental data need to be acquired in the near-nozzle region (i.e. at axial distances $x/D = O(1)$, where D is the nozzle diameter). The availability of these data would enable to assess the effect of superheat on the atomisation process and eventually to formulate these dependencies into a theoretical model for flash-atomisation. Second, in order to properly analyse the data, the data-reduction procedure should establish a direct link with the theory of bubble nucleation and/or of superheated evaporation. Note that, to-date, a direct connection between the purely fluid mechanical process of atomisation and the kinetics of phase transition (nucleation rate) has only been postulated (e.g., [Kurschat et al., 1992](#)), but never verified against experimental data. Furthermore, a different phase change mechanism was proposed for retrograde fluids (e.g., [Vieira and Simoes-Moreira, 2007](#)).

In light of these considerations, the present study aims at providing a comprehensive and accurate experimental database on superheated atomisation for model validation purposes. The database includes data on spray morphology as well as on droplet size, velocity and temperature distributions. As a first step towards the development of a superheated atomisation model, the transition threshold and the spray contour data (i.e. the spreading angle versus axial distance) are correlated as function of the controlling parameters for nucleation. The analysis is extended to both standard and retrograde fluids to find out whether a common phenomenology can be identified in all cases. If feasible, literature data are also included to assure the generality of the conclusions.

The outline of the paper is as follows. Section 2 reviews briefly the most relevant non-dimensional parameters governing flash atomisation and bubble nucleation processes. Section 3 discusses the different flash atomisation regimes and briefly outlines the available theoretical models and/or empirical correlations. The objective is to identify the range of disintegration modes, whose onset and lateral spreading might be solely controlled by thermodynamic parameters. Section 4 describes the test facility and post-processing algorithm. Finally, Section 5 discusses the modelling strategy, the experimental results and the plausibility of the proposed model.

2. Nucleate boiling

As mentioned in Section 1, atomisation in superheated fluids occurs mostly through nucleate boiling. The superheat level can be described through two parameters, displayed in [Fig. 1](#). The first parameter (ΔT – alias the degree of superheat) is defined as the difference between the fuel injection temperature and the saturation temperature at the assigned back pressure:

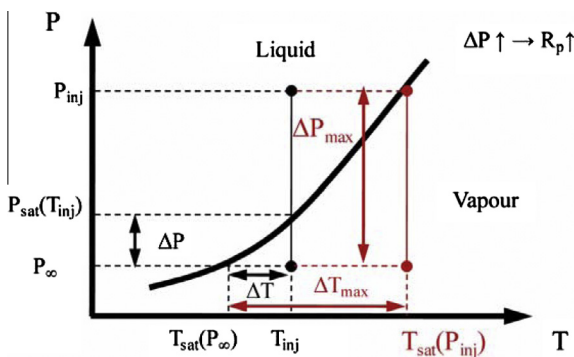


Fig. 1. Flashing parameters.

$$\Delta T = T_{inj} - T_{sat}(p_{\infty}) \quad (1)$$

The second parameter R_p is defined as the ratio between the saturation pressure at the fuel injection temperature and the prescribed back pressure:

$$R_p = \frac{p_{sat}(T_{inj})}{p_{\infty}} \quad (2)$$

Denoting with k_b the Boltzmann constant, the thermodynamic relation

$$\Delta \mu = k_b T \ln(R_p) \quad (3)$$

shows that R_p is directly related to the difference in chemical potential, which represents the “generalised driving force” for the phase transition process. Hence, R_p (rather than ΔT as customarily suggested) is the most adequate choice to measure the degree of departure from thermodynamic equilibrium in a superheated liquid. In the realm of Classical Nucleation Theory (CNT), the number of stable vapor nuclei generated per unit volume and time J is proportional to

$$J_{CNT} \propto \sqrt{\frac{2\sigma}{\pi m}} \exp\left(-\frac{\Delta G^*}{k_b T_{inj}}\right) \quad (4)$$

where m is the mass of a liquid molecule and ΔG^* represents the formation energy of the critical cluster

$$\frac{\Delta G^*}{k_b T_{inj}} = \frac{16\pi\sigma^3}{3(\Delta\mu)^2} \quad (5)$$

Following [Girshick and Chiu \(1990\)](#), let us introduce a dimensionless surface tension Θ :

$$\Theta = \frac{a_0\sigma}{k_b T_{inj}} \quad (6)$$

where a_0 is the surface area, defined as $a_0 = (36\pi)^{1/3}(v_m)^{2/3}$. The volume of a molecule v_m can be rewritten in terms of macroscopic quantities as $v_m = M/(\rho_l N_A)$ with ρ_l denoting the liquid density, M the molar mass and N_A the Avogadro constant. The parameter Θ measures the relative importance between surface energy (i.e. the energy required for the creation of a new interface) and thermal energy. Combining Eqs. (3)–(6), the nucleation rate can be expressed as:

$$J_{CNT} \propto \sqrt{\frac{2\sigma}{\pi m}} \exp\left[-\frac{4}{27} \frac{\Theta^3}{(\ln R_p)^2}\right] \quad (7)$$

Note that Eq. (7) represents simply the non-linearised version of CNT. The linear version – where the pressure difference ($p_{sat}(T_{inj}) - p_{\infty}$) appears instead of $\ln(R_p)$ (e.g., [Blander and Katz, 1975](#)) – is no longer applicable at highly superheated conditions (i.e. at large R_p values). Therefore, throughout this paper, Eq. (7) will be used for the analysis and data reduction procedures of the experimental data.

The classical nucleation theory has been widely criticised for being an equilibrium theory and for modelling the critical bubble nucleus by macroscopic thermodynamics and its surface by the planar surface tension (e.g., [Oxtoby and Evans, 1988](#); [Oxtoby, 1998](#)). Specifically for nucleate boiling applications, CNT was also criticised for predicting a finite energy barrier at the spinodal and for failing to predict the superheat of boiling at relatively low temperatures ([Briggs, 1951](#)). Several modifications of CNT have been proposed to take into account the effect of dissolved gas ([Tucker and Ward, 1975](#); [Lubetkin and Blackwell, 1988](#)), to correct for the erroneous temperature dependence of CNT through scaling laws ([McGraw, 2000](#)) and to improve the accuracy of the predicted nucleation rates ([Delale et al., 2003](#)). It is beyond the purpose of this paper to assess the accuracy of bubble nucleation

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