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Vaporization process of liquid ammonia injection: Droplet modelling and experimental data

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Introduction

Direct injection is frequently employed in the combustion applications as internal combustion engine and gas turbine. Liquid injection aims to inject the fuel directly inside the combustion chamber and to vaporize it as fast as possible but also due to the heat of vaporization to cool down the ambient temperature to enhance the charge and the thermal NOx emissions. The fuel spray is first broken up into small droplets to increase the surface between liquid and air. Then, the vaporization of droplets is greatly significant for the spatial distribution of fuel vapor/air, the ignition, and the combustion itself. However, the use of new carbon-free fuels such as ammonia with completely different thermodynamics properties needs fundamental studies to improve the knowledge and its application itself.

Pelé et al. [1] explored the sprays of liquid ammonia with a current Bosch GDI injector. The geometry of the ammonia sprays for different conditions of air densities and temperatures was compared to the sprays of classic fuels such as gasoline and ethanol. The impact of the flash boiling ($P_{saturation}(T_{fuel}) > P_{ambient}$) was investigated on the spray morphology. Some numerical studies [2,3] have reproduced the ammonia sprays and found a good agreement on the spray morphologies between numerical and experimental results. However, local features and atomisation levels require further theoretical development for calibration-free models. Zhang et al. [4] have shown that no obvious differences in terms of spray macroscopic and microscopic properties between the results from the normal evaporation model and the flash boiling model used. The vaporization process is a complex phenomenon, especially in the case of flash boiling. Back to a simplified configuration as one unique droplet model allow us to better understand the physical basis of the vaporization process of ammonia with or without flash boiling. The model of droplet vaporization developed in this work is compared to experimental data obtained in a single-hole injector.

Materials and Methods

Droplet Vaporization

To understand the vaporization of ammonia, an example of the process is represented in the state diagram, Figure 1. Classic vaporization operates in the stable liquid phase. The liquid-vapor equilibrium is assumed around the droplet. The evaporation model used from [5] results from the Navier-Stokes equation :

$$\dot{m} = -2\pi D r_d \rho_{air} ln(1 + BM) Sh \#(Eq.1)$$

where $\dot{m}$, D, r_d, ρ_{air}, BM and Sh represent respectively the mass flow rate, the diffusion coefficient, the droplet radius, air density, the Spalding mass transfer number, and the Sherwood number. The calculation of the BM is determined from the mole fraction assumed as the ratio of saturation pressure over the ambient pressure. This ratio is logically between 0 and 1 supposing that the saturation pressure is lower than the ambient pressure, a condition of stable liquid phase. The classic vaporization corresponds to process 2→3.

However, in the case of flash boiling, the liquid is metastable, and the current mole fraction calculation with the saturation pressure is not accurate because the saturation pressure is higher than the ambient pressure (mole fraction higher than 1). However, it can be assumed that only fuel vapor surrounds the droplet and consequently, the vapor mass fraction of the fuel is equal to 1. Nevertheless, this consideration makes resolution unfeasible because the Spalding number BM goes to infinity.

To solve this problem, the following model from [6] studying the evaporation of aqueous ammonia droplets is employed. Cai et al. [7] introduced a corrective factor, φ to take the mass diffusion in the droplet into account in the model:

$$\dot{m} = -2\pi D r_d M \left(\frac{x^V P_{sat}(T_d)}{R T_d} - \frac{x^\infty P_{amb}}{R T_{amb}} \right) Sh\varphi \#(Eq.2)$$

P_{sat} is estimated by the Peng-Robinson equation and x^V, x^∞ are the mole fractions in the vapor phase and far away from the droplet, respectively (in this study: $x^V = 1$ (for flashing pure fuel) and $x^\infty = 0$), T_d is the droplet temperature. This equation makes the consideration of vapor-liquid equilibrium like; the global condition of the droplet is the ambient pressure (point 1 in Figure 1), but locally a thin layer of saturated fuel is considered at the saturation pressure (higher than the ambient pressure) to make the liquid-vapor equilibrium (Point 1'). During the vaporization in flash boiling condition, from 1'→2, the

state of the liquid follows the saturation curve. When the saturation pressure drops to the ambient pressure (Point 2), the classic model can be reused.

To obtain the droplet temperature, the heat transfer is considered as followed:

$$mC_p \frac{dT_d}{dt} = h4\pi {r_d}^2 (T_{amb} - T_d) + \Delta H^{Vap} \dot{m} \#(Eq.3)$$

Where m the droplet mass, C_p the heat capacity of the droplet, h the heat transfer coefficient and ΔH^{Vap} the latent heat. The initial conditions of the droplet are the experimental conditions of ambient pressure and fuel temperature for a r_d of 5µm. This radius corresponds to the measurement of some droplet size distribution as obtained in [2,3] for a multi-hole injector with ammonia at similar conditions of pressure and temperature. The primary analysis has shown that the initial droplet radius does not impact the final temperature but only the vaporization duration. The modelled temperature of vaporization is considered the equilibrium temperature when the stationary regime is reached.

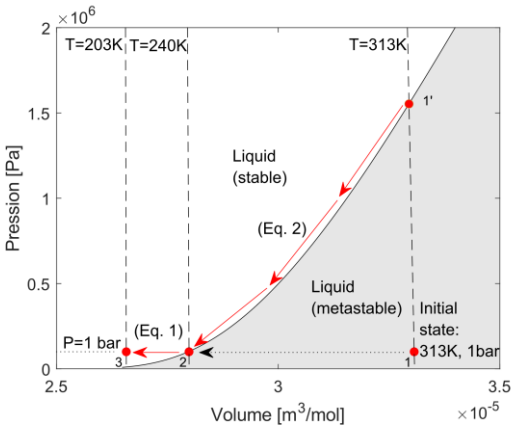

Figure 1. Example of the vaporization process of an ammonia droplet represented with the state diagram

Experimental conditions

Liquid ammonia is injected through a single-hole injector, Spray M ECN injector, in a closed vessel. The cooling effect in the chamber caused by the flash boiling process and the vaporization is measured by using a 25 µm thermocouples type K near the spray. When the ammonia is injected, the temperature measured drops and reaches a minimal value. This minimum temperature is considered the temperature of the vaporization of the spray. Liquid ammonia is pressurized at 70 bar in a tank by means of pressurized helium. The fuel temperature is maintained using a temperature control system connected to a liquid jacket surrounding the injector. To investigate the liquid ammonia spray in a broad range of flash boiling conditions, different combinations of ambient pressure (1 bar to 15 bar) and fuel temperature (-10°C and 50°C) were considered, providing the R_p (P_{sat}(Tf)/ P_{amb}) range from 0.59 to 15.4.

Results and Discussions

Figure 2 shows the comparison between the evolution of the spray temperature obtained experimentally with thermocouples and that obtained numerically. Figure 2.a and Figure 2.b represent, respectively, the evolution of the spray temperature versus the superheat degree R_p and versus the ambient pressure. These results show a very good agreement between the experimental measurements and the numerical model. Figure 2.a shows experimentally a non-monotonic evolution of the spray temperature as a function of R_p and the data from the simple model predict the same trend. Figure 2.b indicated also that the minimum spray temperature increases with the increase of P_{amb}. From these results, it can be observed that for the condition P_{amb} = 1 bar, the change of fuel temperature from -10°C to 40°C does not have a sensitive impact on the drop of temperature. Consequently, the spray temperature depends mainly on the ambient pressure while the influence of the fuel temperature is negligible. These results show that the use of simple equilibrium evaporation model is viable to model the spray under non-flashing and even under flash boiling conditions and that the experimental measurement method using thermocouples is relevant. More conditions will be carried out in future work especially to characterize the droplet diameter.

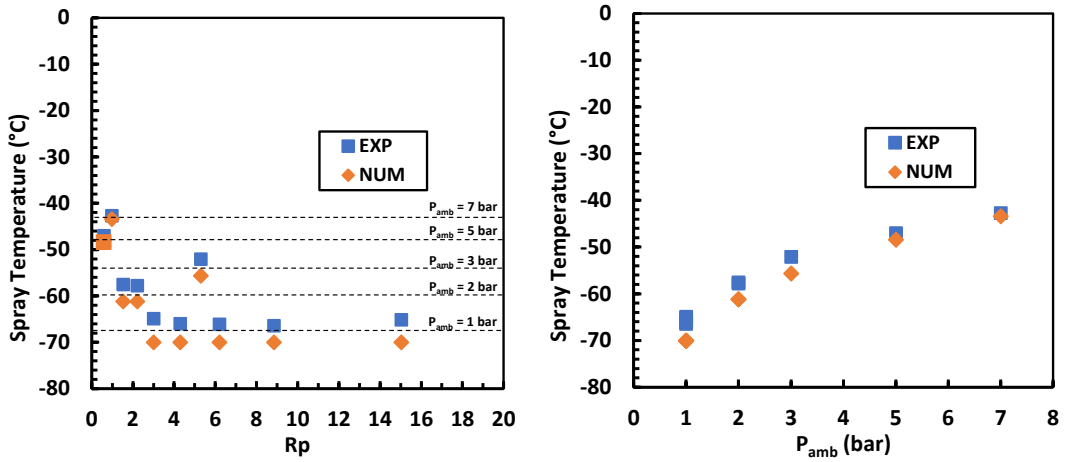

Figure 2. Evolution of spray temperature (a) versus the superheat degree and (b) versus the ambient pressure.

Conclusions

The cooling effect due to the significant vaporization of latent heat was successfully obtained via thermocouple measurements and compared with a numerical simulation based on an equilibrium evaporation model for one droplet. The additional equation for the flash boiling condition allows us to solve the model while the first model only tends to infinity. The results show a very good agreement and highlight the use of both models is viable to model the spray under flash boiling and non-flashing conditions and that the experimental measurement method using thermocouples is relevant. From the results, a more in-depth analysis of these results, using experimental data and numerical simulation results, will be carried out in future work.

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