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2nd Symposium on Ammonia Energy

ASSESSMENT OF BREAKUP MODELLING FOR LAGRANGIAN SIMULATION OF AMMONIA SPRAY IN FLASH BOILING CONDITION

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Introduction

With the aim of expanding the knowledge on liquid ammonia sprays, this work investigates the injection process of ammonia through Computational Fluid Dynamics (CFD) using the Lagrangian particle method, within the Reynolds Averaged Navier Stokes (RANS) approach for turbulence modelling. Pelé et al. [1] characterized the spray morphology, penetrations and sizing in different conditions using a GDI injector, and these data are used as reference for the comparison. Numerical results and experimental data are compared in terms of liquid and vapor tip penetration, local values of Sauter Mean Diameter (SMD) and global spray morphology. In order to explore also the flash boiling phenomenon, results of CFD simulations of ammonia spray and the comparison with experimental data are presented for different conditions, ranging from non-flashing regimes to flash boiling conditions. A preliminary CFD study has been carried out in two conditions [2], in order to compare evaporating and flashing conditions. The breakup model constants need to be tuned for each regime, and in this work, a correlation for Rayleigh-Taylor (RT) model parameters is proposed. In parallel, a flash boiling model for Lagrangian sprays has been developed to eliminate the need for breakup model calibration. This study highlights that capturing spray local SMD values across all the regimes is still challenging, especially with a new fuel such as ammonia, whose properties differ by a large amount from more established values for hydrocarbons.

Materials and Methods

Experimental set-up

Experimental imaging data have been presented and discussed extensively in [1], and only a brief description of the available data is reported here, for the sake of comprehensiveness. A 2.5 l constant volume chamber is used for experimental measurements where the back-pressure can be increased up to 30 bar (by an air compressor) and the ambient temperature warmed-up up to 473 K (by wall heating resistances). The ammonia is pressurized up to 120 bar, by means of pressurized Helium. The injector is a current Bosch gasoline direct injector comprised of 7 holes of 150 μm diameter. The temperature and injection duration were controlled. The Schlieren technique was setup to follow the liquid and vapor spray development. Post-processing of 100 raw images was performed. The high sensitivity to refractive index gradients makes it possible to identify the limit of the line of sight between the vaporized fuel and the ambient gases [3]. The sensitivity is a function of the light intensity and is adjustable by a diaphragm in front of the camera; a small diaphragm opening increases the sensitivity. In addition, droplet size measurement with a Malvern Spraytech droplet size analyser was done at different locations in the spray: in the central point, and on the spray boundary close and far from the injector nozzle as indicated in Fig. 1.

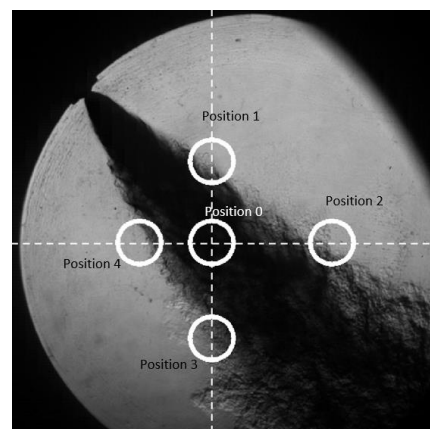


Fig. 1. Example of the position of the measurement of the droplet size distribution for ammonia spray.

Numerical set-up

A numerical model has been built with the CONVERGE v3.0 CFD code, for transient analyses using the U-RANS approach and the standard $k-\epsilon$ turbulence model. Numerical schemes accuracy is second-order in space and first-order in time. Mesh resolution is controlled by a combination of prescribed refinements, to maximize computational efficiency, with a minimum mesh size of 0.25 mm around the injector nozzle. Ammonia spray is modeled with the Lagrangian particle approach [4], with blob model for the injection, and Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) models for breakup. In addition, appropriate sub-models for droplet turbulence dispersion, collision and phase change are included. Particular attention is paid to the phenomenon of flash boiling, easily experienced with ammonia at relatively low ambient pressures, adopting the model by Price et al. [5].

Results and Discussions

Here a comparison of experimental and numerical results is presented, with chamber pressure varying from 2 bar to 15 bar, and air temperature and fuel temperature at 293 K. Global spray parameters such as liquid and vapor tip penetration and spray morphology are relatively easy to reproduce, and here are not reported for the sake of conciseness. On the contrary, local features and atomization levels require more attention since flash boiling and evaporating regimes are very different. The Sauter mean diameter comparison is shown in Fig. 2, with experimental results reported in blue and CFD results in red. The D32 experimental data are useful to calibrate and optimize the model, and this is confirmed by the good agreement between numerical and experimental results.

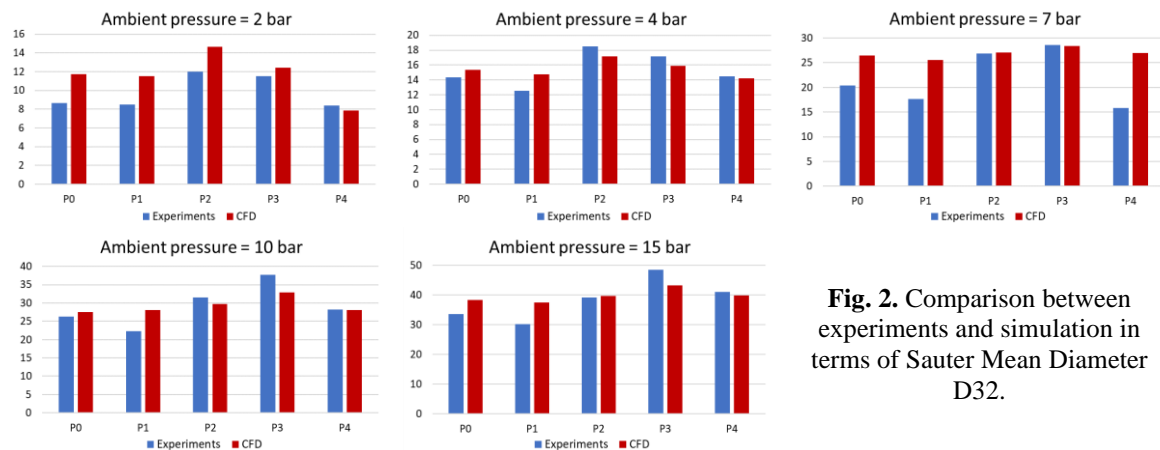


Fig. 2. Comparison between experiments and simulation in terms of Sauter Mean Diameter D32.

KH breakup model parameters are kept constant (KH time constant = 17.5 and KH size constant = 1.75) from a preliminary calibration carried out in evaporating conditions. Then it was necessary to adapt the coefficients of the RT breakup model moving from the evaporating regime to the flashing one. In particular, a correlation for RT time and size constants has been developed, as shown in Fig.2. The RT time constant correlation shows an increasing linear trend as the ambient pressure increases. The RT size constant correlation indicates two linear trends whose slope changes in the vicinity of ammonia vapor pressure at 293 K (8.57 bar).

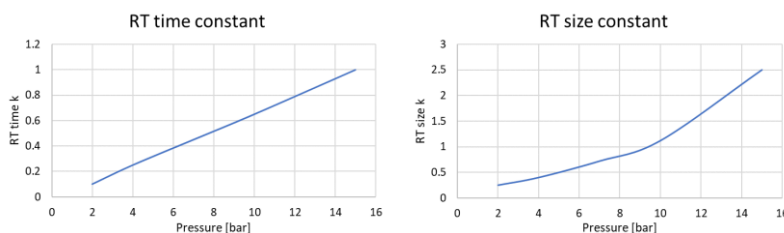


Fig. 3. Correlations for RT time and size constant as a function of ambient pressure.

Conclusions

In this work, CFD results of ammonia spray simulations and their comparison with experimental data are presented, in order to compare flash boiling and evaporating regimes. Global spray parameters such as liquid and vapor tip penetration and spray morphology are relatively easy to reproduce, while local features and atomization levels will require further theoretical development for calibration-free models. Capturing spray local details (such as SMD) across all the regimes is still challenging, especially with a new fuel such as ammonia. Thanks to the correlation proposed for the RT breakup constants as a function of the ambient pressure, CFD simulations can faithfully reproduce the ammonia atomization process both in evaporative and in flash boiling conditions.

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