3D-CFD Simulation of a GDI Injector Under Standard and Flashing Conditions

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Abstract. In the optimization of GDI engines, fuel injection plays a crucial role since it can affect the combustion process and, thus, fuel efficiency and pollutant emissions. The challenging task is to obtain the required fuel distribution and atomization inside the combustion chamber over a wide range of engine operating conditions. To achieve such goals, flash-boiling can be exploited. Flash-boiling is a phenomenon occurring when fuel temperature exceeds saturation temperature or, similarly, when ambient pressure is lower than saturation one. Under these conditions, which can occur inside the injector or directly in the combustion chamber, the fuel undergoes extremely accelerated breakup and quickly evaporates. The proposed manuscript shows the application of an alternative flashboiling model, recently implemented by Siemens-PLM in STAR-CD V.2019.1, to be applied in 3D-CFD Lagrangian simulations of GDI sprays. Results are validated against experimental data, provided by the SprayLAB of the University of Perugia, on a single-hole research injector. The new flash-boiling model consists of three main parts: an atomization model able to compute droplet initial conditions and the overall spray cone angle; an evaporation model and, finally, a droplet break-up model; the last two models are designed to simulate all the physical events occurring when droplets are injected into the combustion chamber. As for the investigated operating condition, vessel pressure and temperature are 40 kPa and 293K, respectively; as for the fuel (n-Heptane) temperature, it ranges from 303.15 K to 393.15 K, on equal injection pressure (10 MPa). The numericalexperimental comparison is carried out in terms of liquid penetration, imaging, and droplet sizing.

1 INTRODUCTION

In the last decade, besides the increasing level of hybridization [1], many efforts have been dedicated to increase the efficiency of the internal combustion engine while decreasing tailpipe emissions. As for spark ignition engines, the reduction of the specific fuel consumption is mainly limited by abnormal combustion onset. Therefore, attention of engine manufacturers is primarily focused on knock mitigation by means of several techniques such as improved cooling [2], adoption of a variable compression ratio [3], bore reduction [4], use of cooled EGR [5] and water (or water/methanol) injection [6-9], unconventional valve strategies [10] and, finally, Gasoline Direct Injection (GDI) systems [11]. In this panorama, a crucial role is played by CFD analyses which allow to reduce time- and cost-to-market thanks to a proper prediction of the knock onset. Simulations are based, on the one hand, on reliable knock models [12-16] and, on the other hand, on a robust numerical framework able to fairly reproduce flow field, cycle-to-cycle variability, heat transfer, spray, film formation, fuel chemistry and combustion [17-28].

As for GDI systems, besides a knock tendency reduction via the cooling effect of the mixture, they allow the adoption of a stratified charge which leads to a reduction of the specific fuel consumption at part-load and low revving speed conditions. A stratified charge is usually obtained by means of late injections [29], which in turn are feasible thanks to the remarkable injection pressures promoted by GDI systems. In fact, a higher injection pressure promotes a stronger spray break-up. Alternatively, to promote break-up and, hence, evaporation of the spray, injection can be carried out under flash boiling conditions.

Flash boiling occurs when fuel is injected in an ambient characterized by a static pressure lower than the fuel saturation pressure for a given temperature and it causes instability of the fluid operating under superheated conditions. The rapid reduction in pressure or the increase in superheat cause the fuel to enter a metastable state with a significant superheated thermal energy, which is absorbed via the rapid flash-boiling process. As a result, a fast vapor nucleation inside the liquid takes place; during the injection process the vapor bubbles grow up and burst due to the liquid pressure sudden drop from the nozzle to the ambient level. Flash boiling can occur inside the nozzle where the gaseous phase creates an under-expanded jet of fuel vapor at the nozzle exit, together with liquid droplets. This occurs due to the high injection pressure typically used with gasoline direct injection. In fact, in Gasoline Direct Injection engines operating under part load and early injection conditions, the in-cylinder pressure can fall below the atmospheric level at the start of the injection [30], while temperature can raise due to the presence of EGR. Spray morphology and air-fuel mixing are strongly influenced by the flash boiling phenomenon, and the effect of different injector configurations with different types of fluid on flash boiling were explored [31-37].

In this work, a flash boiling model recently implemented in STAR-CD V.2019.1 [38] is tested and validated against experimental data provided by the SprayLAB of Perugia University. A single-hole research injector is analyzed in a constant volume chamber characterized by a pressure of 40 kPa, in order to replicate an engine part-load operation. To evaluate the effect of the fuel (n-Heptane) temperature on the flash boiling phenomenon, two different conditions are investigated: a subcooled one and a flashing one, with injection temperatures equal to 303.15 K and 393.15 K, respectively. The numerical framework is based on the Arbitrary Lagrangian-Eulerian (ALE) approach, in which computational parcels are introduced directly at the nozzle exit, hence the choice of droplet initial conditions is extremely important to achieve fully representative simulations of the spray [39]. Numerical simulations are validated against experimental data in terms of imaging, liquid penetration curves, and Phase Doppler Anemometry (PDA) data. In the paper, a methodology to evaluate droplet initial conditions from experimental momentum measurements is firstly presented. Secondly, a detailed description of the new flash boiling model is carried out. Thirdly results on both subcooled and flashing condition are discussed. Finally, conclusions on the present work are outlined.

2 A METHODOLOGY FOR DROPLET INITIALIZATION

Evaluation of droplet initial conditions, in terms of diameter and velocity, is a crucial aspect in the ALE approach. Droplet characteristics at the nozzle exit have a large impact on spray penetration and morphology, as well as on the distribution of diameters and velocities along the envelope of the jet. A possible approach to evaluate droplet initial conditions involves Eulerian Multiphase nozzle internal flow simulations, as described in [40-41]. Since the internal nozzle geometry was not available for the investigated injector, an alternative approach developed at the SprayLAB of the University of Perugia was exploited, which is based on experimental momentum measurements as described in [42-43]. The global spray momentum flux measurement is a widely diffused technique to understand the characteristics of the fuel flow. The total momentum flux is measured through the evaluation of the jet impact force on a target flat surface, located at a given distance from the injector tip.

$$\dot{M} = F \tag{1}$$

Definitions of both the momentum flux \dot{M} and the mass flux \dot{m} at the nozzle exit are reported in equations (2) and (3), where ρ is the fuel density, A_{ef} is the effective area and v_{eff} the effective injection velocity:

$$\dot{M} = \rho \, A_{eff} \, v_{eff}^2 \tag{2}$$

$$\dot{m} = \rho \, A_{eff} \, v_{eff} \tag{3}$$

With traditional injector analyzers it is possible to evaluate the mass flux \dot{m} . To calculate the effective area, it is necessary to estimate the contraction coefficient C_A defined as the ratio between A_{eff} and the geometric area of the nozzle A_0 . Combining equations (2) and (3) it is possible to write the C_A coefficient as:

$$C_A = \frac{\dot{m}^2}{\rho A_0 \, \dot{M}} \tag{4}$$

Then from the mass flux it is possible to calculate the discharge coefficient C_d defined as:

$$C_{d} = \frac{\dot{m}}{\dot{m}_{theoric}} =$$

$$\frac{\dot{m}}{A_{0}\sqrt{2(p_{inj}-p_{amb})\rho}}$$
(5)

The effective injection velocity can be evaluated from the velocity coefficient C_v , which depends on the C_d and C_a as follow:

$$C_{\nu} = \frac{C_d}{C_a} \tag{6}$$

$$v_{eff} = C_v \, v_{theoric} \tag{7}$$

This approach, based on experimental outcomes, provides significant information used to initialize the droplets in the Lagrangian simulations through a simple blob model. The initial droplet velocity is calculated as in the equation (7), while initial droplet diameter D_{eff} is evaluated from the contraction coefficient and the geometric diameter D_{geom} as follow:

$$D_{eff} = D_{geom} \sqrt{C_a} \tag{8}$$

3 A NOVEL FLASH BOILING MODEL

In GDI engines, at specific conditions, flash boiling can occur both inside and outside the nozzles and it massively impacts spray characteristics. However, internal nozzle flow simulations via a Eulerian approach imply significant computational efforts and require detailed CAD geometry of the injector. To provide an accurate prediction of droplet characteristics at nozzle exit under flash boiling conditions, 0D submodels can be adopted. In STAR-CD, the flash boiling atomization and evaporation models developed by Price [44-45] are implemented in combination with the vapor bubble breakup model proposed by Senda [46]. The latter considers flash boiling effects on droplet breakup after injection.

3.1 Flash boiling atomization model

Experimental outcomes show that the amount of flash boiling is mainly determined by superheat degree ΔT_{SD} , defined as:

$$\Delta T_{SD} = T_{inj} - T_{sat,\infty} \tag{8}$$

where T_{inj} is the injection temperature and $T_{sat,\infty}$ is the saturation temperature at ambient pressure. It is assumed that the flash boiling atomization model is activated when superheat rises above a predefined threshold value, for example 10 K. When flash boiling occurs, the injected droplet velocity is obtained from:

$$U_{eff} = \frac{A_n}{\dot{m}} \left(P_s - P_{\infty} \right) + U_{vena} \tag{9}$$

where A_n is the nozzle area, \dot{m} is the mass flow rate of injection, P_s is the saturation pressure at the fuel injection temperature, and P_{∞} is the ambient pressure. The velocity at the vena contracta U_{vena} is obtained from:

$$U_{vena} = \frac{\dot{m}}{A_n \rho_l C_c} \tag{10}$$

where ρ_l is the density of the liquid, and C_c is the contraction ratio defined as the ratio between the mean velocity and the U_{vena} . In this work C_c is calculated with an empirical formula. The spray cone angle is modelled as [45]:

$$\theta = a\beta^2 + b\beta + c \tag{11}$$

where β is a non-dimensional parameter that depends on the ratio between the saturation pressure and the ambient pressure as well as on the surface tension of the fuel. In the equation (11), default values of the coefficients *a*, *b* and *c* are -3.208, 366.61 and -10324 respectively. At flash boiling conditions, vapour is generated inside the nozzle and the resulting volume flowrate \dot{V}_{vap} is calculated as:

$$V_{vap} = N_{nuc} f V_b S_{nozzle}$$
(12)

where N_{nuc} is the nucleation site density per unit surface area, V_b is the bubble departure volume, f is the bubble departure frequency, and S_{nozzle} is the inner surface area of the nozzle orifice. The liquid volume flowrate is calculated as:

$$\dot{V}_{liq} = \dot{V}_{total} - \dot{V}_{vap} \tag{13}$$

Making the hypothesis that the liquid volume flowrate corresponds to the volume of the droplet exiting the nozzle, it is possible to evaluate the initial droplet diameter as:

$$D_d = \left(\frac{6\,\dot{V}_{liq}}{\pi}\right)^{\bar{3}} \tag{14}$$

The flash boiling atomization model estimates the effective velocity of the droplets U_{eff} , their diameter at the nozzle exit D_d , and the cone angle θ taking into account flash boiling effects such as vapor generation inside the nozzle and reduction of efflux section.

3.2 Flash boiling evaporation model

In addition to the mass transfer \dot{m}_{sc} predicted by the standard evaporation model, driven by heat transfer from ambient gas to droplets, evaporation due to flash boiling is predicted with an additional term \dot{m}_{sh} [44]:

$$\dot{m}_{sc} = AP \frac{ShD_i}{T_f R_f D_d} \ln \left(\frac{P - P_v}{P - P_s}\right)$$
(15)

$$\dot{m}_{sh} = \frac{A\alpha\Delta T_{SD}}{H_l} \tag{16}$$

where A is the droplet surface area, P is the ambient pressure, Sh is the non-dimensional Sherwood number, D_i is the binary diffusion coefficient, T_f is the temperature of the vapor film, R_f is the specific gas constant of the vapor film, P_v is the partial vapor pressure in the cell, P_s is the saturation pressure of the fuel, H_l is the latent heat of vaporization, and α is the overall heat transfer coefficient given by empirical functions [47]:

$$\alpha = 760 \ \Delta T_{SD}^{0.26} \ if \ 0 \\ \leq \Delta T_{SD} \ \leq 5$$

$$\alpha = 27 \ \Delta T_{SD}^{2.33} \ if \ 5 \\ \leq \Delta T_{SD} \ \leq 25$$

$$\alpha = 13800 \ \Delta T_{SD}^{0.39} \ if \ \Delta T_{SD} \ \geq 5$$
(17)

3.3 Flash boiling droplet breakup model

Flash boiling can occur outside the nozzle as well, promoting droplet break-up and leading to significantly smaller droplets. In this paper the bubble nucleation and growth model of Senda [48] is adopted for the simulation of droplet breakup due to flash boiling occurring inside droplets outside of the nozzle. Firstly, bubbles are created through a nucleation process within the droplets, whose bubble number density N is obtained from:

. . .

$$N = C \exp\left(\frac{-\Delta A}{\Delta T_{SD}}\right) \tag{18}$$

where *C* and ΔA are model constants having values of 1.11x1012 and 5.28, respectively. Bubble growth is secondly modelled by solving the following equation:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 = \frac{1}{\rho} \left(P_w - P_\infty \right)$$
(19)

and

$$P_{w} = P_{s} + \left(P_{r0} + \frac{2\sigma}{R_{0}}\right) \left(\frac{R_{0}}{R}\right)^{3n} - \frac{2\sigma}{R} - \frac{4\mu_{l}\dot{R}}{R} - \frac{4k\dot{R}}{R^{2}}$$
(20)

where R is the bubble radius, R_0 is the initial bubble radius (with 10 µm default value), P_{∞} is the ambient pressure, P_{r0} is the pressure at the nozzle orifice, μ_l is the liquid viscosity, σ is the surface viscosity coefficient set by default to 1.25x10-5 Ns/m. Droplet breakup due to flash boiling only occurs when the bubble volume fraction ε exceeds a threshold volume fraction ε_{max} set to 0.55:

$$\varepsilon = \frac{V_{bubble}}{V_{bubble} + V_{liquid}} > \varepsilon_{max}$$
(20)

When droplet breakup occurs, the number of child droplets generated is taken as twice the number of bubbles.

4 OPERATING CONDITIONS AND NUMERICAL SETUP

In this work a single-hole research injector is simulated under both standard and flashing conditions, with the aim to evaluate the new flash boiling model. The injector is characterized by a step-hole geometry, with a nominal orifice diameter equal to 175 μ m. Operating conditions for both standard and flashing tests are reported in Table 1:

Parameter	Subcooled Case	Flashing Case
Fuel	n-Heptane	n-Heptane
Injection Pressure	10 MPa	10 MPa
Fuel Temperature	303.15 K	393.15 K
Vessel Pressure	0.04 MPa	0.04 MPa
Vessel Temperature	293.15 K	293.15 K

Table 1. Investigated operating condition

The computational domain for 3D-CFD simulations consists of a 70x70x160 mm blockshaped vessel. Numerical grid comprises hexahedral cells and it is characterized by a coneshaped refinement along the jet envelope, where minimum cell size is equal to 0.5 mm in order to obtain both a moderate computational cost and a reduced grid dependency [49].

As for the turbulence modeling a RANS approach is adopted in all the simulations and, specifically, the k- ε RNG two-equation turbulence model [50] is adopted. A coupled Eulerian-Lagrangian approach is exploited to enable the numerical modeling of a dispersed multi-phase flow. The second order MARS numerical scheme is adopted for temperature, momentum, and turbulent quantities. In all the simulations 30 parcels are injected every time-step; this last is equal to 1e-6 s in order to keep the maximum Courant number well below unity. The computational domain is initialized with experimental pressure and temperature values, and all the boundaries are set as non-slip adiabatic wall. One single-component fuel n-Heptane is injected, whose properties are inherited from the NIST database for both liquid and vapor phase [51].

In all the simulations the experimental injection mass flow rate profile, provided by the SprayLAB of Perugia University, is adopted. In the numerical framework the syringe-like effect described in [52] is considered in order to obtain a faithful numerical representation since the very early stage of the injection.

Primary break-up uses a simplified Blob Model, while for secondary break-up the Reitz-Diwakar model [53] is adopted; values of the model constants are calibrated in the subcooled case and then they are retained in the flashing one, with the aim to evaluate the reliability of the flash boiling breakup model contribution to the estimation of the reduction of droplet size due to bubbles burst inside the liquid droplets.

5 NUMERICAL RESULTS

In the subcooled case, droplet initialization is based on experimental momentum and mass flow rate outcomes, while at flashing conditions the flash boiling atomization model automatically evaluates droplet properties at the nozzle exit. As for the spray semi-cone angle, in the subcooled case it is imposed equal to 10 deg according to the experimental imaging; for the flashing case, the semi-cone angle value is calculated by the flash boiling

atomization model. Experimental tests are carried out with an injection pressure equal to 10 MPa and an excitation time equal to 1 ms for the momentum and 1.5 ms for the mass flow rate. Experimental curves are depicted in Fig.1



Fig. 1. Experimental mass flow rate and force provided by SprayLAB

The resulting hydraulic coefficients obtained with the previously described methodology are reported in Table 2:

Table 2. Estimated values for the injector hydraulie coefficients		
Ca	0.703	
Cd	0.581	
Cv	0.826	

Table 2. Estimated values for the injector hydraulic coefficients

A first comparison between experimental and numerical outcomes is carried out in terms of imaging. For the sake of brevity, only three snapshots are chosen and reported in Figs. 2 and 3.



Fig. 2. Comparison in terms of imaging between experimental outcomes and numerical simulations at (a) 300 μ s, (b) 650 μ s, and (c) 1300 μ s after the start of injection at subcooled conditions.



Fig. 3. Comparison in terms of imaging between experimental outcomes and numerical simulations at (a) $300 \ \mu$ s, (b) $650 \ \mu$ s, and (c) $1600 \ \mu$ s after the start of injection at flashing conditions.

As visible in Figs. 2 and 3, at subcooled conditions the main spray characteristics such as jet penetration and cone angle are well represented by the simulations; as for the flashing operating point, it is possible to state that there is a slight overestimation of the cone angle value even if the global morphology of the spray is well predicted. To quantitatively validate the numerical framework, a comparison between numerical and experimental liquid penetration curves is reported in Fig. 4.



Fig.4. Liquid penetration comparison for (a) subcooled and (b) flashing cases.

It is useful to point out that, on the numerical side, the maximum penetration is considered for the comparison. In other words, the distance along the injector axis between the farthest droplet and the tip is reported in Fig. 4. Error bars are shown in the experimental curves to point out the standard deviation values. Numerical liquid penetrations closely reproduce experimental results in both cases; a slight underestimation of the penetration in the last stage of the injection is reported for the flashing case, due to the previously commented overestimation of the cone angle. Since a reduction of the droplet size is expected when flash boiling occurs, the last comparison is carried out in terms of PDA data. PDA analysis is carried out along the nozzle axis at 20 mm, 30 mm, 40 mm, and 50 mm far from the injector tip; comparisons between numerical and experimental mean droplet diameter (D10) and velocity magnitude are depicted in Figs. 5 and 6. It can be seen that both D10 and velocity values are well predicted by the numerical simulations at all the measurement stations; it is useful to point out that PDA values are filtered in specific time interval with the aim to analyze the characteristics of the spray in the static phase of the injection. As for the flashing case, the adopted model is able to predict the reduction of droplet diameters due to flashing along the axial direction.



Fig. 5. Comparison between simulations and experiments in terms of (a) D10 and (b) velocity magnitude at subcooled conditions.



(a)

Fig. 6. Comparison between simulations and experiments in terms of (a) D10 and (b) velocity magnitude at flashing conditions.

6 CONCLUSIONS

In the present paper, a validation of a flash boiling model to be adopted in ALE simulations, implemented in the last version of the commercial code STARCD, is performed on a single-hole research injector. Numerical results are validated against experimental outcomes provided by SprayLAB of Perugia University; a methodology to evaluate droplets initial conditions based on experimental momentum measurements is depicted. The main conclusions of this work can be drawn as follows:

- experimental momentum tests are very valuable to calculate droplet properties at the nozzle exit, such as initial diameter and initial velocity. Static values of mass flow rate and force on a target surface are exploited to evaluate the nozzle hydraulic coefficients, which are used as inputs for the Lagrangian simulations.
- for both subcooled and flashing conditions, numerical results show a good agreement with experimental data, in terms of imaging, liquid penetration and PDA data (D10 and velocity magnitude).
- as for the flash boiling atomization model, a slight overestimation of the cone angle in the flashing case can be noticed, according to the imaging comparison. This is confirmed by the penetration curves where, in the flashing case, a slight underestimation of the liquid length emerges.
- as demonstrated by the comparison between numerical and experimental values of D10, the flash boiling breakup model is able to predict the reduction of droplets size along the envelope of the spray due to vapor bubble nucleation and burst inside the liquid droplets.

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