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Assessment of the Cavitation Models implemented in OpenFOAM® under DI-like conditions

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Abstract

Direct injection engine performance is strictly correlated to the fluid dynamic characteristics of the injection system. Actual DI engines, both Diesel and gasoline, employ injector characterized by high injection pressure that, associated to micro-orifice design, result in cavitation flow conditions inside injector holes. The cavitation has a beneficial effect on the atomization process and a negative one on the physical erosion generated by the vapor bubble collapse.

In order to quantify both effects with a numerical approach, the reduced dimension and the complex flow structures reduce the efficacy of an experimental approach, thus the cavitation model used is of primary importance.

The present work addresses the validation of the mixture model-based cavitation models that are implemented in OpenFOAM®, with particular focus on the Schnerr and Sauer model, using the experimental results, available in literature, for a two-phase flow in an optically accessible nozzle under diesel-like conditions.

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1. Introduction

Cavitation consists in the generation of vapor cavities dispersed in the main liquid flow that occurs when the pressure drops below the fluid vapor pressure. When the pressure increases, these cavities implode generating intense shock-waves, that are cause of loud noise, strong vibrations and destructive effects on the metallic surface.

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The cavitation inside high pressure injectors holds a very important role on the definition of their overall performance [1-8] having a positive effect on droplet atomization [9] and a negative effect on spray stability [1] and injector lifetime [10]. The physical erosion of the injector internal surfaces can be explained by the presence of very high pressure and flow rate gradients that lead to the generation of vapor bubbles very close to the injector solid boundaries.

Due to the small size of the involved components, the CFD approach can be useful in assessing the cavitation risk and its effects. Among the different simulation methods, the two-phase homogeneous mixture models (HMM) are the most used since they allow to model a large number of bubbles with an affordable computational cost, even if they are unable to define a sharp interface between the vapor and the liquid phases [11]. The HMM assume the multiphase flow to be an homogeneous mixture of two incompressible components, the liquid and the vapor phase, and apply either a barotropic equation of state or a transport equation to solve the density variation in the flow.

In the barotropic cavitation models, the mixture equations are solved and the local mixture density (ρ_m) is assumed to be dependent on the local sound velocity of the mixture, that in turn depends on the local pressure and the void fraction. The barotropic cavitation models are able to properly predict the choke effect on the flow rate, but as Ducoin et al. [12] stated, they are not able to properly predict the dynamics of the cavitating flows, especially for cases with unsteady cavitation, because of the importance of cavitation in vorticity production.

In the transport equation model (TEM) the continuity equation of the mixture is substituted by a transport equation for the volume or mass fraction of one of the phases. The continuity equation for the vapor's volume fraction is:

$$\frac{d}{dt} \rho_v \alpha_v + \nabla \cdot (\rho_v \alpha_v \mathbf{u}) = R \quad (1)$$

The mass source term (R) is a function of the fluid properties and the phase transition process, and it can be written as the net rate between two terms, the term R_v representing the mass exchange from liquid to vapor phase (evaporation rate), and the term R_c which models the mass exchange from vapor to liquid phase (condensation rate):

$$R = R_v + R_c \quad (2)$$

Various authors have proposed different formulations for the source terms (see Ducoin et al [12] for an overview of the principal formulations). Some authors (Merkle et al. [13], Kunz et al. [14]) have chosen to directly model vaporization and condensation rate with a formulation similar to the chemically reacting flows. Other authors, like Singhal [15], Zwart [16] or Schnerr and Sauer [17], have preferred a more physical approach. They suppose that the vapor created by the cavitation could be described by a cloud of perfectly spherical identical bubbles:

$$\alpha_v = \frac{n \frac{4}{3} \pi \frac{\mathfrak{R}_B^3}{2}}{1 + n \frac{4}{3} \pi \frac{\mathfrak{R}_B^3}{2}} \quad (3)$$

where n is the parcels' volumetric density and \mathfrak{R}_B is the bubble's radius. Then they correlate the evolution of the vapor fraction with the bubble's dynamic described by the Rayleigh-Plesset equation (R-P), which was simplified neglecting the surface tension, the viscosity and the second order time dependence:

$$\frac{d\mathfrak{R}_B}{dt} = \sqrt{\frac{2}{3} \frac{p_B - p}{\rho_l}} \quad (4)$$

where p_B is the bubble's pressure, assumed to be uniform and equal to the vapor's pressure. It must be kept in mind that in this family of models the equation (4) is not solved, but it is simply used as a source term for the change of phase, and thus the position of the single bubble is not traced.

The conceptual correlation between vapor fraction and bubble diameter can be used to define a correlation between the cavitation onset/development and a damage risk index. For example Brusiani et al. [18], focusing their attention on the cavitation phenomenon analysis inside nozzles characterized by micro-orifice design, used the ANSYS Fluent implementation of the Zwart mass transfer model in order to have a direct match between bubbles life and possible surface damage.

The present paper is focused on the analysis of the HEM-TEM cavitation models implemented in OpenFOAM® v.2.3.0. Among the three available models (Merkle, Kunz, Schnerr and Sauer), this paper is focused on the Schnerr and Sauer model since is the only one based on the R-P equation. This analysis aims to be a preliminary work in order to implement the methodology defined by Brusiani et al [18]. in an open source framework.

2. Schnerr and Sauer model

The Schnerr and Sauer model [17] defines the source term of eq. (1) as:

$$R = C_{civ} \frac{\rho_l \rho_v}{\rho_m} \alpha_v (1 - \alpha_v) \operatorname{sgn}(p - p_{sat}) \frac{3}{\mathfrak{R}_B} \sqrt{\frac{2}{3} \frac{|p - p_{sat}|}{\rho_l}} \quad (5)$$

where the mixture density ρ_m is defined as the weighted average between the density of the liquid (ρ_l) and the vapor (ρ_v) phases:

$$\rho_m = (1 - \alpha_v) \rho_l + \alpha_v \rho_v \quad (6)$$

The bubble radius \mathfrak{R}_B is obtained from eq. (3):

$$\mathfrak{R}_B = \left(\frac{1 - \alpha_v}{\alpha_v} \frac{3}{4\pi n} \right)^{\frac{1}{3}} \quad (7)$$

Where the parcels density (n) is taken constant and its value is of the order of 10^{13} bubbles per volume unit. It must be noted that the Schnerr and Sauer model doesn't use the source term in the form of eq. (2). It defines a single equation, valid for both the condensation and the evaporation effects. The application of this equation as a source or a sink term depends on the value of the fluid pressure relative to the vapor pressure. The coefficients C_c and C_v are not present in the original formulation of the model: they are usually introduced in some CFD implementations in order to enhance the evaporation or the condensation effect, and usually they are proposed to be equal to one.

The authors of the model suggest that a small fraction of vapor must ever be present. This small gaseous fraction "contaminating" the liquid is both a physical and a numerical necessity. From a numerical point of view, it is evident that the source term R of eq. (5) is null when the mixture is composed by a pure component only. So the model is incapable to express a phase change even if the cavitation condition onset ($p < p_{sat}$) is reached. From a physical point of view, in every fluid a not condensable gas part, acting as cavitation nucleation site, is present. Strictly speaking, the radius of the cavitation nuclei and the particle density of the bubbles depend on many factors, such as the temperature, the difference between the local pressure and the vapor pressure, the purity of the chosen fluid [20]. The model doesn't differentiate between not condensable gas and vapor phase, the authors simply assume that the "contaminating" part is composed by a vapor phase which can be described as a group of spherical particles having diameter d_{Nuc} and a volume density n .

Table 1. Diesel oil data.

	Liquid	Vapor
Density (kg/m ³)	832	0.13
Viscosity (m ² /s ²)	7.81e-6	4.35e-7
Vaporization pressure (Pa)		5400

The nucleation volume fraction (α_{nuc}) is defined as:

$$\alpha_{nuc} = \frac{n \frac{4}{3} \pi \frac{d_{Nuc}^3}{2}}{1 + n \frac{4}{3} \pi \frac{d_{Nuc}^3}{2}} \quad (8)$$

In the original model it is not clear if this volume fraction must be transported or if its value must be used as a lower limit for the vapor phase.

3. Reference experimental case

The cavitation model implemented in OpenFOAM® v.2.3.0 has been validated against the experimental data by Winklhofer et al. [19].

In the cited paper the mass flow rate was obtained for three different nozzles under respectively non-cavitating, incipient and full cavitating flow. The nozzles have the same inlet section and length, but differ for the contraction ratio: the J-hole has no contraction, the U-hole has a ratio of 5%, and lastly the W-hole has a contraction ratio of 10%. The nozzles (Fig. 1a) have been obtained by erosion from a 0.3 mm thick steel sheet that is sandwiched between two sapphire glasses, for providing an optical access: as a consequence the section is rectangular and the resulting flow is quasi 2D. The length before and after the injector's section has been chosen in order to obtain an unperturbed flow. The authors chose to fix the inlet pressure at 100 bar and to vary the outflow pressure in the range 10-80 bar. The fluid used is generic Diesel oil, so the necessary thermodynamic properties have been assumed according to Table 1.

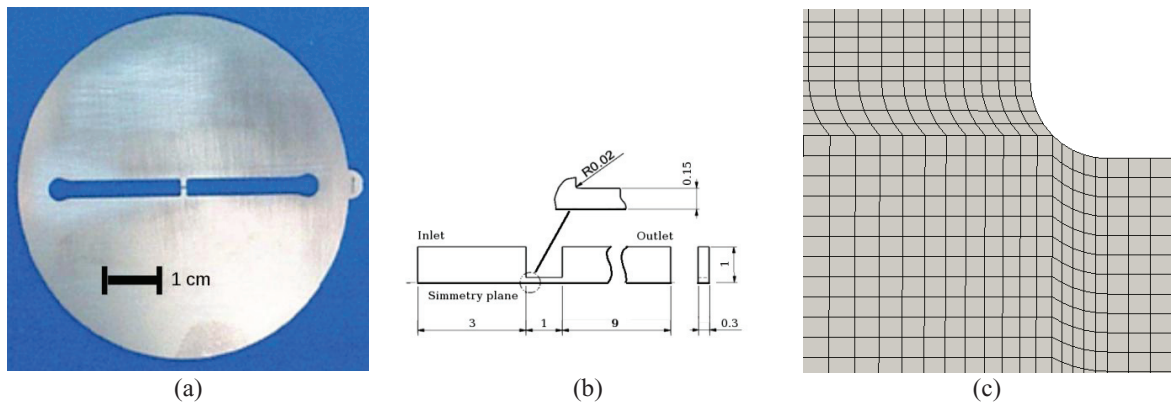


Figure 1: Definition of the computational domain: (a) view of the experimental nozzle, (b) dimensions of the simulated domain, (c) particular of the grid in the nozzle region.

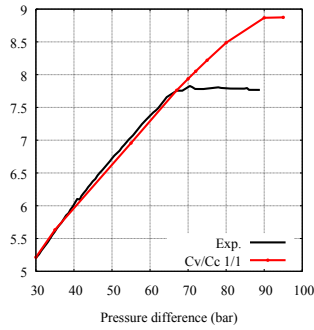


Figure 2: Mass flow versus pressure drop – J-Hole (unitary condensation and vaporization coefficients)

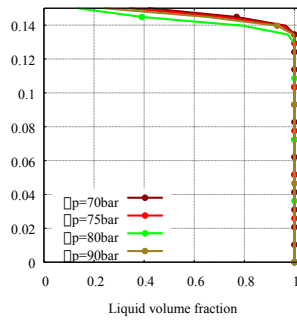


Figure 3: Liquid volume fraction in a section at 0.02 mm from the hole inlet – J-Hole

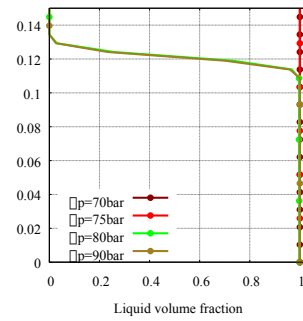


Figure 4: Liquid volume fraction in a section at 0.75 mm from the hole inlet – J-Hole

4. Numerical case methodology

After a tuning process finalized to find out the best trade-off between the necessity to limit the total number of cells, hence the computational cost, and a proper reproduction of the experimental geometry, the authors have chosen a fully three-dimensional symmetric domain with a depth equal to the experimental one, but of reduced length (Fig. 1b).

The domain discretization has been performed using the `blockMesh` utility: a particular care has been devoted to define the round inlet (Fig. 1c) and the sharp outlet of the injector hole. The mesh is composed of around 250000 hexahedral cells. Inside the injector nozzle the cells are almost square along both the axial direction and its orthogonal direction with a size of $5\ \mu\text{m}$. Due to the quasi-2D nature of the flux the cell's size on the third direction is larger than $5\ \mu\text{m}$. The small size and the regularity of the cell inside the injector nozzle, have allowed to not apply any wall layer.

The turbulence model was initially set to the $k-\varepsilon$ model with standard wall functions at the solid surfaces. At the boundary inlet a constant total pressure condition was applied ($p_{INLET} = 100\ \text{bar}$) together with a turbulent intensity of 5%, while at the boundary outlet a variable static pressure was set, accordingly with the pressure difference adopted in the experimental test, with a zero-gradient outflow condition.

The chosen solver (`interPhaseChangeFoam`) is a fully transient solver that uses the PISO algorithm for the pressure-velocity coupling. The discretization schemes chosen are the second order implicit for the time, the QUICK scheme for the liquid volume fraction and the central differencing scheme for the remaining equations. The time step has been fixed in the order of $10^{-8}\ \text{s}$ due the characteristic time of the cavitation phenomenon.

Since the cavitation inside the injector is highly fluctuating, the resulting volumetric flow rate has been measured at the inlet boundary after a sufficient time has been elapsed from the achievement of the stationary flow. The mass flow rate is then deduced under the phase-incompressibility hypothesis.

5. Schnerr and Sauer model validation

The OpenFOAM® implementation of the Schnerr and Sauer model requires four mandatory parameters: the vaporization coefficient (C_v), the condensation coefficient (C_c), the diameter of the cavitation nuclei (d_{Nuc}) and the density of the cavitation nuclei (n). It is useful to highlight that the term d_{Nuc} is used to define the α_{nuc} value, and it doesn't represent an inferior limit to the value of the bubble radius. Also α_{nuc} is added to the evaporation mass source term, but is not transported. According to the model all the parameters concur to the development of the cavitation phenomenon: the optimal combination of the values requires some analysis. In the following part of the paper the main results of these models compared to the experimental data by Winklhofer et al. [19] will be discussed.

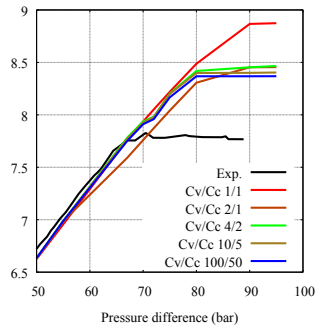


Figure 5: Mass flow versus pressure drop – J Hole - Effect of the condensation and the vaporization coefficient values

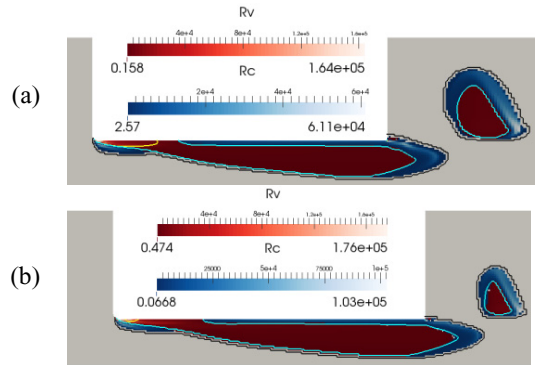


Figure 6: Distribution of gaseous (R_v) and liquid (R_c) phase sources for $\Delta p=90$ bar Black isoline $\alpha_t=1$; cyan isoline for pressure $p=p_{\text{vap}}$; yellow isoline $p=0$ bar. C-Ratio constantly equal to 2: a) $C=10/5$, b) $C=100/50$

5.1. Vaporization and condensation coefficients

Accordingly to the guidelines proposed in [17], the cavitation nuclei ($n=1.6e+13$ $1/m^3$) and their diameter ($d_{\text{Nuc}}=2$ μm) have been set. In Fig. 2 the simulation results for the J-hole obtained with the condensation and evaporation coefficients values equal to 1 (i.e. using the model accordingly to the original formulation) have been reported. The mass flow choke effect is over-predicted. In Fig. 3 it is visible that the cavitation occurs at the hole entrance for a pressure drop of 70 bar, delayed with respect to the experimental data, but it fails to develop until at least a pressure drop of 80 bar, as can be seen in Fig. 4.

For increasing the vapor volume fraction downstream the cavitation inception, the evaporation must be promoted and the condensation inhibited. Under the assumption of maintaining the same proportionality between the two values ($C=C_v/C_c=2$), the parameters C_v and C_c were varied over a large range.

As can be seen in Fig. 5, the increase of the coefficient values led to the advance of the cavitation condition, but in relative terms the benefit obtained by this increment rapidly becomes insignificant. With the simple increase of the values of C_v and C_c is not possible to bring the numerical results to the experimental ones. Comparing Fig. 6a and Fig. 6b it is to note that the increase of the C_v coefficient is useful in order to reduce the extension of the non-physical pressure zone (the yellow isoline).

5.2. Effect of the turbulence model

In the open literature it was observed that the turbulence effect is of great importance on the cavitation phenomenon. Some models include the turbulence effect directly into the source term (for example Singhal [15]), while other models modify the pressure value in order to take into account the energetic contribute of the kinetic turbulence energy.

In order to verify if the overestimation of the mass flow rate with respect to the experimental data depends on the turbulence model, the RNG k- ϵ and the SST k- ω models have been tested using the same grid with the best parameter setup previously defined. For the RNG k- ϵ model the wall treatment is the same of the k- ϵ model, for the SST k- ω model the wall treatment on the lateral wall has been changed to the one provided for k- ω models, and deactivated on the the upper wall of the hole, due to the small value of y^+ obtained (Fig. 7). As can be seen in Fig. 8 the use of a model, such as the RNG k- ϵ model, that accounts for the curvature effect of the flow improves the prediction. The intermediate results obtained with the SST k- ω are due to a suboptimal resolution of the wall effects, particularly on the lateral walls of the injector hole. This leads to an underestimation of the mass flow rate in non-cavitating conditions and to a delay of the incipient cavitation condition. To be able to respect the condition $y^+\leq 1$ on the lateral wall, a reduction of the grid size is required.

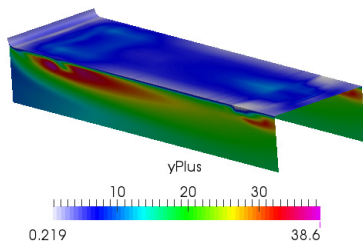
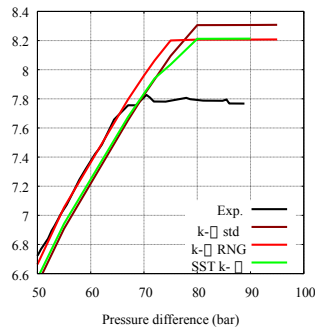
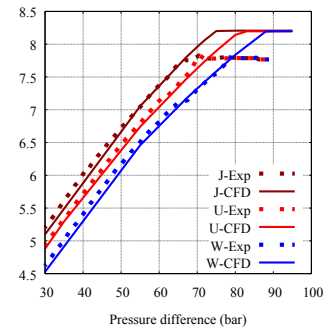
Figure 7: y^+ value for $\Delta p=80$ bar. SST $k-\omega$ 

Figure 8: Effect of the turbulence model

Figure 9: Assessment of the cavitation model, best results RNG $k-\epsilon$

Since the choked mass flow rate is the same of the RNG case and due to the modest curvature effect that characterized the real case authors assume the RNG $k-\epsilon$ model as the best compromise between result and the computational cost.

6. Conclusion

In Fig. 9 the best results obtained using a RNG $k-\epsilon$ model with $C_v=200$, $C_c=100$, $n=1e+15$ $1/m^3$ and $d_{nuc}=2$ μm are reported. As can be seen the model is capable of correctly predicting the mass flow rate in a non-cavitating condition, of reconstructing the effect of the convergence and the global effect of the cavitation, but it fails to correctly predict the mass flow rate in choked conditions.

In the authors' opinion this lack of the cavitation model is due to the absence of the sonic velocity formulation in the model based on the transport equation. Of consequence the flow rate block shown before for all the analyzed cavitation models is not properly a sonic block but rather a fluid-dynamic block. This could explain the systematic error between the numerical results and the experimental data, for any model based on the transport equation. Moreover the solver is still an incompressible solver, and the results are obtained in terms of volumetric flow rate, so the chosen value for the density of the fluid can slightly modify the results in terms of mass flow rate. There is also an uncertainty about the effective properties of the Diesel oil used by Winklhofer, not explicitly reported in the paper [19].

Some final notes regarding the parameter used:

- The values of the coefficients of evaporation and of condensation must be high enough and with a C-ratio ($C = C_v / C_c$) around 2.
- The value of the parameter α_{nuc} was considered the primary target. By many tests and simulation results an optimum value of α_{nuc} was found to be in the range $10^{-6} \div 10^{-3}$. Exceeding this range would mean bringing in the system a mixture having two well marked phases, with the risk of stationing of a part of the pilot gas in an unwanted area. Reducing the value under the minimum threshold can be risky if α_{nuc} is so small that it can be confused with a zero from the machine during calculations. These considerations have led to determine a value $\alpha_{nuc}=4 \cdot 10^{-3}$, i.e. a feeding liquid having a 0.4% of pilot vapor phase.
- d_{nuc} is limited at least upwardly: it is unthinkable to introduce, in a confined flow, so large cavitation nuclei that could create a stopper in the injector hole. In the present case it may be reasonable to accept cavitation nuclei in a range $10^{-9} \div 10^{-3}$ m. Under these conditions, continuing to believe acceptable nuclei with radius of 1 μm , the term n loses its independence and it's automatically defined by the other two parameters (about $n \approx 10^{15}$ $1/m^3$).

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