Numerical modelling of flashing flow phase change in convergent-divergent nozzle: A sensitivity analysis

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Abstract. A sensitivity analysis of a computational fluid dynamics (CFD) model of flashing flow phenomenon including the thermal non-equilibrium effect is proposed in the present paper. The model uses a two-phase mixture approach and the phase-change process is based on the difference between the vaporization pressure and the vapour partial pressure. Thermal non-equilibrium effect is included in the model by a sub-routine for the boiling delay. A two-dimensional axisymmetric convergent-divergent nozzle is used as benchmark for the proposed study. Such geometry is representative of well-known applications in nuclear, refrigeration and energy engineering (e.g., primary flow in the motive nozzle of ejectors). The results are compared to experimental data and previous numerical results available in literature. Present results show good agreement with global and local experimental fluid dynamic quantities used to validate the model. The paper includes in the first part a brief description of physical phenomenon of flashing flow, the experimental benchmark geometry and operating conditions. In the second part, the physical model and the numerical modeling approach are reported, showing the validation and the results related to the sensitivity analyses of the artificial coefficients characterizing the modelling approach.

1. Introduction

The flashing flow, a phase change phenomenon, is encountered in accelerated flow inside nozzles with the boiling delay phenomenon (thermal non-equilibrium effect) [1, 2]. In general to model flashing flow, CFD approaches must take into account the two aspects including: (i) the phase change phenomenon during flashing flow and (ii) the two-phase interaction during the evaporation process between the liquid and the vapour phases. For the phase change during vaporization process, there are two main categories including: (i) the nucleation process is considered in models providing a better agreement to behavior of the real fluid-flow, but experimental data must be supported to control the source term of the nucleation equation (Table 1); (ii) models assume constant bubble size or number density and neglect the nucleation process (Table 2). For the interaction between two phases during the vaporization process, there are two approaches including: (i) the Eulerian-Eulerian model and (ii) the mixture model. Within the Eulerian-Eulerian model, the conservation equations are solved for each phase and then interfacial terms are considered for coupling two phases. Conversely, the mixture approach assumes the same velocity of individual phases in flow over short length scales (viz. homogeneous flow). In the mixture model, the average velocity field of the mixture flow is derived by a single momentum. Volume fraction is, thus, extracted by solving the individual equation for the second phase. In some cases such as high-speed flows, relative motion between two phases becomes more significant and must be taken into
account. Several models for velocity differences between two phases are suggested in literature, including: the drift-flux model [36], the mixture model [37], the algebraic-slip model [38], the suspension approach [39], the diffusion model [37, 40] and the local-equilibrium model [41]. This paper performs an improved CFD model for flashing flows, which includes the thermal non-equilibrium effect. In the proposed CFD model, the mixture two-phase approach is considered with the phase change process, assuming constant bubble size distribution, based on the difference between the vaporization pressure and the vapor partial pressure.

In this paper, the first part is devoted to the physical phenomenon of flashing flow and the experimental benchmark of a circular convergent-divergent nozzle is presented along with operating conditions. The second part introduces the physical model and the numerical modelling approach. Validation of the numerical approach and a sensitivity analysis of artificial coefficients are reported in the last part.

Table 1. Flashing Flow Simulation with Nucleation Models: a literature survey

| References and code | Numerical model | Benchmark for validation |
|---------------------|-----------------|--------------------------|
| [3] CFX 4.2         | - Eulerian model with Scalar transport equation for bubble number density using wall nucleation as source term. - Nucleation rate is determined by model of Jones [4-7]. | - Flashing flows in pipes and nozzles [8]. |
| [9] FLUENT 6.2.16   | - Eulerian model. - Effects of bubble nucleation and interfacial heat transfer to phase change process, momentum and energy conservation are considered | - Flashing phenomenon is accounted in depressurization process of a piping system at Rusal Auginish. |
| [10] NEPTUNE-CFD    | - Eulerian model. - unphysical heat transfer coefficient - A modified version of Jones’ model [4-7] is used for nucleation effects to vapor generation rate, momentum and energy transfer. | - Critical flow in nozzle [11] with initially subcooled inlet and flashing outlet. - Experimental test from [12] with cavitation developments downstream an orifice. |
| [13] CFX 14.5       | - Eulerian model. - Interphase momentum transfer with drag, lift, lubrication, virtual mass and turbulent dispersion forces. - Interphase mass transfer is derived by interfacial heat transfer - Nucleation models of [7] RPI model [14-16], Riznic model [17, 18], Rohatgi model [19] are used to bubble number transport equation. | - Vertical circular convergent-divergent nozzle from [20]. |
| [21] STAR-CD        | - Mixture model with barotropic phase change - The bubble growth is modeled by Rayleigh-Plesset equation. | - A single-hole diesel injector with different needle’s lifts. |
Table 2. Flashing Flow Simulation Neglecting Nucleation Process

| References and code | Numerical model and assumptions | Experimental benchmark and remarks |
|---------------------|---------------------------------|-----------------------------------|
| Laurien and his colleagues [22-24] CFX 4.2 | - Eulerian model  
- Assuming bubble number density is used for growth of bubble size by. | - Cavitation flow in pipes. |
| [25] CFX | - Eulerian model  
- Bubble diameter is is fixed to 1mm | - Edward blowdown test |
| [26] CFX 14.0 | - Eulerian model  
- Nucleation process is neglected by assuming constant bubble number density. | - Transient pressure release in vertical pipe with flashing flow of [27]. |
| [28] FLUENT 12.0 | - Mixture model with slip phenomenon between two phases  
- phase change phenomenon is driven by pressure [29] and temperature  
- Rate of phase change is based on sonic velocity equation [30]. | - Convergent-divergent motive nozzle of [31] inside a two-phase ejector. |
| [32] CFX 14.5 | - Same model as in [26] | - Flashing of initial sub-cooled water flow in vertical convergent-divergent nozzle from [8]. |
| [33] CFX | - Same model as in [26] uses different models for bubble number density (mono-disperse assumption and poly-disperse method). | - An overview of previous works with assumptions of both mono-disperse approach and poly-disperse approach. |
| [34] In-house code | - Mixture model.  
- Mass transfer models consider (i) pressure phase change model from [35] and (ii) thermal phase change model.  
- Modelling cavitating flow on a cylindrical head form and a Clark-Y hydrofoil geometry to confirm empirical coefficients of phase change model. | - Circular convergent-divergent nozzle geometry with operating conditions in Abuaf et al. [8] is used as experimental benchmark. |

2. The phenomenon of flashing flow

Figure 1a presents the thermodynamic diagram of boiling process of water. This process happens at constant pressure in a saturation region under thermal equilibrium conditions (further details in [42]). However, in high-speed flows, as ejector-based systems, the phase change phenomenon inside nozzles shows thermal non-equilibrium behaviours. Particularly, the depressurization inside the nozzle leads to have superheated water and, consequently, a phase change occurs. The bubble nucleation growth in this case is related to the non-equilibrium effects [43]. In general, the flashing flow, phase change process driven by sudden depressurization, is separated in 3 stages, as presented in Figure 1b and summarized in the following:

1. **Stage 1.** After the pressure of flow drops below saturation line, the nuclei existing in cavities of wall and in the flow start growing. The surface tension forces dominate the behaviour of the bubbles at this stage, in which growth of the nuclei is limited (this stage is named delay period in [44] or idle period in[45]).

2. **Stage 2.** When the diameter of the bubbles reaches a critical radius (reference in [43]), the growth of the bubble is dominated by the pressure difference between the bubble surface and the surrounding water. Rayleigh-Plesset equation as in [46] can be used to approximate the bubble growth rate in this stage.
3. **Stage 3.** Heat transfer around the bubble interface, combined with turbulence fluctuations and relative motion between phases, will have a big influence to boiling process in this stage.

a) Thermodynamic diagram of phase change of water with equilibrium assumption

![Thermodynamic diagram of phase change of water](image1)

b) Start of vaporization

![Start of vaporization](image2)

**Figure 1.** Physical behaviour of flashing flow

3. **Experimental benchmark**
The experimental measurements proposed by [8] have been used to validate the numerical results. In this benchmark, net vapour generation rates with non-equilibrium conditions are measured. Particularly, this benchmark includes a circular convergent-divergent nozzle, with sub-cooled water at the nozzle inlet and flashing flow at the outlet (Figure 2 presents the detailed dimensions of the nozzle). Abuaf has designed the converging-diverging nozzle with 49 pressure taps and two windows for observation at the exit point. Experimental data used to validate include (a) distributions of the pressure along nozzle, (b) the average vapour fraction, (c) inception point of the flashing and (d) radial void fraction profiles at axial positions. Table 3 describes the operating conditions of the experiments. For more information the experimental conditions, reader may refer to [8].

![Figure 2. Vertical circular convergent-divergent nozzle in Abuaf et al. [8]](image)

Table 3. Operating conditions and case code names in [8]

| Case code name | Upstream pressure [Pa] | Inlet temperature [K] | Outlet pressure [Pa] | Flashing inception pressure [Pa] | Saturation pressure [Pa] | Mass flow rate [kg/s] |
|----------------|------------------------|-----------------------|----------------------|----------------------------------|-------------------------|----------------------|
| BNL284         | 530000                 | 422.35                | 456000               | 404700                           | 466000                  | 7.3                  |
| BNL309         | 555900                 | 422.25                | 402500               | 393500                           | 464800                  | 8.8                  |
| BNL273         | 573500                 | 421.85                | 442100               | 419200                           | 459800                  | 8.7                  |
| BNL268         | 575200                 | 422.05                | 443000               | 405700                           | 462300                  | 8.7                  |
| BNL304         | 577700                 | 422.15                | 441000               | 399700                           | 463500                  | 8.8                  |
| BNL278         | 688600                 | 421.95                | 434100               | 425700                           | 461000                  | 11.7                 |
| BNL296         | 764900                 | 421.95                | 432600               | 417000                           | 461000                  | 13.1                 |

4. Physical model
Model of flow

In this study, the mixture model with slip effect in ANSYS-FLUENT 16.0 is used with assumptions of pseudo single-phase flow. With this assumption, the same governing equations (mass, momentum and energy conservation) are used for both phases. For more information about this model, [47] is referred.

Phase change model

The transport equation for the phase change is given by:

\[
\frac{\partial (\alpha_v \rho_v)}{\partial t} + \nabla \cdot (\alpha_v \rho_v \vec{v}_m) = \dot{m}
\]  \hspace{1cm} (1)

The source term \( \dot{m} \) to consider the evaporation-condensation flux at the interface is defined:

\[
\dot{m} \left[ \frac{kg}{m^3 s} \right] = FA_1 \beta \frac{M}{\sqrt{2 \pi R T_{sat}}} (P_v - P^*)
\]  \hspace{1cm} (2)

Where \( \beta \) is the accommodation coefficient, \( M \) the molar mass [kg/kmol], \( R \) the universal gas constant [kJ/kmol K]. The turbulence effects to flashing process is taken into account via vaporization pressure in (3)

\[
P_v = P_{sat} + 0.195 \rho k
\]  \hspace{1cm} (3)

In Eq. (2), \( P^* \) is the value of the pressure inside saturation region and should be close to saturation pressure \( P_{sat} \) and \( k \) the turbulence kinetic energy [m^2s^-2]. Interfacial area density \( A_i \), presented in (4)

\[
A_i [m^{-1}] = (6\alpha_v)^{2/3}(\pi N_b)^{1/3}
\]  \hspace{1cm} (4)

Numerical set-up and boundary conditions

The computational domain is represented by 2D-axisymmetric approach and a structured quadrilateral elements grid has been set up. Figure 3 and Table 4 present mesh and boundary conditions used in the simulations. In the benchmark cases, there is no reversed flow observed at the outlet and only outlet static pressure can be imposed to generate the depressurization inside the nozzle. Please note that a grid independency study has been performed to ensure accuracy. In this study, the \( k - \omega \) SST with Standard option for the near wall treatment is chosen in combination with flashing model.
Figure 3. Mesh and boundary condition of convergent-divergent nozzle

Table 4. Boundary conditions

| Boundary | Flow boundary | Turbulence boundary |
|----------|---------------|---------------------|
| Inlet    | Total pressure| Turbulence intensity and hydraulic diameter |
| Outlet   | Static pressure|                      |
| Wall     | Adiabatic wall | Wall function        |
| Axis     | Axisymmetric  | Axisymmetric         |

The proposed approach performs PISO scheme for Pressure-Velocity Coupling algorithm and Second Order Implicit scheme for the transient term. The spatial discretization of different quantities is presented in Table 5. In this simulation, the time step is $10^{-5}$s with convergence criteria: (i) relative error of mass flow rate between inlet and outlet <2% and (ii) the maximum residual below $10^{-6}$ for all equations is imposed. Artificial coefficients such as bubble number density and maximum of $dp = P_{\text{sat}} - P^*$ are set at the values of $4 \cdot 10^8$ and 75Pa, respectively. The mass flow rate error can be explained by the use of artificial coefficients and the mesh approximation, as reported below. Further investigation on this aspect can be done to improve the accuracy of the numerical results. The phase change process is triggered by a vapour fraction of $10^{-5}$ imposed at the inlet. An analysis of mesh convergence has been performed for the BNL309 case with four different meshes including: (i) 21350, (ii) 53184, (iii) 109728 and (iv) 214650 elements, with a ratio of the elements $N_{i+1}/N_i \approx 2$ and the value of $y^+$ ranging from 6 to 16 for all tested meshes. Finally, mesh of 109728 elements is applied for further calculations.
Table 5. Numerical method

| Discretization | Scheme |
|----------------|--------|
| Transient formulation | Second Order Implicit |
| Pressure-Velocity Coupling | PISO |
| Gradient | Green-Gauss Cell Based |
| Pressure | PRESTO! |
| Density | |
| Momentum | |
| Volume Fraction | |
| Turbulence Kinetic Energy | |
| Specific Dissipation Rate | |
| Energy | Second Order Upwind |

5. Numerical results

Validation

The numerical results, obtained with the present model, are validated with available measurements in [8]. The nucleation stage has been neglected in this model when imposing \( N_b = 4 \cdot 10^8 \) and introducing an accommodation coefficient to tune the boiling delay effect. In this part of paper, different results are compared and reported including mass flow rate, vapour volume fraction, pressure drop and vapour volume fraction profile.

Table 6 shows comparison between the computed mass flow rate and the experimental data for all the operating conditions. There is an agreement between numerical results and experiment when average and maximum relative errors equal to 4.7% and 6.8%, respectively. The accommodation coefficient \( \beta \) was imposed to a value close to unity for all cases.

Table 6. Comparison of Experimental Mass Flow Rate and CFD Mass Flow Rate

| Cases       | Accommodation coefficient \( \beta \) | Experimental Mass Flow Rate (kg/s) | CFD Mass Flow Rate (kg/s) | Relative error |
|-------------|--------------------------------------|----------------------------------|--------------------------|----------------|
| 1           | 0.8                                  | 7.3                              | 7.7                      | +5.4%          |
| BNL309      | 1.2                                  | 8.8                              | 8.8                      | +0.2%          |
| BNL273      | 1.05                                 | 8.7                              | 9.3                      | +6.8%          |
| BNL268      | 1.0                                  | 8.7                              | 9.2                      | +5.7%          |
| BNL304      | 1.11                                 | 8.8                              | 9.1                      | +3.4%          |
| BNL278      | 1.15                                 | 11.7                             | 12.3                     | +5.1%          |
| BNL296      | 1.18                                 | 13.1                             | 13.9                     | +6.1%          |
Comparison of average vapour fractions and absolute pressures along the nozzle with experimental data is performed and shown in Figure 4. A general agreement of the present model with the measurements is observed for all tested cases. Average vapour starts from close to zero at the convergent part and increases near the nozzle throat region \((x=0.3045\text{m})\) up to the nozzle outlet. Besides, the present model shows a good prediction of the average vapour volume faction for tested cases BNL268, BNL273, BNL284, BNL304 and capability of model to correctly capture the flashing inception position is confirmed. There is an agreement with measured data of absolute pressure at convergent section, whereas a slight difference at the divergent section is observed. For all the analysed fluid dynamic quantities, the proposed CFD flashing model shows a good prediction with respect to measurements.

BNL268

BNL273

BNL278

BNL284
Figure 4. Averaged vapor fraction and absolute pressure along nozzle
Radial vapour distribution for case BNL309 is presented in Figure 5 and Figure 6 from the near the nozzle throat at $x=0.306m$ to near the nozzle outlet at $x=0.577m$. There is a comparison between the present model and experimental data at different sections across the nozzle. At $x=0.306$ (position A), the present flashing model shows a peak near the wall region, whereas, vapour volume fraction value of measurements equals to zero, implying a later flashing inception. In the present model, the turbulence effects near the wall to phase change process is taken into account leading to a good agreement with the measured data in sections from $x=0.319m$ to $x=0.577m$ at near wall region.

**Figure 5.** Radial void fraction profile at positions along divergent nozzle

Section A ($x=0.306m$)  

Section B ($x=0.319m$)  

Section C ($x=0.332m$)  

Section D ($x=0.344m$)
Sensitivity analysis of artificial coefficients

A systematic procedure to evaluate effects of artificial coefficients including $dp$ and the accommodation coefficient, $\beta$, is performed. In this approach, one coefficient will be fixed to perform sensitivity analysis on the other quantity. Generally, higher vapour volume fraction at divergent sections is observed when the either $\beta$ or $dp$ increases, as shown in Figure 4. Besides, the pressure at the throat region also increases corresponding to the increase of artificial coefficients. For static pressure variable along nozzle, it can be observed how the increase of artificial coefficients leads to an increase of pressure in correspondence of the throat region. This behaviour can be associated to an earlier vaporization process. Indeed, if water flow is incompressible from convergent part to throat, giving an explicit relation between static pressure and velocity, at throat level the flow becomes compressible and static pressure is not linked to velocity trend anymore and pressure does not keep decreasing further with the increase of velocity. The influence of the artificial coefficients including the pressure drop $dp$ and the accommodation coefficient, $\beta$, have been reported in Figure 7 for cases BNL268, BNL273, BNL284, BNL304, BNL309, respectively. A similar trend among different cases is observed when varying coefficients. The importance of accommodation coefficient $\beta$ is highlighted by the sensitivity analysis presented here, showing a coherent behavior for different operating conditions.
BNL268

a) Vapour profile and static pressure along nozzle with fixed $dp = 75\text{Pa}$

b) Vapour profile and static pressure along nozzle with fixed $\beta = 1.0$

BNL273

a) Vapour profile and static pressure along nozzle with fixed $dp = 75\text{Pa}$

b) Vapour profile and static pressure along nozzle with fixed $\beta = 1.05$
BNL284

a) Vapour profile and static pressure along nozzle with fixed $dp = 75\text{Pa}$

b) Vapour profile and static pressure along nozzle with fixed $\beta = 0.8$
BNL304

a) Vapour profile and static pressure along nozzle with fixed $dp = 75\text{Pa}$

b) Vapour profile and static pressure along nozzle with fixed $\beta = 1.11$

BNL309

a) Vapour profile and static pressure along nozzle with fixed $dp = 75\text{Pa}$

b) Vapour profile and static pressure along nozzle with fixed $\beta = 1.2$
6. Conclusion
A CFD flashing model for flashing flows has been performed and validated. The model is based on the two-phase mixture model considering the slip effect and the thermal non-equilibrium effect (viz. boiling delay phenomenon). The model has been validated by using the available measurements of a circular convergent-divergent nozzle. Generally, there is an agreement in the comparison between numerical results and measured data including (a) mass flow rate (e.g., maximum relative error below 6%), (b) average vapour fraction and (c) static pressure along the nozzle and (d) radial vapour volume fraction profiles at different positions along nozzle. Besides, sensitivity analyses of artificial coefficients have been performed. With the accommodation coefficient and the difference between saturation pressure and vapour partial pressure at the interface, an earlier flash inception point is observed from numerical results when increasing the coefficients.

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