Prediction of the bubble nucleation rate in a quasi-stable cavitating nozzle using 2D computational fluid dynamics and enhanced classical nucleation theory

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Most of the numerical studies of the cavitation process available were simulated based on the Rayleigh-Plesset equation, which has a presumed value for the number of bubble nuclei in the domain. However, in the computational domain for most cases, the bubble nuclei density varies, depending on the hydrodynamics and different bubble nucleation rates. Therefore, the modeling of the bubble nucleation rate based on the number of molecules required to form a critical cluster, which is affected by the hydrodynamics in the domain, is one of the challenges that must be overcome for bubble nuclei density prediction. In this work, an enhanced Classical Nucleation Theory (CNT) model was written as in-house code for integration in Computational Fluid Dynamics (CFD) to estimate the water vapor bubble nucleation rate across a quasi-stable cavitating flow nozzle. The enhanced CNT model included microscopic factors that specifically address water vapor bubble nucleation. Because these factors vary in the radial direction, this work was extended into the 2D domain to estimate the bubble nucleation rate in both the axial and the radial directions. The bubble nucleation rate was estimated through various numbers of molecules (depending on the hydrodynamics in the domain) required to form a critical cluster. The Population Balance Model was used to estimate the bubble nuclei density based on the bubble nucleation rate. The simulated results indicated that the bubble nucleation rate was highest at the throat of the nozzle, especially near the wall of the nozzle. Thus, a higher bubble nuclei density was found near the wall after the throat of the nozzle.

Keywords: bubble nucleation rate; number of bubble nuclei; CFD

1. Introduction

Nucleation of vapor bubbles occurs either by increasing the temperature of the liquid above its boiling point (superheated liquid) or reducing the external pressure below the saturated vapor pressure of the liquid (stretched liquid). This phenomenon, which is also known as cavitation, can be easily found in many places, such as marine propellers and fuel injectors.

Computational Fluid Dynamics (CFD) has been widely used in various industrial applications to predict the hydrodynamic flow in the relevant computational domain, such as in a nozzle (Cai, Fang, Xu, & Liu, 2007; Ding, Wang, & Chen, 2014; Peralta, Chew, & Wilson, 2011; Tian & Lu, 2013). In the numerical study of cavitation processes, the mathematical model based on the Rayleigh-Plesset equation is often used in the numerical simulation of cavitating flow due to its simplicity. Singhal, Athavale, Li, and Jiang (2002) has developed a full cavitation model by introducing vapor generation and condensation rates as source terms in the vapor transport equation. The effect of noncondensable gases was included in the model. The phase change rates in the model depend only on the pressure difference, vapor and gas mass fraction, density, turbulence kinetic energy, surface tension and empirical constant. This model was also integrated into CFD codes and successfully validated with experimental results. There are also several cavitation models proposed by other researchers, including Kunz, Boger, Stinebring, Chyczewski, Lindau, Gibeling, Venkateswaran, and Govindan (2000) and Shin, Yamamoto, and Yuan (2004). The factors considered in these cavitation models were similar to the model suggested by Singhal et al. (2002). In these models, the microscopic factors that influence the nucleation and growth of vapor bubbles, for example, cluster surface tension and the Zeldovich factor, were not included in the cavitation model. Therefore, the work required for forming a critical cluster was difficult to determine using the model. To date, there are limited numerical investigations on the cavitation of water in the bubbly flow considering the nucleation of vapor bubbles (Goncalves & Patella, 2009; Lindau, Kunz, Boger, Stinebring, & Gibeling, 2002; Preston, Colonius, & Brennen, 2002). Delale, Okita, and Matsumoto, (2005) successfully attempted to integrate the enhanced Classical Nucleation Theory (CNT) into the cavitating flow model in 1D steady state bubbly flow. However, one of the bubble nucleation determining factors, that is, the critical bubble radius, must be pre-set before the numerical simulation of the cavitating study. There are also works that attempted to include thermodynamic effects in the numerical study of cavitating...
flow (Goncalvés, and Patella, 2010; Vortmann, Schnerr, & Seelecke, 2003).

CNT has been widely used in the studies of nucleation processes in various areas, such as in crystallizers, atomizers and bubble nucleation studies (Liška, Holubová, Černošková, Černošek, Chromčíková, & Plško, 2012; Lubetkin, 1995; Shukla, Mandal, & Ojha, 2001). In the early works of bubble nucleation studies, CNT was used for modeling a unary system (single component), either for dissolved gas bubbles or vapor bubbles (Lubetkin, 1995). This CNT model has been used by several researchers to calculate the cavitation pressure of water. From their calculations, large negative pressure (few hundreds of MPa) was required to initiate bubble nucleation in pure water without dissolved gas and impurities (Caupin & Herbert, 2006). Similar values were obtained using other methods of calculations for the cavitation pressure of water, such as the thin-wall approximation and density functional theory. However, the cavitation pressure values reported in the literature are widely scattered, with a maximum negative pressure of −120 MPa at 40°C reported (Zheng, Durben, Wolf, & Angell, 1991). The calculated negative pressure was larger than the values reported from experimental data due to impurities in water (Herbert, Balibar, & Caupin, 2006). In addition, the onset of nucleation for water with dissolved gas occurred at a much higher pressure (less negative) compared to the pressure for pure water, as discussed above. This happened due to the lowering of surface tension by the dissolved gas, which acted as a surfactant in this case and thus reduced the work of bubble formation (Lubetkin, 2003). Therefore, the effect of dissolved gas and impurities was suggested to be added into the CNT mathematical model as a correction factor. This correction factor was dependent on the quality of water, which can be determined by comparison with the experimental results (Delale, Hruby, & Marsik, 2003). The modification of the CNT model for bubble nucleation has enabled it to be used for predicting the nucleation process in water. Delale, Okita, and Matsumoto (2005) has also successfully tested and validated this enhanced version of the CNT model to predict the 1D steady-state cavitating nozzle flow. Later, the use of CNT was further extended to a multicomponent system (Vehkamäki, 2006). Another approach to predict the bubble nucleation rate in water for gas and vapor proposed by Kwak and Oh (2004) was based on a unified approach. This approach considered different factors of the bubble nucleation of gas and vapor.

To date, most of the cavitation processes have been described using the reduced Rayleigh-Plesset cavitation model, whereby the nuclei number density is predefined in the domain, regardless of the hydrodynamic effects. The famous CNT is one of the methods used in the effort to determine the bubble nucleation rate according to the hydrodynamic conditions. However, the coupling of CNT and the bubbly liquid flow model is complex and hinders the prediction of the bubble nuclei density, especially in the 2D flow domain. The prediction of bubble nuclei density is important for the modeling of bubble growth and mass transfer in the domain. In addition, modeling of the bubble nucleation rate based on the number of molecules required to form a critical cluster (which determines the critical cluster size) is also one of the challenges to obtain the bubble nucleation rate. Therefore, the main objective of this work is to model the bubble nucleation rate for water flowing across a 2D cavitating nozzle under quasi-stable condition in both the axial and the radial directions. Hence, the bubble nuclei density in the computational domain could be predicted. This study was accomplished with the aid of an enhanced CNT and CFD coupling approach. In addition, in-house code for bubble nucleation rate modeling was developed in the current work. The Population Balance Model (PBM) is applied to further estimate the distribution of the bubble nuclei. In addition, the bubble nucleation rate is estimated through the computed number of molecules required to form a critical cluster. Because the main focus of the current work are modeling the bubble nucleation rate using the coupled CFD and enhanced CNT model; bubble mass transfer and growth are not included in the current work.

2. Mathematical modeling

2.1. Governing equation

A multifluid model based on the Eulerian–Eulerian approach, as used by other similar works (Yan, Li, & Luo, 2012), was used in this work to describe the fluid flow across the nozzle. This model was assumed to be capable to describe the simple shear flow in the 2D domain. In addition, the 2D domain was sufficient to describe the flow in the nozzle because it is symmetric in the radial direction. Because the mass transfer between the two phases was not considered in the current work, the continuity equation for the system is expressed as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$  (1)

where \( \rho \) is the density of the solution, \( \mathbf{u} \) is the Reynolds-averaged velocity vector, and \( t \) is time.

The volume fraction transport equation for liquid phase is given as

$$\frac{\partial}{\partial t} (\alpha_l \rho_l) + \nabla \cdot (\alpha_l \rho_l \mathbf{u}) = 0$$  (2)

where \( \alpha_l \) is the volume fraction of the liquid phase and \( \rho_l \) is the density of the liquid phase.

In the current work, the formation of bubble nuclei was assumed to have an insignificant effect on the hydrodynamics in the computational domain. Therefore, the source term that accounts for bubble nuclei was not included in Equations (1) and (2). The calculation for bubble nuclei formation and distribution was performed by using Population Balance Model based on Classical Nucleation Theory.
2.2. Classical nucleation theory

The nucleation rate, \( J_v \), can be termed as the number of critical clusters formed per unit volume per unit time (nuclei/m³s). CNT states that there is an energy barrier (or the work to form a critical cluster) in the nucleation process. The theoretical expression for the nucleation rate can be written as

\[
J_v = J_0 \exp \left( -\frac{W}{k_BT} \right)
\]

where \( T \) is the liquid total temperature, \( k_B \) is the Boltzmann’s constant, \( W \) is the work to form a critical cluster and \( J_0 \) is a kinetic pre-exponential factor. This expression suggests that the work to form a critical cluster plays an important role in determining the nucleation rate. Thus, the work to form a critical cluster must be perfectly evaluated so that the nucleation rate can be estimated accurately.

In general, for bubble nucleation, the energy barrier is determined by the surface tension of the liquid and also the pressure difference between the bubble and external liquid. The energy barrier is determined as

\[
W = \frac{16\pi}{3} \gamma^3 \left( \frac{1}{P_v} - \frac{1}{P_t} \right)^2
\]

where \( P_v \) and \( P_t \) are the pressure in the bubble and external liquid, respectively, and \( \gamma \) is the surface tension of the liquid-gas surface.

Regarding bubble nucleation, several microscopic parameters, for example, the critical bubble radius, was included in the improved bubble nucleation model based on the CNT (Delale, Hruby, & Marsik, 2003). In the current work, the mathematical model developed by Kwak and Oh (2004) for bubble nucleation was adopted (Equation (5)). They postulated that the physical mechanism behind gas and vapor bubble formation was completely different. The surface energy required to form a gas bubble was constrained by the dissolution due to solvent-solute interaction, while vapor bubble formation was linked with the potential energy between molecules. The expression for vapor bubble nucleation includes the effect from energy to separate a pair of molecules, the number of vapor molecules in the critical cluster, molecular volume, and so on. The equations involved in the calculations of vapor bubble formation was discussed in detail by Kwak and Oh (2004).

\[
J_v = Z_{fv}D_vN_v\exp \left( \frac{1}{2} \eta_{cv}^{2/3} \right)
\]

with

\[
Z_{fv}D_v = \frac{N_v}{\sqrt{6\pi}} \left( \frac{k_BT}{2\pi m_v} \right)^{1/2} \left( \frac{3\nu_m}{4\pi} \right)^{2/3} \beta_v' \exp \left[ \frac{\Delta H_{vap}}{RT} - \frac{\Delta H_f}{RT_f} \right]
\]

where

\[
J_v = \text{Vapor bubble nucleation rate, nuclei/m}^3
\]
\( n_{cv} = \text{Number of molecules required to form a vapor critical cluster} \)
\( N_v = \text{Number density of the liquid, } 3.3428 \times 10^{28} \text{ molecules/m}^3 \)
\( m_v = \text{Mass of the liquid molecules, } 2.99151 \times 10^{-26} \text{ kg} \)
\( \nu_m = \text{Transformed volume of vapor molecules, m}^3 \)
\( \beta_v' = \text{Accommodation coefficient of the vapor molecules to the cluster} \)
\( \Delta H_{vap} = \text{Enthalpy for the evaporation of the solution} \)
\( \Delta H_f = \text{Enthalpy for the freezing of the solution} \)
\( T_f = \text{Melting temperature for the solution, K} \)
\( R = \text{Gas constant, 8.3144621 J/K mol} \)

Water under normal conditions will most likely contain another dissolved gas, such as air, which affects the bubble nucleation rate. Hence, the number of vapor molecules required to form a critical cluster is affected. To extend the application of the nucleation model to account for the dissolved gas in water, the partial pressure of the dissolved gas was added in the model, as shown in Equation (6); this modification is analogous with the modification implemented by Delale et al. (2005). The effect of dissolved air was considered in the current work.

\[
-(P_t - P_v - P_{air})n_{cv}^{1/3} = \frac{k_BT}{\nu_m}
\]

where \( P_{air} \) is the partial pressure of air at atmospheric pressure.

Other than the effect of dissolved air on the number of vapor molecules required to form a critical cluster, it can also affect the surface tension, as it may act as a surfactant. In addition, some other impurities or contaminants may exist as well in the water, which would influence the nucleation rate of the water. Consequently, a correction factor, \( C, \) was introduced into the work of bubble formation, as also introduced by Delale et al. (2005). This correction factor can be obtained by comparing the nucleation rate with the experimental results. Here, the correction factor was determined to be \( 2.396 \times 10^8 \), which was obtained through the nucleation rate results from the work of Delale et al. (2005). The modified bubble nucleation rate is then expressed as

\[
J_v = Z_{fv}D_vN_v\exp \left( \frac{1}{2} \eta_{cv}^{2/3} \right)
\]

2.3. Population balance model (PBM)

The PBM was used in the current work to predict the bubble nuclei density in the computational domain through the bubble nucleation rate and the number of bubble nuclei that exist at the particular position. Because the main focus of
this work was to study the bubble nucleation phenomenon across the nozzle, only the nucleation rate was taken into consideration in the current work in the population balance equation (PBE), where the expression in terms of the number density function \( n(V,t) \) is reduced to

\[
\frac{\partial n(V,t)}{\partial t} + \nabla \cdot [u n(V,t)] = -\frac{\partial}{\partial V} [G(V) n(V,t)]
\]  

(8)

where \( n(V,t) \) is the bubble number density distribution per unit volume (V) for a given time (t). On the right-hand side term, \( G(V) \) is the growth rate of bubble number density, which acted as a source term, in this case, for the bubble nucleation.

The quadrature method of moments (QMOM) was widely used to study the particulate system because it can solve the PBE accurately but requires a lower number of equations. Therefore, QMOM was used in this work to solve the PBE. Based on QMOM, the moments of the particle size distribution (PSD) are approximately obtained as

\[
m_k = \int_0^\infty n(V,t)V^k dV \approx \sum_{i=1}^{Q} w_i L_i^k
\]  

(9)

where \( m_k \) is the kth moment of the number density function, abscissas \( (L_i) \) and weights \( (w_i) \) are determined through the product-difference (PD) algorithm, \( Q \) is the order of quadrature approximation, and \( k \) is the specified number of moments (ANSYS, 2011).

After applying the moment transformation, the PBE is expressed as

\[
\frac{dm_k}{dt} = \int_0^\infty G(V)n(V,t) \cdot V^k dV
\]  

(10)

Equation (10) shows that the rate of change of moment is directly proportional to the bubble nucleation rate in this case.

3. Numerical method

For reasons of comparison with the quasi-stable flow in the cavitating nozzle studied by Wang and Brennen (1998), the geometry and boundary conditions for the current work were changed based on the reference. In addition, the axisymmetric model was used for the nozzle in solver. The normalized area of the nozzle, \( A(x) \), is given by

\[
A(x) = \left\{1 + 0.5 \left[1 - \cos \left(\frac{2\pi x}{L}\right)\right]\right\}^{-1/2} \quad \text{for} \quad 0 \leq x \leq L
\]  

(11)

with \( x \) as the dimensionless normalized length of the nozzle. The normalized length of the nozzle was set as 5 in this study. Thus, the throat of the nozzle is located at \( x = 2.5 \), which is the middle of the nozzle, as shown in Figure 1 (a).

Figure 1 (b) shows the mesh of the computational domain. A total of 13100 cells were generated in the computational domain. In addition, a finer mesh was generated near the wall region. Figure 1 (c) shows the predicted bubble nucleation rate along the axis in the computational domain by using three different mesh densities (1200, 13,100 and 28,500 cells). The results obtained by Mesh 2 and Mesh 3 are both close to each other. Because Mesh 3 requires more computational cost compared to Mesh 2, the computations in current work was performed based on Mesh 2.

Commercial available CFD software, ANSYS FLUENT 14.5, was used in the current work to perform the investigation (Payri, Ruiz, Gimeno, & Marti-Aldaravi, 2015). Table 1 shows the boundary conditions and the settings used in the current work. The governing equations were solved by a coupled pressure-based algorithm and the finite volume approach. The QUICK scheme (Li & Li, 2011) was chosen for the discretization of the governing equations because it can provide third-order accuracy. The 2D space and steady state formulation was used in the simulation. The k-\( \varepsilon \) turbulence model with a standard wall treatment (Vaidyanathan et al., 2003) was used in the current work. Because the flow in the domain was a simple shear flow without a high swirling component or a large pressure gradient, the standard k-\( \varepsilon \) turbulence model was assumed to be capable to provide a reasonably accurate prediction in the simulation. In addition, the standard wall function can also perform well in the simple shear flow condition.

Water, at 20°C, together with dissolved air, was considered to be flowing through the nozzle from the inlet at velocity of 10 m/s. Several properties of water at this temperature were assumed to be constant, such as the density of water, at 1000 kg/m³; the viscosity of water, at 0.001 Ns/m²; and the vapor pressure of water, at 2340 Pa. The volume fraction of dissolved air was set as \( 2.5 \times 10^{-6} \) in current work because the cavitation in the nozzle would be quasi stable flow as reported by Wang and Brennen (1998). The dissolved air was assumed to have a negligible effect on the hydrodynamics in the nozzle. The effect of the dissolved air was included in the bubble nucleation rates model as discussed.

To use the equations (Equations (6) & (7)) for the calculation of bubble nucleation rate, a user-defined function (UDF) was adopted. An in-house code (written in UDF) to for the calculation of bubble nucleation rate was developed. This code was incorporated with the commercial CFD codes to be coupled along with the hydrodynamics equations. Thus, the UDF was integrated in the PBM in the solver. Consequently, the bubble nucleation rate based on enhanced CNT was coupled with CFD-PBM. The bubble nucleation rate can be calculated directly from the hydrodynamics simulated from the CFD codes. One of the unique aspects of the use of this method to calculate the bubble nucleation rate was that the varied number of molecules that was required to form a critical cluster in
the domain could be computed. The number of molecules is a very important parameter that greatly affects the work of formation of the critical cluster and, consequently, the bubble nucleation rate. The equation for the calculation of the number of molecules required to form a critical cluster was found to depend on the pressure at a specific position. Therefore, the hydrodynamics profile in the nozzle is important to determine the bubble nucleation rate.

For comparison, two additional parameters were introduced in the current work. First, a dimensionless parameter, namely, pressure coefficient, $C_p$, was introduced. This parameter has been widely used in cavitating flow analysis to determine the pressure profile across the nozzle with regards to the inlet flow velocity. The pressure coefficient is defined as

$$C_p = \frac{(P_l - P_i)}{0.5 \rho_l U_i^2}$$

where $P_l$ and $U_i$ are the liquid pressure and velocity at the inlet of the nozzle, respectively. This expression is analogous to the definition of the cavitation number, which is used to characterize the potential of the flow to cavitate.

Meanwhile, the second parameter is the number of vapor molecules required to form a critical cluster. This parameter acted as the main factor to determine the bubble nucleation rate because it will directly affect the work of formation of the critical cluster. The parameter can be calculated by using Equation (6), as suggested by Kwak and Oh (2004).
Table 1. Boundary conditions and settings for the numerical simulation.

| Property                  | Boundary Conditions and Settings                        |
|---------------------------|---------------------------------------------------------|
| Materials                 | Water, density = 1000 kg/m³                              |
| Dimensionality            | 2D                                                      |
| Solution method           | Coupled pressure-based solver                           |
| Solution formulation      | Implicit                                                |
| Time dependence           | Steady state                                            |
| Turbulence model          | k-ε model, standard wall function                       |
| Velocity inlet            | Velocity = 10 m/s, Temperature = 20°C                   |
| Volume fraction of gas    | 2.5 × 10⁻⁶                                             |
| phase                     |                                                         |
| Pressure outlet            | Pressure = 0, Temperature = 20°C                        |
| Population balance model  | Quadrature method of moments (QMOM)                     |

4. Results and discussion

4.1. Model validation

The CFD simulation coupled with the improved CNT was used to simulate the case of cavitating nozzle flow based on the conditions discussed by Wang and Brennen (1998). The hydrodynamic profiles of the simulated results in the present investigation were compared with the results obtained from Wang and Brennen (1998) for the case without dissolved air. The comparisons in flow velocity and pressure coefficient along the axis of the nozzle are plotted in Figure 2 and Figure 3, respectively. Based on the figures, the results from the current work exhibit good agreement with the results obtained from Wang and Brennen (1998), with the highest fluid flow velocity at the throat of the nozzle recorded as 14 m/s, while the lowest pressure coefficient was found to be −1.0 m/s. There is a slight difference in the fluid flow velocity and the pressure coefficient near the nozzle exit. Under 2D simulation, uniform inlet velocity profile would develop in both radial and axial direction. Therefore, the velocity profile at axis in 2D simulation is higher as compared velocity profile in 1D simulation since 1D simulation neglects the velocity profile development in radial direction. Because the simulation results in the axial direction were validated, the results in the radial direction were assumed to be valid because the same governing equations were used for the simulation. In addition, this approach has been applied in several similar works available (Cai, Fang, Xu, & Liu, 2007; Ding, Wang, & Chen, 2014; Tian & Lu, 2013).

Figure 2. Distribution of the flow speed along the axis of the nozzle in the axial direction in the current work (dotted line) and the results from Wang and Brennen (1998) (solid line).

Figure 3. Distributions of the pressure coefficient $C_p$ along the axis of the nozzle in the axial direction in the current work (Dotted line) and the results from Wang and Brennen (1998) (Solid line).

Figure 4. Distributions of the nucleation rate $J$ along the axis of the nozzle in the axial direction in the current work (diamond dots) and the results from Delale et al. (2005) (solid line).
Figure 4 shows the bubble nucleation rate profile of water vapor along the axis of the nozzle. Based on the figure, the result for the current work was compared with the simulation result from Delale et al. (2005), who also attempted to integrate CNT into the cavitation simulation with the same geometry but in the 1D domain. Both works exhibited the same maximum bubble nucleation rate along the axis of the nozzle, which was recorded to be $10^{10}$ nuclei/m$^3$ s at the throat of the nozzle. In their study, bubble nucleation only occurred between positions $2 < x < 3$. According to Equation (3), the onset of cavitation is actually determined by the work of formation for a critical cluster. In the current study, this work of formation for a critical cluster is represented by the number of molecules required to form a critical cluster. However, Delale et al. (2005) used the critical cluster size to indicate the work of formation for a critical cluster. They set a fixed value for the critical cluster size in their study. In other words, the onset of cavitation was dependent on the preset minimum pressure difference. Therefore, the bubble nucleation was ignored for the case when the pressure difference has not achieved the minimum value. Their approach caused the bubble nucleation rate to increase and decrease sharply at the onset and end of cavitation because only the pressure difference in this region was sufficient to create a critical cluster.

The predicted bubble nucleation process in the current work occurred almost throughout the entire nozzle, with a
significant rate at the throat of the nozzle. In the current work, the mathematical model of the number of molecules required to form a critical cluster, which was specifically designated for vapor bubble nucleation, as suggested by Kwak and Oh (2004), was used. The computed number of molecules required is used to determine the bubble nucleation rate in the domain. Therefore, the onset of bubble nucleation does not depend on the predefined minimum pressure difference.

4.2. CFD analysis

Using the approach of coupling CFD and bubble nucleation theory in the 2D computational domain, the distribution of various parameters, including the bubble nucleation rate, pressure, and number of bubble nuclei, can be estimated both in the axial direction and the radial direction. The bubble nucleation rate is strongly dependent on the pressure drop across the nozzle, whereby the hydrodynamics information can be obtained through the CFD approach. In this section, the distribution of pressure and velocity, the number of molecules required to form a critical cluster, and the bubble nucleation rate are presented.

4.2.1. Velocity and pressure

The contour plots of the velocity distribution for water flowing across the nozzle are shown in Figure 5. Based on Figure 5, the water flows in at a velocity of 10 m/s and the speed increases at the throat of the nozzle to nearly 14 m/s due to the constriction. Subsequently, the speed of the water flow gradually reduces again to approximately 10 m/s. The increase and decrease of velocity of the water was predicted based on the laws of mass and momentum conservation, with the assumption of an incompressible fluid flow.

Figure 6 (a) shows the contour plot of the pressure distribution in the nozzle. Based on the law of momentum conservation because there was no external force applied to the fluid flow and because of the difference in height, the

![Contour plots of velocity and pressure](image)

Figure 7. Number of molecules required to form a critical cluster: (a) contour plot across the nozzle and (b) along the axial direction at the throat of the nozzle ($2 < x < 3$) and at radial positions of $y = 0, 2$ and 4.
increase of velocity in fluid flow must be compensated by a pressure drop. As a consequence of the increase of the velocity of the water flowed across the nozzle, the pressure of the water at the throat of the nozzle has dropped to nearly $-46$ kPa in the current work, that is, as if the nozzle was being stretched.

Furthermore, Figure 6 (b) shows the liquid pressure in the axial direction at the radial positions of $y = 0, 2$ and 4. Based on the figure, the lowest liquid pressure is decreasing from the middle of the throat ($y = 0$), at approximately $-44.0$ kPa, towards the wall of the nozzle, recorded at approximately $-45.5$ kPa at $y = 4$. The difference in the vapor and liquid pressures, $\Delta P$, is larger when the liquid pressure is lower. According to Equation (6), the difference in the vapor and liquid pressures is the main factor that determines the number of molecules required to form a critical cluster. Therefore, the pressure difference was the key to initiate the bubble nucleation process. In addition, the pressure difference also acted as driving force for bubble nucleation, whereby the larger pressure difference would generate a higher bubble nucleation rate.

4.2.2. Number of molecules required to form a critical cluster

Figure 7 (a) shows the contour plot of the number of molecules required to form a critical cluster. The number of molecules required decreases towards the throat of the nozzle and increases after the region. Figure 7 (b) shows the number of molecules required to form a critical cluster at the throat of the nozzle for the radial position of $y = 0$, 2 and 4 in the axial direction. The graph shows that the number of molecules required is not constant in the radial direction and that the number of molecules decreases when approaching the wall. The lowest number of molecules required decreases from approximately 1150 at the axis ($y = 0$) to approximately 1140 at $y = 2$ and further decreases to approximately 1100 at $y = 4$. The same trend is observed in the axial direction for the above positions. The profile of the numbers of molecules required to form a critical cluster was dependent on the pressure difference in the vapor and liquid pressures, $\Delta P$. A higher pressure difference was determined to require a lower number of molecules to form a critical cluster.

![Figure 8](image-url)

**Figure 8.** Bubble nucleation rate: (a) contour plot across the nozzle and (b) along the axial direction at the throat of the nozzle ($2 < x < 3$) and at the radial positions of $y = 0, 2$ and 4.
4.2.3. Bubble nucleation rate

The contour of the bubble nucleation rate across the nozzle, which was the main parameter under study in the current work, is presented in Figure 8(a). Based on the figure, the bubble nucleation rate was predicted to be the highest at the throat of the nozzle. Figure 8(b) shows the bubble nucleation rate at the throat of the nozzle in the axial direction at radial positions of \( y = 0, 2 \) and 4. The maximum bubble nucleation rate increases from the middle of the throat (\( y = 0 \)) at approximately \( 1 \times 10^{10} \) nuclei/m\(^3\) s to approximately \( 1.3 \times 10^{10} \) nuclei/m\(^3\) s at \( y = 2 \) and further increases to \( 3 \times 10^{10} \) nuclei/m\(^3\) s at \( y = 4 \). The trend of the bubble nucleation rate exhibited a similar trend to the number of molecules required to form a critical cluster. Hence, the real maximum bubble nucleation rate was determined not only to be \( 10^{10} \) nuclei/m\(^3\) s, as predicted by Delale et al. (2005); in addition, the rate was found to be \( 5.8 \times 10^{10} \) nuclei/m\(^3\) s at the wall of the throat of the nozzle, as shown in Figure 8(a).

The higher pressure difference between the vapor and liquid pressures reduces the number of molecules required to form a critical cluster, thereby increasing the nucleation rate. Figure 8(a) shows that the liquid pressure is lowest at the throat of the nozzle in the axial direction, while in Figure 8(b), the pressure difference, \( \Delta P \), increases in the radial direction. Therefore, the bubble nucleation rate was found to be highest at the throat of the nozzle and increased in the radial direction.

4.2.4. Bubble nuclei distribution

The distribution of bubble nuclei formed across the nozzle is presented in Figure 9(a). From the figure, the bubble nuclei developed significantly at the region after the throat of the nozzle. This behavior was due to the high bubble nucleation rate at the throat of the nozzle. Consequently, a significant number of bubble nuclei were formed and dispersed across the nozzle. Therefore, the bubble nuclei distribution was determined by both the local bubble nucleation rate and also the hydrodynamics in the nozzle. In accordance with the bubble nucleation rate profile (high bubble nucleation rate near the wall of the throat of the nozzle), a high density of bubble nuclei was found to be concentrated near to the wall of the nozzle.

Figure 9. Number of bubble nuclei: (a) contour plot across the nozzle and (b) along the axial direction at the throat of the nozzle (2 < \( x < 3 \)) and at the radial positions of \( y = 0, 2 \) and 4.
The number of bubble nuclei estimated at the throat of the nozzle in the axial direction at the radial positions of $y = 0, 2$ and $4$ is presented in Figure 9 (b). Generally, the number of bubble nuclei formed increases sharply at the throat of the nozzle and remains almost constant after the throat. The number of bubble nuclei formed after the throat of the nozzle increases from approximately $6 \times 10^{7}$ at $y = 0$ to approximately $8 \times 10^{7}$ at $y = 2$ and further increases to approximately $1.7 \times 10^{8}$ near the wall of the nozzle at $y = 4$. The number of bubble nuclei formed in the radial direction was found to be different due to the differences of the bubble nucleation rate in the radial direction.

The bubble nuclei distribution estimated in the current work was predicted using the Population Balance Model (PBM). The PBM was capable to consider the local bubble nucleation rate, and the nuclei existed at particular positions and times within the computational domain. This approach could predict the bubble nuclei distribution, which is an important element to estimate the mass transfer from liquid to gas phase when a bubble is formed.

4.3. Bubble nucleation rate at different inlet velocities

Figure 10 shows the bubble nucleation rate along the axis of the nozzle at different inlet velocities. A similar approach was used to predict the bubble nucleation rate along the axis of the nozzle at different inlet velocities of 5 m/s, 10 m/s and 15 m/s. From the figure, the bubble nucleation rate is generally higher for cases with a higher inlet velocity. The highest bubble nucleation rate is recorded as $1 \times 10^{-6}, 1 \times 10^{10}$ and $1 \times 10^{21}$ with inlet velocities of 5 m/s, 10 m/s and 15 m/s, respectively, at the throat of the nozzle ($x = 2.5$). The bubble nucleation rate increases with the inlet velocity because a higher inlet velocity will generate a higher pressure drop at the throat of the nozzle. Hence, the higher bubble nucleation rate is developed due to the high pressure drop.

5. Conclusion

The bubble nucleation rate in a quasi-stable cavitating nozzle flow in the 2D computational domain was successfully estimated via the coupling of CFD and the enhanced CNT. In addition, the bubble nucleation rate was estimated using the computed number of molecules required to form a critical cluster. Because the pressure was found to be lowest at the throat of the nozzle, the bubble nucleation rate was predicted to be the highest at the throat of the nozzle (up to $6 \times 10^{10}$ nuclei/m$^3$ s). Furthermore, PBM was used to predict the bubble nuclei density across the nozzle. In addition, the bubble nucleation rate was determined to increase with inlet velocity through the same approach. Because the use of a 1D simulation cannot represent the bubble nucleation phenomenon in the cavitating nozzle, the prediction of the bubble nucleation rate and the nuclei distribution in the 2D domain is important because these properties increase in the radial direction. Because bubble growth modeling was not included in the current work, it will be implemented in future work.

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Nomenclature

- $A(x)$: Normalized area of the nozzle
- $C$: Correction factor
- $D$: Rate of molecules striking on a surface area of the cluster, molecules/m$^2$·s
- $G (V)$: Growth rate of the bubble number density, number/m$^3$·s
- $\Delta H_{\text{evap}}$: Enthalpy for the evaporation of the solution
- $\Delta H_{\text{f}}$: Enthalpy for the freezing of the solution
- $J$: Bubble nucleation rate, nuclei/m$^3$·s
- $J_0$: Kinetic pre-exponential factor
- $k_B$: Boltzmann’s constant, J/K
- $k$: Specified number of moments
- $L$: Abscissas
- $m_k$: kth moment of the number density function
- $m_v$: Mass of vapor molecule, kg
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