Cavitation modelling using real gas state equation: A conceptual study

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Abstract. The prediction of the onset of cavitation to allow investigations of the flow in off-design conditions during design is unavoidable for a variety of applications. Numerical modeling of the cavitation phenomena is however computationally challenging due to the nature of the phenomena. High density ratios, steep pressure gradients, the presence of multiple phase including phase change and hence to occurrence of real gas thermophysical behavior would cause a computational effort unmanageable during design. Today’s models are therefore greatly simplified representations of the reality. Conservation equations are usually solved using a mixture approach with flow properties being a volume fraction weighted average of two incompressible fluids thus neglecting real gas effects. The source term from the phase exchange however usually poses significant stability problems. In this article we will therefore present an approach for cavitation modeling using high-order polynomial real-gas state equations to accurately predict the properties of water at any state. Computational performance is improved by the use of structured tabulation using high order interpolation methods. The numerical results are then compared against measurement data and conventional cavitation model results.

1. Introduction

Accurate numerical results of cavitation is usually subject to two phase simulations using the mixture approach. The liquid and the gaseous state are thus represented using a phasic average of density and viscosity, reducing the two fluids to a single set of Navier-Stokes equations. The mass exchange between these phases in cavitating regions is further modeled through well known approaches as given by Zwart [1], Kunz [2] and others. These sudden increase in the source term is detrimental to the stability of the iterative solution procedure. Several authors have contributed to improve this behaviour. Stabilization through a diffusive contribution in the phasic equations can be found based on a Favre averaged derivation of the governing equations as shown in [3, 4, 5]. Linearization of the source term, as shown in [6], allows for a partial implicit integration in a pressure correction based framework as demonstrated in [7]. Furthermore, the pressure equation, which is based on the conservation of global mass, has its own variants. It can be defined using what is known as non-conservative form as shown in [7] or the conservative form as shown in [8]. Hence beside the uncertainties in the modeling of the mass exchange, the definition of the underlying conservation equations can vary as well. Although a variety of

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publicly available test cases exist, no complete cavitation theory was yet established. This is also related to the difficulties in identifying the exact local volume fraction from measurement data. In order to remove, at least partially, the uncertainty of the numerical modeling, this paper proposes an approach that removes the classical models for the phase change. Instead of computing mixture properties for density and viscosity, primitive quantities are computed accurately using real gas models. The properties of water at any state is well described using the IAPWS-97 formulation [9]. In the following section, the model is therefore described and applied to of test cases.

2. Governing equations

This section reviews the traditional mixture approach used in numerical algorithms for the prediction of cavitating flows. Their underlying equations are briefly described and discussed. The basic assumption of two incompressible fluids reduces the conservation of mass to a numerically stiff problem, leading to stability issues in cavitating regions. A new compressible formulation is thus proposed, abandoning the questionable mixture approach by accurately describing primitive quantities through real gas formulations.

2.1. Traditional mixture approach

As already introduced, traditional approach for the numerical modeling of cavitating flows use a mixture form of the conservation equations. The governing equations are thus representing a homogeneously mixed flow as defined by an interpenetrating continuum. Although the gas phase is clearly highly compressible, it is assumed incompressible in this formulation. The mixture density (\( \bar{\rho} \)) and viscosity (\( \bar{\mu} \)) are therefore computed based on the volume fraction (\( \alpha \)) as given in Eq. 1. Subscripts \( l \) and \( g \) refer to the liquid and gaseous phase properties respectively.

\[
\bar{\rho} = \alpha_l \rho_l + \alpha_g \rho_g \\
\bar{\mu} = \alpha_l \mu_l + \alpha_g \mu_g
\]  

(1)

Using the above given definition of the mixture quantities, the momentum equation is given in Eq. 2 using a single velocity field (\( u \)) for the mixture.

\[
\frac{\partial \bar{\rho} u}{\partial t} + \nabla \cdot \bar{\rho} u \otimes u = -\nabla p + \nabla \cdot \tau
\]  

(2)

Although, the two fluids are considered incompressible, the value of the mixture density can vary in space and time due to the volumetric averaging of the phasic densities and the unsteady nature of cavitation. Nevertheless, a variety of applications show a quasi steady cavitation bubble, hence it is possible, to numerically predict the impact of cavitation using steady state results.

Two formulations for the conservation of mass are known from literature. The non-conservative form, as used in a previous publication [7], takes the form as given in Eq. 3.

\[
\nabla \cdot u = \left( \frac{1}{\rho_l} + \frac{1}{\rho_g} \right) R_g
\]  

(3)

\( R_g \) is the mass transfer between the liquid and the gaseous phase. The equation is derived through a summation of phasic mass conservation in non-conservative form. When using the phasic conservation equations in their conservative form, the mass exchange has to disappear, since it is simply transferred from one phase to the other. The conservation of mass can therefore be found as shown in [8] and given in Eq. 4.

\[
\nabla \cdot \bar{\rho} u = 0
\]  

(4)
While the non-conservative form shows stability issues due to the non-zero right hand side, the conservative form suffers from sudden density jumps in the convective part. In order to avoid these well known numerical drawbacks, in the next section a compressible formulation of the underlying equations is proposed, showing a consistent approach that accurately describes the physics of cavitating flows for compressible and incompressible regions.

2.2. Compressible real gas approach

The derivation of the governing equations for compressible fluid flows with real gas state equations is given by the authors in great detail in [10]. As opposed to the traditional mixture formulation, the energy equation is solved as well, here in terms of total enthalpy \( h_0 \). This is indispensable to later allow a correct assessment of the thermophysical properties such as density in real gas flows. The governing equations in their general form are:

Continuity Equation

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (5)
\]

Momentum Equation

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = 0 \quad (6)
\]

Energy Equation

\[
\frac{\partial \rho h_0}{\partial t} - \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} \left[ \rho u_i h_0 + q_i - u_j \tau_{ij} \right] = 0 \quad (7)
\]

The term \( q_i \) is the heat diffusion and conveniently modeled using Fourier’s law.

In order to compute the properties of water any state, the IAPWS-97 [9]. This formulation accurately computes the properties of water not only in the liquid region but also in its gaseous state close to the two-phase region where real gas effects are no longer negligible. The formulation is split up into five different regions as shown in Fig. 1.

![IAPWS regions in the p-T diagramm](a) IAPWS regions in the p-T diagramm

![IAPWS regions in the p-v diagramm](b) IAPWS regions in the p-v diagramm

Figure 1: IAPWS regions

Region 1, 2 and 4 are of special interest when running cavitating flows. Region 1 is the liquid region, region 2 accounts for the properties of real gas and region 4 is the two-phase region in the phase transition. For cavitating flows, the vast majority of the domain is assigned to region 1, i.e. the liquid region. In regions of sudden pressure drop, the flow exhibits transition into the two phase region 4 and if expanded even further extends to region 2. The properties in the two phase region 4 are obtained using the definition of the void fraction as given in Eq. 8 based on static enthalpy \( h \).

\[
x = \frac{h(T, p) - h_l(T_{Sat}, p_{Sat})}{h_g(T_{Sat}, p_{Sat}) - h_l(T_{Sat}, p_{Sat})} \quad (8)
\]
The specific volume \( (v) \) is then defined through a linear combination of the saturation properties.

\[
v = xv(p_{\text{Sat}}, T_{\text{Sat}}) + (1 - x)v_g(p_{\text{Sat}}, T_{\text{Sat}})
\]  

(9)

To show exemplary the complexity of the state equations of the IAPWS-97 formulation, the definition of the specific volume for the gaseous region 2 is given below.

\[
v_2(p, T) = \frac{R_s T}{p} \pi \left( \gamma_o \pi + \gamma_r \pi \right)
\]  

(10)

The function is divided into an ideal gas contribution \( \gamma_o \pi \) and a residual part \( \gamma_r \pi \) accounting for real gas effects. \( \pi = p/p^* \) is a normalized pressure with \( p^* = 1 \text{MPa} \). The ideal gas and residual part are defined as:

\[
\gamma_o \pi = \frac{1}{\pi}
\]  

(11)

\[
\gamma_r \pi = \sum_{i=1}^{43} n_i I_i \pi^{I_i - 1} (\tau - 0.5)^J
\]  

(12)

With \( \tau = T^*/T \) and \( T^* = 540K \) and \( n_i, I_i, J_i \) being predefined coefficients. It becomes immediately clear that accounting for real gas effects increases the complexity of the state equation drastically. Iterative methods are required to solve for temperature given the enthalpy and pressure from the governing equations. These iterative methods with the highly polynomial expressions of the IAPWS-97 formulation require stable methods and was solved in the presented framework using Newton-Raphson root finding method as described in [10].

3. General description of numerical framework

The coupledNumerics solver [11] was adopted for all the computations. This framework solves the Navier-Stokes equations, given in Eq. 5, Eq. 6 and Eq. 7, in a (U)-RANS formulation and being based on the latest C++-17 version, it allows easy customization and implementation of new models extending the functionality to the specific purpose of the application.

The governing equations are discretized using a collocated, pressure-based approach in finite volume discretization environment. However, different to traditional methods, these equations are not solved sequentially (segregated). In particular the pressure velocity coupling, \( (u, v, w, p) \), is solved using a coupled (monolithic) approach. In this method the coupling of Eq. 5 and Eq. 6 is fully implicit and the resulting coefficients are stored in a single matrix, see Eq. 15.

\[
AX = B
\]  

(13)

\[
A = \sum_{p=1}^{N_{\text{cell}}} (A_p + A_{nb,p})
\]  

(14)

where:

\[
\begin{bmatrix}
A_{uu} & a_{uu}^{nb} & a_{uw}^{nb} & a_{up}^{nb} & u_p \\
A_{uv} & a_{uv}^{nb} & a_{uw}^{nb} & a_{up}^{nb} & v_p \\
A_{wu} & a_{wu}^{nb} & a_{uw}^{nb} & a_{wp}^{nb} & w_p \\
A_{wu} & a_{wu}^{nb} & a_{uw}^{nb} & a_{wp}^{nb} & p_p
end{bmatrix}
+ \sum_{p=1}^{N_{\text{cell}}} \begin{bmatrix}
a_{uu}^{nb} & a_{uw}^{nb} & a_{up}^{nb} & u_{nb} \\
a_{uv}^{nb} & a_{uw}^{nb} & a_{up}^{nb} & v_{nb} \\
a_{wu}^{nb} & a_{uw}^{nb} & a_{wp}^{nb} & w_{nb} \\
a_{wu}^{nb} & a_{uw}^{nb} & a_{wp}^{nb} & p_{nb}
end{bmatrix}
= \begin{bmatrix}
b_u \\
b_v \\
b_w \\
b_p
end{bmatrix}
\]  

(15)
The adopted monolithic algorithm allows efficient computations for all Mach ranges as well as for fluid-solid simulations (CHT, FSI). Further details considering the coupled assembly of the Navier-Stokes equations can be found in [12, 13, 14]. The extension to real gas is given in detail in [10] and therefore not repeated here.

4. Results

4.1. NACA-0012

The NACA-0012 testcase was previously investigated by the author’s using traditional cavitation models based on a mixture formulation of the Navier-Stokes equations and results have been published [8]. Water is entering the domain with a speed of 16.91 m/s. At the outlet, the static pressure is set to 51957 Pa. Turbulence is modeled using the Menter-SST formulation [15] with automatic wall functions and an inlet turbulence intensity of 3% with an eddy viscosity ratio of 10. The computational mesh is shown in Fig. 2 and consist of 9940 hexahedra elements.

![Figure 2: NACA-0012 Domain](image)

The distribution of the density on the plane can be seen in Fig. 3. A very sharp interface is found using the proposed real gas cavitation modeling.

![Figure 3: Mixture density](image)

The pressure distribution is plotted against experimental data and results obtained using the mixture formulation of previous publications as shown in Fig. 4. A reference run using purely incompressible formulation, i.e. without cavitation, is shown in black. As expected, the measurement results can not be captured when not properly accounting for the properties changes in the two phase region. The proposed approach can accurately describe the water properties in these cavitating conditions. In an earlier paper by the authors [8], results have been published using the traditional mixture approach. As reference and comparison with the proposed method, these results are also shown in Fig. 4 in red. The solution using the proposed real gas approach is given in green. It can be demonstrated that the proposed method shows excellent agreement with measurement results and the standard cavitation approach.

4.2. SHF Pump

As second test case the SHF Pump described in [16] is investigated. The pump has a shrouded impeller and an annulus for the water collection which then turns in the axial direction (bulb), i.e. there is no spiral casing. Therefore the computation of a single passage with a vaneless diffuser represents a meaningful approximation of the experimental setup.
The impeller diameter is 330 mm, with a rotation speed of 3000 rpm and a nominal flow rate is $Q_n = 0.157 m^3/s$. The computational domain for this preliminary study is quite coarse, with approx. 100'000 cells for the single passage as depicted in Fig. 5. It corresponds to the one investigated in previous publications, like [17] and [18]. Turbulence is modeled with the Menter SST turbulence model [15] using automatic wall functions.

Although quite coarse, this setup is sufficient to assess the methodology. More in depth investigations with finer mesh, various turbulence models and computational setups as well as head-drop curves at different flow rates will be performed in a second phase and published later.

The investigations were performed imposing flow rate at inlet and average pressure at outlet. This shows a small backflow zone at the outlet, but should not affect the analysis of the cavitation behavior. Fig. 6 shows the head drop as function of NPSH for experimental data ([16], [17] and [18]) and computations. The head is slightly overestimated (fully incompressible case) while the 3% NPSH is slightly underestimated. With respect to the NPSH of the head-drop the experiments have a certain spread and a tolerance of 0.5 m. Accordingly, it can be stated that for this preliminary investigation (coarse mesh) the results are satisfactory. Two important aspects are worth to be mentioned at this point about the computational procedure. First, using
the real gas approach the computations are considerably more stable than using a cavitation model with phasic equation. Every presented operating point was computed from a constant initial solution (and thus without cavitation), independent on the imposed NPSH and on the cavity extension. Within 200 to 300 iterations a stable head was achieved (see Fig. 7).

Second, no additional parameter is needed for the computations of cavitating conditions, thus clearly simplifying the case setup.

The cavitation bubble presents a very similar behaviour and evolution with NPSH as observed in the experiments (Fig. 7): first the bubble develops starting at the hub. Reducing NPSH the bubble becomes uniform along the blade span. Further reduction leads to an extension of the shroud-side region. In all computations the bubble starts, as observed in the experiments, from the leading edge.

5. Conclusions
A method for the prediction of cavitation using real gas state equations was described. This preliminary conceptual study shows the capabilities and potential of the proposed approach in combination with a pressure based coupled solver. Being able to properly account for the compressibility resulted in a robust numerical algorithm. The problematic source term, usually introduced by the modeling of the phase change in a mixture formulation, is removed through an accurate representation of the thermophysical properties based on the IAPWS-97 formulation. Proof of concept was given based on a cavitating NACA profile and using a centrifugal pump configuration. For both cases the results are satisfactory and good base to start more in depth investigations including mesh size, domain configuration/setup and turbulence model.

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Figure 6: Head drop curve for Q=Qn
Figure 7: Cavitation region

OP 1 = 14.7 NPSH, OP 2 = 9.7 NPSH, OP 3 = 6.7 NPSH

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