Multiscale Cavitation Sub-Grid Modeling via Population Balances as Linear Stochastic Processes

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Abstract

Keywords:

1. Introduction

Phenomenological Multiscale Cavitation Model. Dispersed cavities are tracked over multiple size scales, ranging from the smallest inception scale to a macroscopic scale where the assumption of spherical cavities no longer holds. The cavities grow and shrink as a consequence of competing effects of vapor pressure and surface tension. While the vapor pressure is constant for all cavities, the opposing surface tension depends on the specific cavity scale. The rate of bubble growth or shrinking therefore differs across scales.

The number density of bubble size scales is tracked across the different scales. Instead of a fixed time step, a diffuse time step is introduced, causing a broader variation in bubble dispersion over its evolution. The number density is therefore interpreted as a statistical mean over an effective average time step.

Employing a simplified Raleigh-Plesset equation, the growth or collapse rate is effectively constant, which makes the radius evolution linear in time. Accordingly, the radius change over a time step is directly proportional to the chosen time step. Consequently, number densities evolve through linear transfers between discrete scales. A Markov-chain formulation exploits this by encoding the evolution in a transition operator acting on the number-density vector.

In the following I denote a vector with in bold face $\mathbf{a}$ and its elements as a_i. The inner product is denoted as $\mathbf{a} \cdot \mathbf{b}$. A matrix is denoted with a capital letter Ω, while its elements are denoted as Ω_{ij}. The matrix-vector product is either denoted as $\Omega\mathbf{a}$ or using the Einstein notation $\Omega_{ij}a_j$, implying a summation over double indices. The element-wise multiplication of two vectors is $\mathbf{a} \circ \mathbf{b}$, and taking the element-wise cube of a vector uses $\mathbf{a}^{\circ 3}$.

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2. Theory

Bubble evolution on discrete scales.
The changes in sizes are governed by the Rayleigh-Plesset equation:

$$R\frac{d^2}{dt^2}R + \frac{3}{2}\left(\frac{d}{dt}R\right)^2 = \frac{p_g + p_v - p_l}{\rho_l} - \frac{4\nu_l}{R}\dot{R} - \frac{2\sigma}{\rho_l R} \tag{1}$$

Disregarding the viscous term and the acceleration term, bubble size changes are governed by pressure differences and surface tension, where $p_b = p_v + p_g - 2\sigma/R$ and the relevant pressure difference is $p_b - pl$. Since the remaining equation only defines the (squared) magnitude of the bubble growth rate, its direction must be determined separately. Hence, the absolute value of the pressure difference determines the growth rate magnitude, while the sign of the pressure difference sets whether the bubble grows or collapses. Furthermore, it is assumed that the cavity pressure and the liquid pressure change at a much slower rate, and hence $dR/dt \approx \dot{R}$.

$$\dot{R} = \pm\sqrt{\frac{2}{3}\frac{|p_b - p_l|}{\rho_l}} \tag{2}$$

where " $+$ " is used for evaporation, i.e. $p_b > p_l$, and " $-$ " for condensation.

discretizing.
I consider R_i, $i \in [0, M]$, the discrete scales of cavitation bubbles, representing different bubble sizes. The scale R_0 is reserved for cavitation nuclei. The respective scales are bounded by r_i, $i \in [0, M+1]$, with $r_0 = 0$, $r_1 = r_{min}$ and $r_{M+1} = r_{max}$. The volumetric bin size grows by a factor $\Gamma \geq 1$:

$$r_{i+1}^3 - r_i^3 = \Gamma(r_i^3 - r_{i-1}^3) \tag{3}$$

The representative scale R_i is defined as the cubic mean of adjacent bin edges for $i \in [1, M]$, and as zero for the nuclei bin $i = 0$. Setting the nuclei radius to zero ensures that this scale supplies bubble numbers without contributing to the vapor fraction.

$$R_i = \begin{cases} \sqrt[3]{\frac{r_i^3 + r_{i+1}^3}{2}} & i \in [1, M] \\ 0 & i = 0 \end{cases} \tag{4}$$

The bubble pressure is evaluated at each representative radius R_i for $i \in [1, M]$ with equation (5). At the nuclei scale, p_{b0} is constrained by two conditions: it must supply nuclei, when R_1 cavitates, and it must condensate, when R_1 condensates, avoiding spirious oscillations of number density between the two lowest scales. By setting the absolute pressure difference $p_{b0} - p_l$ to be a fraction of the pressure difference $p_{b1} - p_l$, both requirements are fulfilled. The resultant bubble pressure is defined in equation (6). The growth rate follows from the radius rate-of-change equation (2) for each representative scale.

$$
p_{bi} = p_v + p_g - \frac{2\sigma}{R_i}, \qquad i \in [1, M] \tag{5}
$$

$$
p_{b0} = \beta p_{b1} + (1-\beta) p_l, \qquad 0 < \beta < 1 \tag{6}
$$

the diffuse time step.

Since all bubbles in a given bin i have the same size R_i, they grow simultaneously with rate $\dot{R}_i$, and the number density n_i occupation moves collectively to another bin j. **[if all bubbles were in R_0, would the evolution then be similar to Schnerr-Sauer's model?]** This is not depicting particular interesting dynamics.

Instead, I am introducing the diffuse time step, where δt denotes the mean in the interval $[\delta t^-, \delta t^+]$, where $\delta t^\pm = \delta t * (1 \pm \epsilon)$, $0 < \epsilon \leq 1$. All bubbles in a given bin are exposed to the pressure difference for a duration between δt^- and δt^+, and hence their size differences covers an interval $[\dot{R}_i \delta t^-, \dot{R}_i \delta t^+]$. This effectively spreads the number density evolution across several bins. Therefore, the number density can be regarded as stochastic variable.

The discrete time step δt and its range ϵ predominately control, if number densities travel across bins. Two conditions must be met, in order to facilitate the least dynamics: In case of evaporation, the growth of the second-biggest bin must reach the biggest bin. In case of condensation, the shrinking bubbles in the largest bin must reach the second-largest.

$$
\delta t > \frac{1}{1+\epsilon} \max \left\{ \frac{r_M - R_{M-1}}{|\dot{R}_{M-1}|}, \frac{R_M - r_M}{|\dot{R}_M|} \right\} \tag{7}
$$

The Markov Chain.

The linearity of the bubble growth allows to model the redistribution of bubble numbers across scales through a Markov chain, see equation (8). The number density vector at a new time step n_i' is calculated as the product of the transition matrix Γ_{ij} and the recent number density vector n_i. The transition matrix holds transition fractions $0 \leq \Gamma_{if} \leq 1$. The lower-triangular entries (highlighted in red) are evaporation coefficients, while the upper-triangular (the blue ones) are condensation coefficients.

$$
\begin{pmatrix}
\Gamma_{00} & \Gamma_{01} & \Gamma_{02} & \Gamma_{03} & \ldots \\
\Gamma_{10} & \Gamma_{11} & \Gamma_{12} & \Gamma_{13} & \ldots \\
\Gamma_{20} & \Gamma_{21} & \Gamma_{22} & \Gamma_{23} & \ldots \\
\Gamma_{30} & \Gamma_{31} & \Gamma_{32} & \Gamma_{33} & \ldots \\
\ldots & \ldots & & &
\end{pmatrix}
\begin{pmatrix} n_0 \\ n_1 \\ n_2 \\ n_3 \\ \ldots \end{pmatrix}
=
\begin{pmatrix} n_0' \\ n_1' \\ n_2' \\ n_3' \\ \ldots \end{pmatrix} \tag{8}
$$

If I have conservation of total bubble number, $\sum_i^M \Gamma_{ij} = 1$.

For the calculation of the transition coefficients, I take a starting point in bin i. In the following I am developing the $i-$th column in the transition matrix.

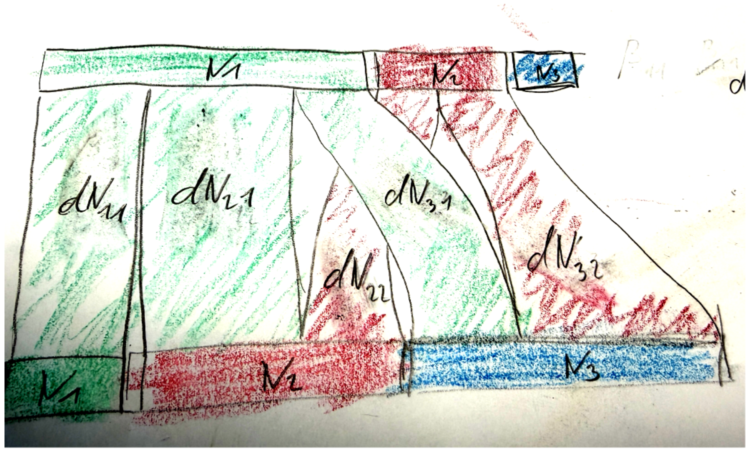

Figure 1: Caption

$$\delta R_i^- = min(\dot{R}_i \delta t^-, \dot{R}_i \delta t^+) \tag{9}$$
$$\delta R_i^+ = max(\dot{R}_i \delta t^-, \dot{R}_i \delta t^+) \tag{10}$$

Let $a_i, b_i, a_i \leq b_i$, be the bins in which the smallest and the largest size changes fall:

$$a_i = k : r_k < R_k + \delta R_i^- \leq r_{k+1} \tag{11}$$
$$b_i = k : r_k < R_k + \delta R_i^+ \leq r_{k+1} \tag{12}$$

if $a_i = b_i$

$$\Gamma_{ii} = 1 \tag{13}$$
$$\Gamma_{jk} = 0, \quad \forall j, k \neq i \tag{14}$$

with $\delta R_i^+ - \delta R_i^- = 2\dot{R}_i \epsilon \delta t$

$$\Gamma_{ai} = \frac{r_{a+1} - (R_i + \delta R_i^-)}{2\dot{R}_i \epsilon \delta t} \tag{15}$$
$$\Gamma_{ji} = \frac{r_{j+1} - r_j}{2\dot{R}_i \epsilon \delta t}, \quad j \in [a+1, b-1] \tag{16}$$
$$\Gamma_{bi} = \frac{R_i + \delta R_i^+ - r_b}{2\dot{R}_i \epsilon \delta t} \tag{17}$$
$$\Gamma_{ji} = 0, \quad j \in [0, a-1], j \in [b+1, M] \tag{18}$$

$$\frac{d}{dt}\mathbf{n} = \lim_{dt \to 0} \frac{\mathbf{n}(t+dt) - \mathbf{n}(t)}{dt} \approx \frac{(\Gamma - \mathbb{1})\mathbf{n}}{\delta t} \tag{19}$$

macroscopic volume mass source $\dot{m}$.

$$\frac{d}{dt}(\alpha\rho_v) = \dot{m} \tag{20}$$

$$\dot{m} = \frac{4}{3}\pi\rho_v \sum_{i=0}^{M} \left(R_i^3 \frac{d}{dt} n_i + 3 n_i \frac{d}{dt} R_i \right) \tag{21}$$

$$= \frac{4}{3}\pi\rho_v \frac{\mathbf{R}^{\circ 3} \cdot (\Gamma - \mathbb{1})\mathbf{n}}{\delta t} + 3\mathbf{n} \cdot \dot{\mathbf{R}} \tag{22}$$

using: $d/dt R_i \approx \dot{R}_i$

The number density.
Let n_i, $i \in [0, M]$ be the number density of the respective scales. assuming spherical bubbles:

$$\alpha = \frac{4}{3}\pi \sum_{i=0}^{M} n_i R_i^3 = \frac{4}{3}\pi\, \mathbf{n} \cdot \mathbf{R}^{\circ 3} \tag{23}$$

In the absence of coalescence modeling, the total number of bubbles per unit volume is a conservative variable, $\sum_{i=0}^{M} n_i = n_{tot}$. When all n_{tot} bubbles are in the largest scale R_M, the entire unit volume is occupied with vapor. Therefore, the greatest bubble scale the total number of bubbles are related through:

$$n_{tot} \frac{4}{3}\pi R_M^3 = 1 \tag{24}$$

model summary.

- The discrete scales are defined with the parameters $N, r_{min}, r_{max}, \Gamma$.
- The magnitude of cavitation inception is controlled with the β coefficient in equation (6). The total number of bubbles is controlled by the largest radius, see equation (24.
- The time step is set through δt and ϵ. For a given ϵ, equation (7) defines the practical lower limit for the time step.