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Theoretical model of ice nucleation induced by acoustic cavitation. Part 1: Pressure and temperature profiles around a single bubble

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ABSTRACT

This paper deals with the inertial cavitation of a single gas bubble in a liquid submitted to an ultrasonic wave. The aim was to calculate accurately the pressure and temperature at the bubble wall and in the liquid adjacent to the wall just before and just after the collapse. Two different approaches were proposed for modeling the heat transfer between the ambient liquid and the gas: the simplified approach (A) with liquid acting as perfect heat sink, the rigorous approach (B) with liquid acting as a normal heat conducting medium. The time profiles of the bubble radius, gas temperature, interface temperature and pressure corresponding to the above models were compared and important differences were observed excepted for the bubble size. The exact pressure and temperature distributions in the liquid corresponding to the second model (B) were also presented. These profiles are necessary for the prediction of any physical phenomena occurring around the cavitation bubble, with possible applications to sono-crystallization.

1. Introduction

1.1. Context and aim of the study

The unstable (inertial) acoustic cavitation of micron size gas bubbles in a liquid medium and especially their violent collapses induce extreme physical conditions (pressures up to tens of GPa, temperatures up to tens of thousands K), inside and in the close vicinity of the bubbles. These conditions are at the origin of spectacular effects like: sonoluminescence, hydroxyl radicals generation, solid surface erosion but also promote the crystallization of solutes in super-saturated solutions or of solvent in super-cooled solutions [1].

In order to keep these phenomena under control, one needs to know exactly the evolution of physical parameters (pressure, temperature, composition) of the gas inside the bubble but also that of the liquid outside as the two are tightly linked one to another.

However, the first concern of most of the studies on acoustic cavitation devoted to interpret sonochemistry and sonoluminescence was the behavior of the gas in the bubble and not that of the surrounding liquid. Thus an approximate way to describe the gas thermal behavior, the heat transfer at the interface and on the liquid side was often adopted in order to obviate the solution of a full set of energy and motion equations in the liquid. In most cases the gas pressure inside the bubble was considered uniform and the motion of the liquid was described by the classical Rayleigh–Plesset equation corrected for liquid compressibility [2–4]. The gas behavior depends strongly on the heat transfer rate across the bubble wall. In a very simplified approach, the slow bubble expansion can be considered as isothermal, while the fast collapse as adiabatic. From that point the basic modeling approach was to describe the gas state by a polytropic equation with a coefficient depending on the Peclet number [5]. As concerns heat transfer in the liquid surrounding the bubble, the simplest assumption was to neglect any thermal gradient and to keep the bubble wall temperature constant at the ambient value [4,6,7]. Another kind of simplified thermal approach was to consider the continuity of the heat flux across the bubble wall and to adopt an arbitrary liquid temperature profile in order to evaluate the heat flux outside the bubble [8,9].

A trend for a more in depth description of the heat transfer between the gas and the liquid was dictated by the recognition of the very important role that plays water vapor in the physics of a collapsing bubble [10–12] and thus the need to take into account the phase change (condensation or evaporation) at the bubble wall and consequently to incorporate a heat balance at the wall in the global model.

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The first aim of this study was to calculate accurately the pressure and temperature at the bubble wall and in the liquid adjacent to the wall just before and just after the collapse, starting from the mathematical description of the gas behavior and of the bubble wall motion already established and validated in the literature.

The second aim was to show the importance of the assumptions concerning heat transfer at the bubble wall and in the surrounding liquid, by considering two different modeling approaches briefly presented below:

(A) Inside the bubble, a thermal gradient was supposed to exist in the gas over a thin boundary layer near the bubble wall, with a thickness varying accordingly to the wall dynamics. A constant bubble wall (liquid–gas interface) temperature equal to the far field liquid temperature was assumed, with no thermal gradient on the liquid side.
(B) Inside the bubble, the same hypothesis as for case A was adopted. Outside the bubble, a non-linear temperature profile in the liquid was introduced, determined as an approximate analytical solution of the heat conduction–advection equation. Moreover, the wall temperature was evaluated from the heat balance at the wall including water liquid–vapor phase change effect.

1.2. Bibliographical review

In this section a short review of the recent literature concerning the pressure and temperature profiles inside and outside the bubble will be given.

Kwak and Na [8] calculated density, pressure and temperature distributions inside an air bubble by solving analytically the conservation PDEs but neglecting the viscous dissipation and water vapor. The time evolution of the bubble radius was obtained from the Keller–Miksis equation. The heat flux on the liquid side of the bubble wall was expressed by the boundary layer approximation with the layer thickness being a fitting parameter.

Yasui [10] used thoroughly the boundary layer approach in order to evaluate the time profiles of gas temperature, gas pressure, water content and bubble wall temperature for an argon bubble. As concerns the heat transfer between the gas and the liquid, he adopted an arbitrary layer thickness on the gas side and an exponential profile on the liquid side with one fitting parameter and he considered a heat balance at the wall including the phase change effect.

Toegel et al. [6] aimed at determining the amount of water vapor trapped in the bubble during the collapse and its impact on sonoluminescence. They used the boundary layer approach and considered a model consisting of 3 ODEs. The bubble wall radius was evaluated by the Keller–Miksis equation which takes water compressibility into account, the amount of water vapor inside the bubble was derived from a Fickian diffusion flux at the wall, the gas temperature was obtained from an energy balance which takes the heat conduction flux at the bubble wall into account. The mass and heat fluxes on the gas side were calculated using a boundary layer thickness evaluated as diffusion length at a characteristic time scale of the bubble motion. The gas pressure was derived from the van der Waals equation of state. The temperature at the bubble wall was supposed constant and equal to the far liquid one.

Kim et al. [9] solved the rigorous set of PDEs on the gas side but adopted the Keller–Miksis equation for the bubble wall motion and considered a priori a parabolic temperature profile in a thermal boundary layer on the liquid side. The thickness of the liquid boundary layer was estimated by means of an ODE obtained by the integration of the advection–conduction heat transfer equation over the layer. On this basis, the temperature profiles inside and outside an air bubble (without water vapor) were finally determined.

The approach of Vuong et al. [13] was very similar, excepted that no arbitrary temperature profile was adopted on the liquid side. The heat transfer equation in the liquid was transformed by the Plesset–Zwick method and simplified assuming a thin boundary layer (large Peclet's number) in order to obtain finally a linear diffusion equation in Lagrangian boundary layer coordinates which was solved numerically. Vuong et al. [13] used this model to determine the radial gas temperature profiles and bubble wall temperature time profiles for an argon bubble.

Yuan et al. [14] also transformed the advection–conduction equation on the liquid side into a purely diffusive one by means of the Plesset–Zwick variable change but made no further simplification to solve it. He calculated numerically the radial profiles of gas pressure, temperature, velocity and density for a bubble containing only air. The equations of liquid motion were not solved, the Keller–Miksis equation was used to describe the wall dynamics and the liquid compressibility was neglected in the heat transfer equation.

As concerns the heat transfer on the liquid side, Hauke et al. [15] adopted the less restrictive approach as compared to the already cited works. They solved numerically the full set of governing PDE on the gas side and the heat advection–conduction equation on the liquid side (neglecting only the liquid compressibility in the heat transfer equation) using the Keller–Miksis formulation to describe the bubble wall motion. They provided the radial profiles of temperature, pressure and water vapor content inside the bubble as well as the radial temperature profile outside the bubble.

In the context of therapeutic ultrasound, cavitation and bubble dynamics imply very high acoustic pressures and frequencies as well as elevated temperatures. In such conditions, the mass and heat transfer at the bubble wall are particularly important. To address the relevant physics, a reduced-order model of a single, spherical bubble was proposed by Kreider et al. [12] that incorporates phase change at the liquid–gas interface as well as heat and mass transport in both phases. Two approaches for heat transfer on the liquid side were modeled and compared. In the "scaling" approach (SCL model), uniform liquid temperature was assumed everywhere outside of a boundary layer near the bubble wall and a Fickian expression was used for calculating the thermal flux within the boundary layer. A fitting parameter was needed for estimating the boundary layer thickness. In the second approach the Plesset–Zwick analytical solution was used for describing thermal conduction in the presence of advective liquid flow due to bubble wall displacement. The idea of applying the Plesset–Zwick model for heat transfer on the liquid side used in several studies cited above was adopted for this study.

The applied acoustic driving conditions (P_{ac} – acoustic pressure amplitude, f – acoustic frequency, R_0 – initial bubble radius) and the corresponding gas temperature (T_g) as well as gas–liquid interface temperature (T_i) and pressure (P_{li}) at the collapse are presented in Table 1 for the considered publications and compared with the results of this study.

Independently of the conditions considered and thus of the maximal gas temperature obtained in each particular case, all the results shown above can be roughly classified in two groups: a first group where the bubble wall temperature is of the same order of magnitude than the bubble core one [8–10,12] and the second group where the wall temperature is one order of magnitude lower than the core one [13–15]. It is a very marked difference. Furthermore, again in a rough manner, it can be claimed that the results of the first group are based on simplified modeling approaches (boundary layer approximations, arbitrary liquid temperature profiles, analytical solutions) while those of the second group are based on a more comprehensive and rigorous