Ultrasonics - Sonochemistry 41 (2018) 449–457

Contents lists available at ScienceDirect

Ultrasonics - Sonochemistry

journal homepage: www.elsevier.com/locate/ultson

Influence of reactions heats on variation of radius, temperature, pressure and chemical species amounts within a single acoustic cavitation bubble

Kaouther Kerboua, Oualid Hamdaoui*

Laboratory of Environmental Engineering, Department of Process Engineering, Faculty of Engineering, Badji Mokhtar – Annaba University, P.O. Box 12, 23000 Annaba, Algeria

ARTICLE INFO

Keywords:
Acoustic bubble
Thermal balance
Reactions heats
Temperature
Pressure
Free radicals

ABSTRACT

The scientific interest toward the study of acoustic bubble is mainly explained by its practical benefit in providing a reactional media favorable to the rapid evolution of chemical mechanism. The evolution of this mechanism is related to the simultaneous and dependent variation of the volume, temperature and pressure within the bubble, retrieved by the resolution of a differential equations system, including among others the thermal balance. This last one is subject to different assumptions, some authors deem simply that the temperature varies adiabatically during the collapsing phase, without considering the reactions heat of the studied mechanism. This paper aims to evaluate the pertinence of neglecting reactions heats in the thermal balance, by analyzing their effect on the variation of radius, temperature, pressure and chemical species amounts. The results show that the introduction of reactions heats conducts to a decrease of the temperature, an increase of the pressure and a reduction of the bubble volume. As a consequence, this leads to a drop of the quantities of free radicals produced by the chemical mechanism evolving within the bubble. This paper also proved that the impact of the consideration of reactions heats is dependent of the frequency and the acoustic amplitude of the ultrasonic wave.

1. Introduction

During the last decades, an increasing number of authors dedicated their works to the theoretical study of cavitation bubble phenomenon [1–6]. Each study adopted a set of hypotheses regarding the dynamical, kinetical and thermal behaviors of gases within the bubble. This last parameter is of crucial role in the determination of the evolution of reactional system inside the bubble, especially during the collapsing phase. Generally, for simplification purposes, some authors assume that the regime during this phase is simply adiabatic [7–10], neither heat exchange with external media, nor reactions heats are taken into account in the thermal balance. Hence, the variation of temperature would be described by the basic equation of adiabatic regime, governed only by the variation of bubble volume [11]. In the study of Sochard et al. [12], the regime is considered as polytropic during the collapsing phase, thus, the reactions heats are not considered in the simulation of temperature variation.

The chemical mechanism within an acoustic cavitation bubble cannot evolve without absorbing or releasing energy, according to the nature of reactions it includes. Assuming an adiabatic collapse and neglecting reactions heats can then be justified by the simplification of calculation, in case results are not widely affected when reactions heats are taken or not into account. If proved to be true, the temperature is then simply retrieved using the state equation expression corresponding to adiabatic regime [9], while it becomes a more complex expression established through an energy balance considering the pressure forces work, the variation of internal energy and the reactions heats, with emitting an assumption of no energy dissipated to the surrounding liquid media. In the studies of Yasui [13] and Sivasankar and Moholkar [14], the authors established the thermal balance with including the reactions heats of the adopted mechanism in the numerical model.

In this work, we propose to compare the results given by two computational studies of radius, temperature, pressure and chemical species yields variations within an acoustic cavitation bubble during its oscillation. Both approaches include a description of the dynamical behavior of the bubble, the thermal balance inside it and the mass balance represented by the kinetical equations related to the studied mechanism, they differ only in the treatment of the thermal behavior within the bubble. The first approach is based on a simplifying assumption largely adopted, deeming that the temperature varies adiabatically during the collapsing phase, while the second approach is built on a thermal balance taking into account the heats corresponding to the reactions of the chemical mechanism. The modification of this equation has a direct impact on the other parameters variations, as the

* Corresponding author.
E-mail address: ohamdaoui@yahoo.fr (O. Hamdaoui).

http://dx.doi.org/10.1016/j.ultsonch.2017.10.001
Received 11 September 2017; Received in revised form 1 October 2017; Accepted 1 October 2017
Available online 03 October 2017
1350-4177/

Nomenclature

P_∞	Pressure in the liquid media (Pa)
P_A	Acoustic amplitude (Pa)
P_B	Pressure within the bubble (Pa)
P_v	Vapor pressure (Pa)
P_0	Initial pressure (Pa)
P_g	Gas pressure (Pa)
R_g	Ideal gas constant (J/mol K)
R_{max}	Maximum radius (m)
R_0	Ambient radius (m)
T_∞	External media temperature (K)
T_b	Temperature within the bubble (K)
V_0	Initial volume of the bubble (m^3)
X_k	Molar concentration of the kth species (mol/m^3)
n_0	Initial molar amount (mol)
r_i	Reaction rate of the i reaction (mol/s m^3)
w_k	Production rate (mol/s m^3)
A_{fi}	Pre-exponential factor of the ith forward reaction (m^3/mol s) for a two-body reaction and in m^6/mol^2 s for a three-body reactions
A_{ri}	Pre-exponential factor of the ith backward reaction (m^3/mol s) for a two-body reaction and in m^6/mol^2 s for a three-body reactions
E_{afi}	Activation energy of the ith forward reaction (J)
E_{ari}	Activation energy of the ith backward reaction (J)
b_{fi}	Temperature exponent of the ith forward reaction in Arrhenius equation
b_{ri}	Temperature exponent of the ith backward reaction in Arrhenius equation
k_{fi}	Forward rate constant of the ith reaction
k_{ri}	Backward rate constant of the ith reaction
ϑ_{ki}	Stoichiometric coefficient of the kth chemical species in the ith reaction
a	Van der Waals constant (m^6 Pa/mol^2)
b	Van der Waals constant (1/m^3 mol)
c	Sound celerity (m/s)
f	Frequency (Hz)
n	Molar quantity (mol)
R	Bubble radius (m)
t	Time (t)
T	Temperature (K)
V	Volume (m^3)
μ	Dynamic viscosity (Pa.s)
ρ_L	Density of the liquid (kg/m^3)
σ	Surface tension (N/m)
ΔH_i	Reaction heat of the ith reaction (J/mol)
C_{O_2}	Oxygen concentration (mol/m^3)
C_p	Isobaric molar specific heat capacity (J/mol K)
C_v	Isochoric molar specific heat capacity (J/mol K)

differential equations set in each model are dependent. The purpose of this study is to evaluate the extent that the effect of the introduction of reactions heats can have on the values of different parameters over time.

2. Numerical models

The theoretical procedure used to build the numerical models studied in this paper is based on the combination of some differential equations according to the phase of the bubble oscillation, i.e. expansion or collapsing phase, and the assumptions of the model, i.e. either or not the reactions heats are taken into account.

Both computational simulations deem that the expansion phase is isothermal [3,10,15,16]; there is no variation of temperature in this phase, hence, the chemical kinetics knows no evolution. The differential equations that describe the mass balance due to the chemical mechanism are introduced in the simulation programs during the collapsing phase, to study the growth of chemical products amount, especially free radicals. The temperature variation has a major influence on the evolution of the kinetics within the bubble; this parameter is governed by a heat balance. In the first approach, the gases inside the acoustic bubble are assumed to incur a physical adiabatic transformation, thus, the variation of temperature would be described through the expression of state equation in adiabatic regime or Laplace's law, using the adiabatic index [3]. In the second approach, the gases are considered to undergo a chemical transformation, including the reactions heats related to the studied mechanism, with some endothermic and other exothermic elementary reactions [17]. We assume in this approach that the bubble has no thermal exchange with the surrounding media, which defines a chemical adiabatic process. In both approaches, during the expansion phase, the internal energy of the bubble is considered to be constant, indeed, the time derivate of temperature remains null as the process is isothermal. During the collapsing phase, the first one considers that the gases are exposed only to the pressure forces, the internal energy, expressed through the multiplication product of the temperature time variation and the isochoric specific heat capacity of the medium inside the bubble, equals in this case to the work of pressure forces. In the second approach, the internal energy variation during the collapsing phase depends, in addition to the previous term, of the creation of energy due to reactions heats. This is expressed by establishing a thermal balance with no dissipation of energy.

The variation of the volume of the bubble, i.e. the variation of its radius, is studied in both cases through the Keller-Miksis equation [18] describing the dynamical behavior of the bubble during its oscillation. The set of differential equations related to the dynamical, thermal and kinetical evolution of the acoustic bubble and its content constitutes, in each case, a system to resolve numerically by the fourth-order Runge-Kutta method.

The development of each differential equation used in the system is presented in the following.

2.1. State equation

In this work, we resume the approach followed in our previous work [19] regarding the model employed to describe the state of gases within the acoustic bubble during its oscillation. Two hypothesis are considered, the ideal gas with its law [20], almost for simplification purposes, and the real gas model, with the Van der Waals equation [15], more abide by the conditions of temperature attained inside the bubble during its compression. A similar treatment is applied to both cases as explained in what follows.

2.2. Dynamics of bubble oscillation

The dynamics of acoustic bubble is described by the Keller Miksis equation that is derived for the radial oscillations of a bubble trapped in a sound field [18]. It takes into account the viscosity, surface tension, incident sound wave, and acoustic radiation coming from the bubble. Its expression is given by the following formula

$$\left(1-\frac{\dot{R}}{c}\right)R\ddot{R}+\frac{3}{2}\left(1-\frac{\dot{R}}{3c}\right)\dot{R}^2=\frac{1}{\rho_L}\left(1+\frac{\dot{R}}{c}+\frac{R}{c}\frac{d}{dt}\right)[P_B-P(t)] \quad (1)$$

where R is the radius of the bubble, the dots indicate first and second time derivatives, ρ_L is the density of the liquid, c is the speed of sound through the liquid and t is time, P(t) and P_B are given by the expressions