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Insights into numerical simulation of controlled ultrasonic waveforms driving single cavitation bubble activity

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ABSTRACT

A computational study treating cavitation phenomenon within a single bubble undergoing various controlled ultrasonic waveforms is presented in this paper. Numerical simulations using sinusoidal, square, triangular and sawtooth waves crossing an aqueous media, saturated with oxygen, are conducted upon various operational conditions of frequency and amplitude. Bubble radius, temperature and pressure were estimated over time for 64 combined cases. The obtained results show that at relatively low acoustic pressure, i.e. 1.5 and 2 atm, the square wave is proved to generate the highest temperature and pressure inside the bubble, while triangular and sawtooth ones remain the less interesting waveforms for sonochemical application within the same operational conditions. At higher amplitudes above 2.5 atm, this trend is changed, especially at low frequencies, i.e. 200 and 300 kHz, where square wave showed some limitations in attaining the optimal values of the strong collapse within one acoustic cycle.

1. Introduction

Ultrasonic wave travelling through liquid leads to the creation, expansion and implosive collapse of bubbles [1]. This phenomenon knows several application in sonochemistry and sonoluminescence [2,3]. The characteristics of the ultrasonic wave are determinant in leading to the extreme physical and chemical conditions inside the cavitation bubble during strong implosion, in addition to the mechanical oscillation of the bubble. Both generated phenomenon were distinguished previously in term of energy analysis by Moholkar et al. [4] who proposed an ultrasound bath composed of cavitating media and a nanocavitating one, in order to map the energy due to ultrasound itself (mechanical oscillation), and the one due to local activity of the bubble (hot spot from transient cavitation). The effects of acoustic frequency and amplitude on cavitation activity were subject of several research works at both theoretical and experimental levels. Ferkous et al. [5] analyzed in their study the effect of acoustic condition of the ultrasonic wave on the sonolytic degradation of naphthol blue black in water, while Kirpalani and McQuinn [6] reinvestigated the products yields in high frequencies sonochemical reactors. Besides, Tatake and Pandit [7] examined the effect of dual frequency waves on cavitation bubble activity and Brotchie et al. [8] studied the sonochemistry under simultaneous high- and low-frequency irradiation.

Theoretically, several studies proposed numerical models to simulate the cavitation bubble growth and its sonochemical activity, based on various assumptions and different approaches. For instance, Yasui [9] established in 1997 a model for single bubble sonoluminescence in an attempt to explain the single bubble sonoluminescence experimental observations. Ferkous et al. [10] supported their experimental results regarding the sonochemical degradation of naphthol blue black in water by a mathematical model built on bubble dynamics and chemical kinetics equations. The same model has been first presented by Merouani et al. [11] who focused their work on the effect of frequency and acoustic amplitude on the bubble radius evolution. Meidani and Hasan [12] suggested a different theoretical vision considering the coupled momentum of energy and mass transport equations and conducted their study under various amplitudes (0.3, 0.5 and 0.9 bar) and frequencies (20, 25, 35 and 45 kHz). Prosperetti and Lezzi [13] as well as Aymé-Bellegarda [14] studied the response of cavitation oscillating under a Gaussian pulse, while several authors worked on the effect of vapor–gas mixture on the variation of acoustic bubble activity [15,16].

An overall review of the numerical works cited previously exhibits that the ultrasonic wave parameters usually examined are its frequency and amplitude. However, intuitively, only the sinusoidal waveform was considered, and to the best of our knowledge, no controlled shape of ultrasonic wave for cavitation application was invoked before in a computational study.

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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)
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 k^{th} species (mol/m^3)
n_0	initial molar amount (mol)
r_i	reaction rate of the i^{th} reaction ($mol/s\,m^3$)
w_k	production rate ($mol/s\,m^3$)
A_{fi}	pre-exponential factor of the i^{th} 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 i^{th} 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 i^{th} forward reaction (J)
E_{ari}	activation energy of the i^{th} backward reaction (J)
b_{fi}	temperature exponent of the i^{th} forward reaction in Arrhenius equation
b_{ri}	temperature exponent of the i^{th} backward reaction in Arrhenius equation
k_{fi}	forward rate constant of the i^{th} reaction
k_{ri}	backward rate constant of the i^{th} reaction
ϑ_{ki}	Stoichiometric coefficient of the k^{th} chemical species in the i^{th} 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)
R	bubble radius (m)
t	time (s)
T	temperature (K)
V	volume (m^3)
μ	dynamic viscosity (Pa s)
ρ	density (kg/m^3)
σ	surface tension (N/m)

The objective of this paper is to highlight one of the less analyzed wave aspects: the waveform, by proposing four different shapes (sinusoidal, square, triangular and sawtooth ultrasonic wave), whose frequencies and acoustic amplitudes vary in the ranges of 200, 300, 500 and 1000 kHz, and 1, 1.5, 2 and 2.5 atm, respectively. The Acoustic conditions chosen for this study were selected for their relevance in the application intended by this work. These specific values were previously employed by our research group in several theoretical and experimental studies [5,17–19]. Moreover, some intermediate conditions, as 800 kHz, were already examined in simulation and proved to respect the monotonous order found in this paper. The investigation is conducted through mathematical models based on similar assumptions except the waveform. The results, consisting in cavitation parameters variation within an aqueous bubble saturated with oxygen, were compared and several monotonous trends were stood out.

2. Computational simulation model

This work is based on a numerical model formulated as a system of differential equations, describing simultaneously the dynamical, thermal and chemical evolution inside a cavitation bubble, travelled by an ultrasonic wave whose the form is controlled.

The studied media is supposed to be water saturated with oxygen, characterized by constant temperature and pressure of 293 K and 1 atm, respectively [20]. The bubble created within this media is assumed to be spherical with a punctual symmetric distribution, around its center, of different physical and chemical parameters. The initial volume of the bubble is defined by its ambient radius [18], depending at its turn of the acoustic conditions of the ultrasonic wave as reported in Table 1 of our previous work [20]. This volume contains at the beginning of the bubble oscillation two chemical species: H_2O and O_2. Their initial quantities are expressed through Van der Waals state equation given by the formula

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nR_g T \tag{1}$$

The water vapor results of the gas–liquid phase equilibrium, its pressure is temperature dependent and is expressed by Antoine's law

Table 1

Time analysis results: normalized expansion time, implosion time and collapse duration at the various acoustic couples for the four waveforms.

Acoustic conditions		Normalized expansion time (%)				Normalized implosion time (%)				Normalized collapse duration (%)			
Amplitude (atm)	Frequency (kHz)	Sinusoidal	Square	Triangular	Sawtooth	Sinusoidal	Square	Triangular	Sawtooth	Sinusoidal	Square	Triangular	Sawtooth
1.5	200	55	58	50	39	75	82	70	63	20	24	20	24
	300	53	58	50	38	74	82	70	62	20	24	20	25
	500	55	58	50	39	77	83	72	66	22	25	22	27
	1000	54	58	53	43	79	85	78	73	25	27	25	30
2	200	59	65	59	50	84	95	82	79	25	31	23	29
	300	59	62	57	50	83	91	80	77	24	29	23	28
	500	57	61	54	47	80	88	76	74	23	28	22	27
	1000	57	60	55	45	81	88	78	74	23	28	23	28
2.5	200	63	67	64	60	91	–	90	91	28	–	26	31
	300	64	67	63	59	92	–	89	90	27	–	26	31
	500	64	67	61	55	90	99	86	85	26	33	25	30
	1000	59	64	55	48	82	93	78	76	23	29	23	28
3	200	67	69	67	63	98	–	96	97	31	–	29	34
	300	63	68	66	65	93	–	95	97	30	–	28	33
	500	68	78	64	62	99	–	91	94	31	–	27	32
	1000	63	67	60	56	90	99	84	85	27	33	24	29