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Modeling the dynamics of single-bubble sonoluminescence

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Abstract

Sonoluminescence (SL) is the phenomenon in which acoustic energy is (partially) transformed into light. It may occur by means of one bubble or many bubbles of gas inside a liquid medium, giving rise to the terms single-bubble and multi-bubble sonoluminescence (SBSL and MBSL). In recent years some models have been proposed to explain this phenomenon, but there is still no complete theory for the light-emission mechanism (especially in the case of SBSL). In this paper, we do not address this more complicated specific issue, but only present a simple model describing the dynamical behavior of the sonoluminescent bubble in the SBSL case. Using simple numerical techniques within the Matlab software package, we discuss solutions that consider various possibilities for some of the parameters involved: liquid compressibility, surface tension, viscosity and type of gas. The model may be used for an introductory study of SL on undergraduate or graduate physics courses, and as a clarifying example of a physical system exhibiting large nonlinearity.

(Some figures may appear in colour only in the online journal)

1. Introduction

Sonoluminescence (SL) is an intriguing phenomenon, which consists of light emission by small collapsing bubbles inside liquids [1, 2]. Such bubbles are created by ultrasonic waves when the pressure of the liquid is reduced relative to the pressure of the gas present in the medium [3–5]. In general, the appearance of a cavity within a liquid implies the existence of a surface (the wall) dividing the region into two parts, each one occupied by a fluid: the inner cavity consisting of a gas and/or liquid vapor, and the liquid portion outside. The bubble initially expands to a maximum volume, and then collapses. At the final stages of the

collapse, the gas inside the bubble radiates light. It is observed that light emission is enhanced when atoms of noble gas are present inside the bubble.

In the 1990s, Gaitan *et al* [6] created and trapped a single bubble the size of a few microns in the laboratory; it was levitated in a bottle of water under the action of a strong, stationary-wave sound field that periodically emitted flashes of light in each acoustic cycle. The trapping of a single sonoluminescent bubble in the liquid, yielding what is called single-bubble sonoluminescence (SBSL), and the production of repeated cycles of expansion and contraction, excited by ultrasonic acoustic waves, allowed a more accurate study of the phenomenon. This stability of the bubble made more detailed studies about the duration of the flash of light and the size of the bubble possible.

The conversion of the energy of sound waves into flashes of light occurring in such bubbles a few microns in size is an interesting field of research, if one considers the inherent difficulties of the process, the inadequacy of some theories and models proposed, and experimental limitations. Despite the existence of a wide variety of theories and models, the phenomenon has not yet been completely explained, and there are still many open questions. Among them, we can cite the heating mechanism of the gas inside the bubble; the process of light emission; the role of the temperature of the liquid in the intensity of the emitted radiation; the reason why water is one of the ideal fluids for observing the phenomenon. The phenomenon has been studied extensively, but its detailed mechanisms remain unclear.

The study of SL involves topics of physics such as hydrodynamics and thermodynamics, besides electromagnetism, statistical mechanics and atomic physics if one wants to go into the emitting mechanism. Chemical reactions must also be taken into account to explain many aspects of SL. The dynamics of the bubble can be described by the Navier–Stokes equation [7], provided that the initial state of the bubble is defined by a set of physical parameters. The energy of one photon emitted in SBSL, if compared with the energy of one atom vibrating in the sound wave which gave rise to it, typically provides a value of the order of 10^{12} , which shows the high focalization of energy in this effect [8]. The temperature in the interior of the bubble can reach thousands of Kelvins during the collapse phase [9].

In this work we carry out a modeling of SBSL hydrodynamics, using the radius of the bubble as the variable of interest. There are several models that describe the time evolution of the radius of the bubble. The most common are the Rayleigh–Plesset, Herring–Trilling and Keller–Miksis models [2, 10, 11]. All of these models are derived from the Navier–Stokes equation, using different simplifying assumptions [12, 13].

The Rayleigh–Plesset equation describes the behavior of compressible or incompressible fluids, and can therefore be used to compare the effects of the compressibility of the liquid on the time evolution of the bubble radius. Other physical parameters, such as the liquid viscosity, the properties of the gas inside the bubble and the surface tension of the wall can be taken into account in these models.

In order to compare the effects of these factors, we define in this work a useful parameter, the damping factor, which is defined as the ratio of the amplitudes of the first and second oscillations of the bubble. This parameter is relevant, since it compares two values of the radius: one before and the other after light emission. A detailed study of the bubble behavior, including the variation of the wall speed as a function of time, is also carried out.

This work is addressed mainly at (under)graduate students and teachers. The subject requires the domain of calculus and many concepts from various fields of physics at the intermediate level. The work could be useful for physics courses at university level, as well as providing an illustrative example of numerical calculus applied to a highly nonlinear phenomenon. It may also be valuable as an introductory-level text on SBSL addressed to young researchers.

The work is the result of a research project in SL carried out together with undergraduate students.

2. Description of the model

The behavior of a nonrelativistic fluid is described by the Navier–Stokes equation, which is valid at each point of the fluid and can be written as

$$\rho \frac{D\vec{v}}{Dt} = \rho \vec{B} - \nabla p + \mu \nabla^2 \vec{v}, \quad (1)$$

where ρ is the fluid mass density, \vec{v} is the velocity field inside the fluid, $\rho \vec{B}$ is the resultant of body forces (e.g., gravity) per unit volume of the fluid, p is the pressure field inside the fluid and μ is the fluid viscosity. The term $\frac{D\vec{v}}{Dt}$ on the left-hand side of the above equation is the material derivative of the velocity of the fluid element. The material derivative is given by the operator

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla, \quad (2)$$

where the first term on the right-hand side is the time derivative with respect to a fixed reference point of space (the Euler derivative), and the second term takes into account the changes of the velocity field along the movement of the fluid. The quantity \vec{B} on the right-hand side of equation (1) stands for the acceleration originating from the body forces acting on the fluid element, such as gravitational and electromagnetic forces, for example. The second and third terms represent, respectively, the hydrostatic and viscous forces, both per unit volume.

The form the Navier–Stokes equation is written in above means that we are considering the fluid as Newtonian. Now, we remember that the flow inside and around the bubble is restricted to the radial direction, in other words, the problem exhibits spherical symmetry, which in fact is valid even beyond the neighborhood of the bubble, provided that the shape of the flask is spherical, a typical experimental situation. Thus, we take into account only the expansion and contraction motion of the bubble's radius. Besides, we assume as a first approach that the compressibility of the liquid is much smaller than that of the gas inside the bubble. In this case, one derives from equation (1) the Rayleigh–Plesset equation (a dot stands for one time derivative, $\dot{R} = dR/dt$, etc):

$$\rho \left(R\ddot{R} + \frac{3}{2}\dot{R}^2 \right) = p_{\text{gas}} - P_0 - P(t) - 4\mu \frac{\dot{R}}{R} - \frac{2S}{R}, \quad (3)$$

where $R(t)$ is the bubble's radius, $p_{\text{gas}}(t)$ is the variable gas pressure inside the bubble ($p_{\text{gas}}(t)$ is assumed to be uniform in our model), P_0 is the pressure of the liquid measured at any remote point from the bubble (typically, $P_0 = 1$ atm), $P(t)$ is the driven acoustic pressure at the point where the bubble is placed and S is the liquid surface tension at the bubble wall. $P(t)$ is assumed to be sinusoidal and beginning an expansion cycle in $t = 0$, that is,

$$P(t) = -P_a \sin(\omega t), \quad (4)$$

P_a being the amplitude of the driven pressure and ω the ultrasound angular frequency in resonance with the natural oscillations of the flask, such that the driven pressure generates a stationary ultrasound wave that traps the bubble at its center, on a pressure antinode.

Often, the effects of the compressibility of a liquid can be neglected in many problems of hydrodynamics. However, in the case of SBSL this approach is no longer justified, because a large amount of the acoustic energy driven to the bubble is emitted back from it to the liquid, in the form of a spherical shock wave (only a small amount is in fact converted into light), which obviously could not exist in an incompressible medium (the acoustical wave emitted by the

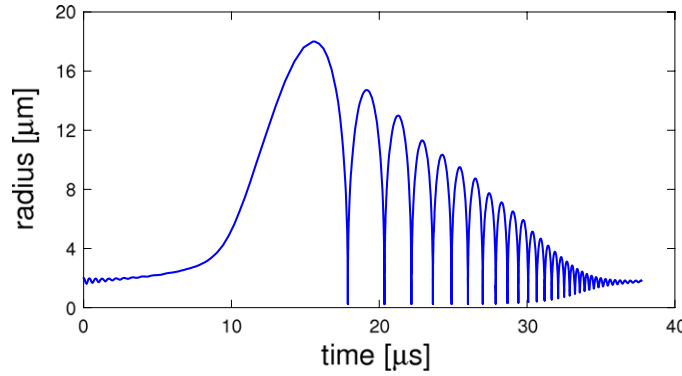


Figure 1. Radius as a function of time for one (acoustically forced) cycle of the motion of the bubble. The liquid is treated as incompressible and the bubble dynamics is described by the Rayleigh–Plesset equation (3).

bubble is experimentally important, since its detection by a hydrophone signals the presence of the trapped bubble at the center of the spherical flask). It follows that when the compressibility of the liquid is considered, a new term is added to the right-hand side of equation (3), leading to the modified Rayleigh–Plesset equation [2]

$$\rho \left(R\ddot{R} + \frac{3}{2}\dot{R}^2 \right) = p_{\text{gas}}(t) - P_0 - P(t) - 4\mu \frac{\dot{R}}{R} - \frac{2S}{R} + \frac{R}{c} \frac{d}{dt} p_{\text{gas}}, \quad (5)$$

where c is the speed of sound in the liquid (which henceforth we will assume to be water).

We adopt a van der Waals equation of state for describing the gas pressure inside the bubble, which reads

$$p_{\text{gas}}(t) = \left(P_0 + \frac{2S}{R_0} \right) \left(\frac{R_0^3 - h^3}{R^3(t) - h^3} \right)^\gamma, \quad (6)$$

where R_0 is the static bubble radius, that is, the ambient bubble radius when it is not acoustically forced, h is the characteristic van der Waals hard-core radius of the gas inside the bubble and γ is the ratio between the specific heat of the gas at constant pressure and at constant volume (the adiabatic index). So, the gas pressure varies with time through the bubble radius, $R(t)$. It was assumed in equation (6) that the gas undergoes so fast a cycle of expansion and collapse, which is adiabatic. However, a more accurate analysis [2] allows one to conclude that the expansion is almost isothermic ($\gamma \approx 1$) and only the final part of the collapse is indeed adiabatic. Our simplified model here considers the whole cycle as an adiabatic process.

In equation (5), the time derivative of the gas pressure is explicitly given by

$$\frac{d}{dt} p_{\text{gas}} = -3\gamma p_{\text{gas}} \frac{R^2 \dot{R}}{R^3 - h^3}. \quad (7)$$

Equations (3) and (5) are second-order differential equations for the radius $R(t)$, which have no analytical solution. So, in order to solve numerically these equations for a given set of parameters and initial conditions, we have used a specific Runge–Kutta routine of the mathematical program, Matlab.

3. Numerical solutions

Let us first consider the case in which the compressibility of the liquid is neglected. Figure 1 shows the solution of equation (3) for a given set of parameters describing some properties of

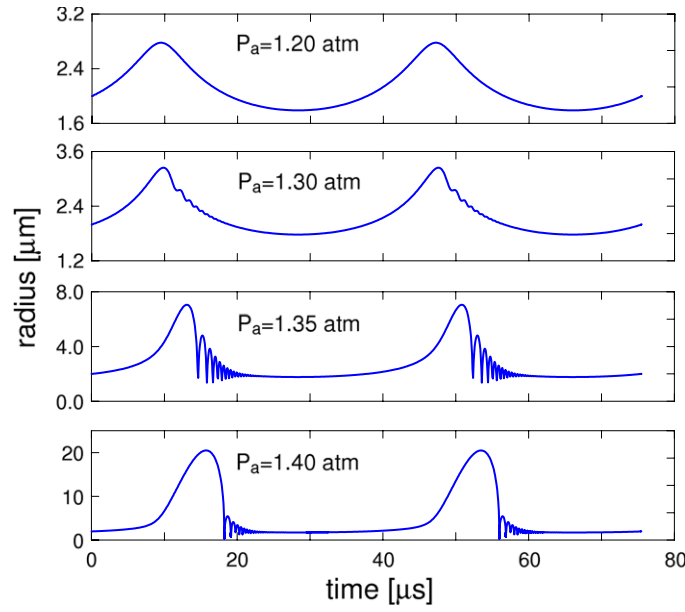


Figure 2. Radius as a function of time for two (acoustically forced) cycles of the subsonic motion of the bubble. The liquid is treated as compressible and the bubble dynamics is described by the modified Rayleigh–Plesset equation (5).

Table 1. Parameters used in the numerical simulation.

Surface tension	$S = 72.8 \times 10^{-3} \text{ N m}^{-1}$
Density (water)	$\rho = 1000 \text{ kg m}^{-3}$
Adiabatic index (argon)	$\gamma = 5/3$
Speed of sound (water)	$c = 1500 \text{ m s}^{-1}$
Viscosity (water)	$\mu = 1.002 \times 10^{-3} \text{ Pa s}$
Ambient pressure	$P_0 = 1.00 \text{ atm}$
Static radius	$R_0 = 2.0 \times 10^{-6} \text{ m}$
Hard core (argon)	$h = R_0/8.86$
Ultrasound frequency	$\omega = 2\pi f; f = 1/T = 26,5 \text{ kHz}$

the gas and the liquid, and at forcing pressure $P_a = 1.42 \text{ atm}$. The parameters used are shown in table 1, where the noble gas argon is considered because it is a well-known fact in the SBSL literature [2] that, after some cycles, argon is the only remaining constituent of the initial air bubble (besides water vapor, which, however, has a lower value for the van der Waals hard-core radius), due to chemical reactions in which the other components participate, carrying them to the water outside. The solution shown in figure 1 is qualitatively similar to the experimental results [8, 2], but quantitatively very different: the experimental afterbounces are much smaller than those that appear in figure 1. This is in agreement with the fact that indeed a considerable amount of energy is lost in the first contraction (collapse), which, as we have already pointed out, is due to sound radiation by the bubble, an effect that is impossible theoretically under the assumptions leading to equation (3).

Figure 2 shows the solutions to the modified Rayleigh–Plesset equation (5) for four different forcing pressures, and the parameters shown in table 1. Under the action of the external forcing, the bubble radius oscillates almost sinusoidally around the equilibrium value R_0 , with small amplitudes and with a period close to that of the external forcing. However,

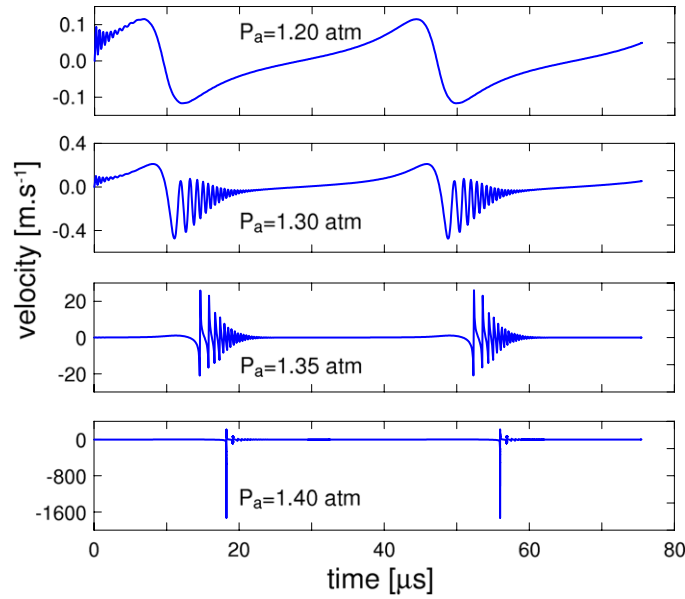


Figure 3. Bubble wall velocity as a function of time for two (acoustically forced) subsonic cycles. The liquid is treated as compressible and the bubble dynamics is described by the modified Rayleigh–Plesset equation (5).

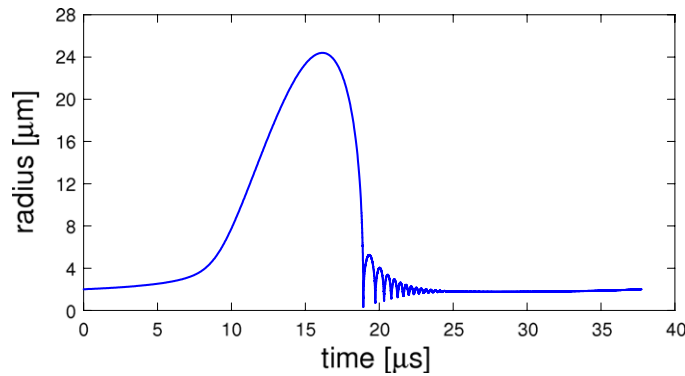


Figure 4. Radius as a function of time for one (acoustically forced) cycle of the supersonic bubble collapse. The forcing pressure is $P_a = 1.42$ atm. The other model parameters used are shown in table 1.

for a critical forcing pressure around $P_a = 1.35$ atm, one observes a nonlinear behavior in the bubble dynamics. As shown in figure 3, in this regime the motion of the bubble is subsonic, except at the forcing pressure $P_a = 1.4$ atm.

The SL phenomenon is expected to occur beyond this threshold. In figure 4 we depict the solution of equation (5) for the bubble radius at the forcing pressure $P_a = 1.42$ atm, just beyond the threshold value. In this example, the initial radius is $R_0 = 2.0$ μm , which is a typical value for the radius corresponding to the mechanical equilibrium bubble under the action of an external ambient pressure (normally ≈ 1 atm). In the first half-cycle of the forcing pressure, its negative values favor an expansion of the bubble. However, the negative peak of

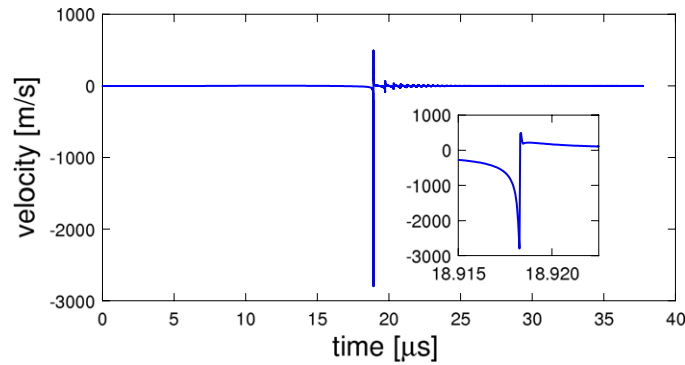


Figure 5. Velocity of the bubble wall corresponding to the solution shown in figure 4.

the pressure (at a quarter-cycle, or $t \approx 9,4 \mu\text{s}$ in figure 4) does not correspond exactly to the instant when the bubble radius is at its maximum, due to the inertia of its expansion. The maximum radius is typically $R \approx 10 R_0$, as shown. Thus, the volume of the bubble is about 10^3 of its initial value, and therefore the gas pressure is reduced by a factor of around 10^3 . At this point, however, the total forcing pressure acting on the bubble is around 1 atm and increasing. The atoms of the rarefied gas close to the wall can no longer balance the external pressure of ≈ 1 atm outside, and then the bubble collapses. This kind of calculation was first carried out by Lord Rayleigh in 1917 [10].

Comparing figures 1 and 4, one observes that when the compressibility of the liquid is taken into account, the experimental results are better reproduced by the model [8, 2]. In SBSL experiments, it is observed that the bubble pulses synchronously with the acoustic field, expanding during a part of acoustic rarefaction cycle and collapsing during the compression phase, with afterbounces like those of figure 4 rather than those of figure 1, confirming the necessity of taking into account the compressibility of the liquid.

A very important aspect of SL regards the velocity of the bubble wall, especially during the collapse. At this stage, if the speed of the bubble wall is comparable or even higher than the speed of sound in the liquid and/or the gas (and this really happens in SBSL experiments), then a shock wave of relatively high intensity is generated inside each of these media. With regard to the liquid, this has been considered above, but with respect to the shock wave inside the gas, this is an issue that we will not address here, due to its complexity. However, it should be noted that some early models for the mechanism of light emission in SBSL had this shock wave inside the bubble as a key ingredient, but these models are no longer believed to be correct [2].

The velocity of the bubble wall depends on some important characteristics, such as the properties of the gas inside the bubble, the initial bubble radius and the properties of the liquid outside the bubble. Figure 5 shows the behavior of the bubble wall speed as a function of time. The collapse ends when the bubble radius approaches the van der Waals hard core of the gas. The gas reaches very high density (near to solid state) and temperature values, and then the flash of light is emitted.

4. The effects of different parameters

As mentioned in the introduction, the damping factor is defined as the ratio of the amplitudes of the first and second oscillation of the bubble during the time evolution. So, the greater the losses due to dissipation in the dynamics of the bubble, the greater the damping factor. In

Table 2. Parameters used in the numerical simulation.

Properties	Damping factor
van der Waals hard core radius, surface tension and viscosity	3.602
van der Waals hard core radius	11.434
Viscosity	11.629
Surface tension	4.063
van der Waals hard core radius and viscosity	11.778
van der Waals hard core radius and surface tension	4.097
Viscosity and surface tension	3.653

order to investigate the effects of the physical properties of the specific gas inside the bubble on the damping factor, as well as the role of the surface tension of the liquid, we carried out several simulations. First, we considered the effects of each of the parameters separately (three simulations). Then, we systematically added the effects of the remaining parameters on the solutions of the equation of motion (5), providing four more simulations. The obtained results are schematically presented in table 2.

In the first line of table 2, we write the value of the damping factor obtained with the full calculation of the bubble dynamics given by equations (5), (6) and (7), which include the conjugated effects of the van der Waals hard core, of the surface tension and the fluid viscosity.

In the second line we consider only the effects of the van der Waals hard core. So, in the limit $S \rightarrow 0$ and $\mu \rightarrow 0$, the equation of motion (5) becomes

$$\rho \left(R\ddot{R} + \frac{3}{2}\dot{R}^2 \right) = p_{\text{gas}}(t) - P_0 - P(t) + \frac{R}{c} \frac{d}{dt} p_{\text{gas}}, \quad (8)$$

while the equation (6) reads

$$p_{\text{gas}}(t) = P_0 \left(\frac{R_0^3 - h^3}{R^3(t) - h^3} \right)^\gamma, \quad (9)$$

and equation (7) remains unchanged.

The third line gives the result obtained when only considering the effects of the fluid viscosity. This is equivalent to taking the limit $h \rightarrow 0$ and $S \rightarrow 0$ in equations (5)–(7). In doing this, we obtain

$$\rho \left(R\ddot{R} + \frac{3}{2}\dot{R}^2 \right) = p_{\text{gas}}(t) - P_0 - P(t) - 4\mu \frac{\dot{R}}{R} + \frac{R}{c} \frac{d}{dt} p_{\text{gas}}, \quad (10)$$

$$p_{\text{gas}}(t) = P_0 \left(\frac{R_0^3}{R^3(t)} \right)^\gamma, \quad (11)$$

and

$$\frac{d}{dt} p_{\text{gas}} = -3\gamma p_{\text{gas}} \frac{\dot{R}}{R}, \quad (12)$$

respectively.

In the fourth line only the effects of the surface tension are taken into account. So, taking the limits $h \rightarrow 0$ and $\mu \rightarrow 0$ in the equations (5) and (6), we find

$$\rho \left(R\ddot{R} + \frac{3}{2}\dot{R}^2 \right) = p_{\text{gas}}(t) - P_0 - P(t) - \frac{2S}{R} + \frac{R}{c} \frac{d}{dt} p_{\text{gas}}, \quad (13)$$

and

$$p_{\text{gas}}(t) = \left(P_0 + \frac{2S}{R_0} \right) \left(\frac{R_0^3}{R^3(t)} \right)^\gamma, \quad (14)$$

respectively, while equation (7) leads to equation (12).

In the fifth line of table 2 we take into account the effects of the van der Waals hard core as well as the fluid viscosity. So, in the limit $S \rightarrow 0$ equations (5) and (6) lead to equations (10) and (9), respectively.

The sixth line shows the results when considering the effects of the van der Waals hard core and of the surface tension. Thus, in taking the limit $\mu \rightarrow 0$, the equation of motion (5) should be substituted by equation (13), while equations (6) and (7) remain unchanged.

Finally, in the seventh line we show the result obtained when the effects of the fluid viscosity and the surface tension are considered. Therefore, in the limit $h \rightarrow 0$ the dynamics of the bubble radius is described by equation (5), while the gas pressure and its time derivative are given by equations (14) and (12), respectively.

As we can see from table 2, the surface tension strongly affects the dynamics of the bubble, when compared with the other two properties considered here, since it substantially reduces the damping factor. According to the experimental results existing in the literature for SBSL [2], the damping factor lies between the two extreme values shown in the table, and closer to the lower values, thus illustrating the importance of including the surface tension in the calculations.

5. Conclusions

In this paper we have presented a model describing the dynamical behavior of a bubble in SBSL. We obtained solutions for the equations of the model in the cases of compressible and incompressible liquids. Comparing figures 1 and 4 with the experimental results, we show that the modified Rayleigh–Plesset equation valid for a compressible liquid, given by equation (5), describes the bubble dynamics with a better accuracy [8], which is due to the experimentally observed acoustic radiation from the bubble, a fact that requires the liquid compressibility to be different from zero.

We introduced the damping factor in order to compare the effects of some properties of the system on the dissipation of energy of the bubble after the collapse (first compression). We observed that the surface tension of the liquid cannot be neglected in any model describing SBSL dynamics, as we summarized in table 2.

It is worth mentioning that chemical effects were not considered in this work. The chemical factors clearly affect the thickness of the bubble wall, thereby also contributing to the generation of a shock wave. Of course, a more realistic treatment must include this. Also, as mentioned above, the process that the bubble gas undergoes is not adiabatic during the whole cycle, as considered here, but instead isothermic during the expansion, which affects the value of the exponent γ . However, as pointed out in [2], just modifying the numerical calculation in order to interpolate between $\gamma = 1$ and $\gamma = 5/3$ is not sufficient to describe the behavior of $R(t)$ completely in all of its details.

In order to solve the equations (3) and (5) we used the routine *ODE45* built in the mathematical program Matlab¹. The package *ODE45* is an explicit method of integration which is based on the Runge–Kutta–Fehlberg method of order 4 or 5. Runge–Kutta methods are widely used in the numerical solution of ordinary differential equations of second order, as well as those of higher order.

The Matlab routines used to generate our results can be requested from any of the authors by e-mail and we hope that the simulations presented here will be valuable for teachers, (under)graduate students and young researchers to become acquainted with single-bubble sonoluminescence and some of its remarkable features.

¹ <http://mathworks.com/products/matlab>

Acknowledgments

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