A computational study of sonoluminescene

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Abstract

This thesis explores the numerical methods for studying nonspherical sonoluminessceing bubbles. It contains derivations of the Rayleigh Plesset equation and perturbations to the equation. It discusses the effect of the n=3 mode and how it can cause bubble collaspe to happen more quickly.

Contents

1 Introduction

In a dark room in 1934 two scientists, H. Frenzel and H. Schultes, tried to speed up the development process of photographs by exposing them to ultrasound. Instead, they discovered bright spots on the photographs, caused by the light emission from bubbles of air in the development fluid. This phenomenon then went on to be named sonoluminescence, or sound induced light. Since then, experimental physicists have been investigating the properties of this mysterious process. Theoretical physicists use sonoluminescence as a means to reach deeper into fluid dynamics.

Sonoluminescence as mentioned before occurs when a bubble induced by sound collapses quickly enough to give off light. The frequencies of the light emitted have experimentally confirmed temperatures up to 5100 K . It is believed by Chen, W. et. a.l in a paper published in 2008 Physical Review that there could be even higher temperatures but go unobserved due to the opacity of water at wavelengths characteristic of very high temperatures. The duration of emitted light is only 35 to 100 picoseconds, while the final size of the bubble is about 5 micrometers. During collapse, an unseen shock wave is produced by the bubble walls exceeding the speed of sound in the liquid. In multi-bubble sonoluminescence, this is and important factor, as each collapsing bubble exerts a force on surroundinrg bubbles.

Sonoluminescence can occur in multi-bubble and single-bubble situations. While multi-bubble sonoluminescence was documented since the early 1910's, single-bubble sonoluminescence was not documented in the lab in the United States until 1990, when Gatian, then a graduate student, trapped a sonoluminescing bubble in a sound wave. This discovery lead to the ability to perform systematic experiments on a single bubble, something which was not possible before. This also led to an explosion of papers on the subject, as theory was able to be more readily tested by experiment and experiment paved the way for more theory. From the time of its discovery until 1990, it is from these papers that physicists started to try and explain the mechanism behind this process.

The theory of light emission considered in this model is that of thermal bremsstrahlung radiation. However, this computational model makes no attempt at simulating the actual emission of light. In this theory, ionized electrons are slowed down by nearby protons and neutrons which, according to classical mechanics, an accelerating particle will radiate. This radiation is the light given off by the bubble. Thermal bremsstrahlung is the process adopted in the hydrodynamic theory of sonoluminescence. It is this theory that simply and accurately explains sonoluminescence.

Sonoluminescence also encompasses areas of chemistry as well as fluid dynamics and thermal physics, . These areas include diffuse equilibrium and chemical reactions occurring in the bubble. The bubble must remain diffusely stable in order to induce sonoluminescence. As far as the chemical reactions are concerned, it is observed experimentally that inert gases produce more intense sonoluminescence. According to a book by Young in 2002 a particularly useful gas for this is Xeon. It seems that when you dope gases with 1 percent Xeon, sonoluminescence is peaked. This fact maybe one of the reasons that air, which is approximately 1 percent Xeon, has such high intensities of emission, as to be seen by the naked eye.

My simulation is based on the hydrodynamic theory of sonoluminessce. Hydrodynamic theory states sonoluminescence is the consequence of well know physical process. This includes colapse under the Rayleigh-Plesset equation, shape stability, diffusive stability, chemical processes in the bubble and light emission as thermal emission from an optically thin body. Predictions of light intensities and time scales are in good agreement with experiment. The specifics of the theory have been worked out by Hilgenfeldt et al. (1999b). Therefore, as the simplest physics of all the theories is involved, I will proceed with this theory. Ruth et al. (2002) have done previous work on a computational model, and they suggest seven areas of future work. One of these areas is to add in water vapor into the model, as it provides a important cooling mechanism in the the hydrodynamic theory. Without water vapor, temperatures exceed 100,000 Kelvin.

There are some problems with the hydrodynamic theory however. The Rayleigh-Plesset equation is only valid in the region where nothing exceeds the speed of sound in the liquid. The walls of the bubble certainly do exceed this speed in the final stages of the collapse. This is one of the reasons that you see bounces after the initial collapse, whereas the Rayleigh-Plesset equation predicts one, defining collapse. The theory also has little to say about why the introduction of inert gasses increases the intensity.

My work sought to understand the importance of intial bubble geometry on the concentration of energy. By modeling bubble collaspes of half of a sphere and perturbations to a spherical geometry, I sought to determine the correct geometry of the intial bubble for sonoluminessence. For this purpose the hydrodymic theory is sufficent and will be what I base my assumptions off of.

Unfortunatly I was unable to numerically integrate the model. However, during the course of reasearch I found a paper [2] which embarked on the same investigation as I sought to. I tried to invesitgate the n=3 mode of their model, but I lacked the appropiate tools to do so. So instead I have recited their dervation and the derivation of the reyliegh plesset equation in the radial frame and volume frame. I then try to predict some effects of the n=3 mode on the solution.

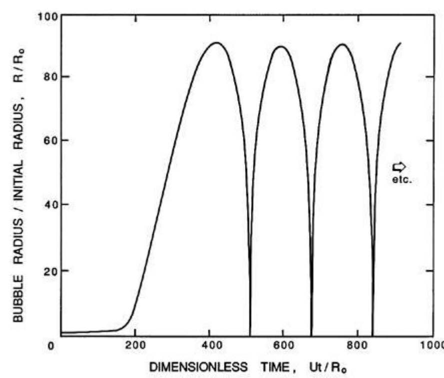
2 Theory

This section develops the mathematical basis for the model and understanding of sonoluminessence in general.The most prominent equation involved in the study of sonoluminescence is the Rayleigh-Plesset equation, an equation derived from the study of bubble dynamics. Bubble dynamics is a description of cavitation in liquids. Starting with Bernoulli's equation and incorporating the ideal gas law, you get the following equation:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 = \frac{1}{\rho}(p_g - P_0 - P(t) - 4\mu\frac{\dot{R}}{R} - \frac{2\gamma}{R})$$

where R is the radius of the bubble, is the density of the liquid, p represents the pressure of the gas and liquid, μ is viscosity of the liquid, and γ is the surface tension. This represents the most basic level of investigation of a bubble, and as such is where all theories of sonoluminescence start. This formulation can also be derived from the Naiver-Stokes equations, the fundamental equations governing fluid dynamics.

A numerical solution of the Rayleigh-Plesset equation predicts bounces after the bubble hits the minimum radius. These bounces are observed to be less pronounced in actual sonoluminessence. The graph below presents a sample solution of the radius as a function of time.



Here, I will take the oppurtunitty to derive the Reliegh-Plesset spherical for a spherical bubble in two frames. The first is the radius frame, the most basic of anyalisis. This will be followed by an equivalent derivation in the volume frame, which is important for the study of non-spherical collaspes. Finally, a presentation of the derivation of non-spherical contributions to the occillating bubble are presented.

2.1 Radial Reyliegh-Plesset Equation

Consider an infinite volume of liquid with a perfectly spherical bubble in it. Let R represents the radius of the bubble and r represents the distance from the center of the bubble to some point in the liquid. If the bubble is occillating due to a standing sound wave in the medium, then we have the following situation.

The expasion of the gas displaces a volume of liquid equal to its volume which must be pushed out at the same velocity as the expasion of the bubble radius because of the incompressibillty of the liquid.This is stated as follows

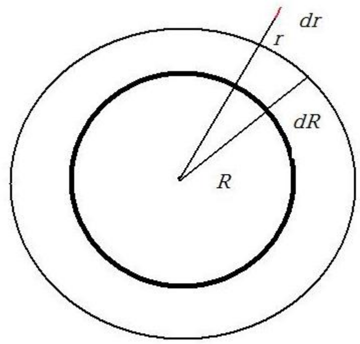


Figure 1: As the bubble expands a radius dR, the liquid is pushed out a radius dr

$$\frac{4}{3}\pi R^2 dR = \frac{4}{3}\pi r^2 dr$$

which implies

$$R^2 \frac{dR}{dt} = r^2 \frac{dr}{dt}$$

which is equal to

$$u(r,t) = \frac{R(t)^2}{r(t)^2}\dot{R}(t)$$

where $u(r,t)$ is the fluid velocity. Next, consider the energy of the system. The work done moving from a radius R_0 to a radius R must be equal to the change in the kinetic energy. Now when the bubble changes radius, there is work done on the bubble by the pressure that would have been at the center of the bubble if the bubble had not been there. Since the pressure changes over a scale much larger then the bubble radius, then this is almost equal to the liquid pressure far from the bubble, which implies $p_\infty = p_0 + P(t)$. This difference between the work done by this pressure and the pressure at the bubble wall p_L is equal to the kinetic energy in the liquid and thus (given by [3])

$$\phi_{KE} = \frac{\rho_0}{2}\int_{r=R}^{r=\infty} 4\pi r^2 u^2 \, dr = 2\pi\rho_0 R^3 \dot{R}^2 \tag{1}$$

Equation (1) is simply the integral of the velocity of the fluid thghout the medium, a simple addition of all the kinetic energies in the fluid. The work done on the gase is equal to this kinetic energy so

$$\int_{R_0}^{R} (p_L - p_\infty) 4\pi R^2 \, dr = 2\pi\rho_0 R^3 \dot{R}^2$$

If you differentiate equation with respect to R you get

$$p_L(t) - p_\infty 4\pi R^2 = 2\pi\rho_0(3R^2\dot{R}^2 + R^3 \frac{\partial}{\partial R}(\dot{R}^2))$$

Now,

$$\frac{\partial}{\partial R}(\dot{R}^2) = \frac{1}{\dot{R}}\frac{\partial \dot{R}^2}{\partial t} = 2\ddot{R}$$

so equation (1) becomes

$$p_L(t) - p_\infty = \rho_0(R\ddot{R} + \frac{3\dot{R}^2}{2})$$

When the pressure p_L is a static componet p_0 and the pressure from a driving force $P(t)$ then you can substitute this in and rearrange to get

$$R\ddot{R} + \frac{3R^2}{2} = \frac{1}{\rho_0}(p_L(t) - p_0 - P(t))$$

This is the radial Rayleigh-Plesset equation. It is a prediction of the radius as a function of time for a bubble in a sound field where the sound field is represented by the P(t) term.

2.2 Volume Rayleigh-Plesset equation

The process for deriving the volume based equation is nearly identical to the radial equation in that they both rely on the equating of kentic energy to work done on the gas. Futhermore the consider the same assumptions for the pressures far away from the bubble. The only real difference is the begining equation which is the statement of how the fluid velocity relates to the given paramter, in this case the volume. For a fluid velocity $u(r,t)$ is related to the volume by

$$u(r,t) = \frac{\dot{V}(t)}{4\pi r^2}$$

where $\dot{V}(t)$ is volume wall velocity. The same argument as for the radial equation leads to the following for the kinetic energy in the liquid

$$\phi_{KE} = \frac{rho_0}{2}\int_{r=R}^{r=\infty} 4\pi r^2 u^2 \, dr = \frac{\rho_0 \dot{V}(t)}{8\pi R}(\frac{4\pi}{3V})$$

equating that to the work done by the pressure in the liquid reveals

$$\int_{V_0}^{V} (p_L - p_\infty)\, dV = \frac{\rho_0 \dot{V}^2(t)}{8\pi}(\frac{4\pi}{3V})^{\frac{1}{3}}$$

Where the radius was converted to a volume from equation 8. Now we differentiate with respect to V and use the fact that

$$\frac{\partial \dot{V}^2}{\partial V} = \frac{1}{\dot{V}}\frac{\partial \dot{V}^2}{\partial t} = 2\ddot{V}$$

to show

$$\frac{1}{8\pi}(\frac{4\pi}{3V})^{\frac{1}{3}}(2\ddot{V} - \frac{\dot{V}^2}{3V}) = \frac{1}{\rho_0}(p_g + p_v - p_\sigma - P(t))$$

This is the Rayleigh-Plesset equaion in the volume frame.

2.3 Non-Spherical Solution

Now we consider the non-spherical collapse of a bubble in an infinite medium of liquid and inside a insonifying feild. This section follows [2] in its derivation. The majority of this derivation is taken from [3]. In order to do this we must consider a bubble surface given the equation

$$r = R(t)[1 + \epsilon(t)P_n(cos\theta)]$$

where ϵ is the amplitude of small oscillations of the shape mode represented by the n-th Legendre polynomial and $R(t)$ is the spherical pulsations. In this way the bubble has a volume part given by $R(t)$ and a shape part or mode given by $\epsilon P_n(cos\theta)$.

Now, assuming irrotational motion in the liquid, a velocity potentail can be defined such that

$$u = \nabla\phi$$

This is laplace's equation and can be evaluated with the appropriate boundry conditions. For this case the normal components of the liquid velocity at the interface must be equal to the bubble-wall velocity. This then implies

$$\phi(r,\theta) = -\frac{\dot{V}(t)}{4\pi r} - \delta(t)(\frac{R(t)}{r})^{n+1}P_n(cos(\theta)$$

with

$$V(t) = \frac{4}{3}\pi R^3(1 + \frac{3\epsilon^2}{2n+1}).$$

The function $\delta(t)$ can be determined from the kinetic boundry condition, so that

$$\delta(t) = \frac{1}{1+n}(R^2\dot{\epsilon} + 3R\dot{R}\epsilon)$$

Now, this is not the most general solution, as a general solution willl include an infinite sum of all the spherical harmonics, however this yeilds additional correction terms of order ϵ^2 which are associated with the influnce of the other orders. This equation will be used to study the influences of only the n-th order perturbation.

Now, consider the energy balance of the bubble. The energy of the liquid must be equal to the energy of the gas which implies

$$\Delta E_{kin.gas} + \Delta E_{pot.gas} = \Delta E_{kin.liquid} + \Delta W_{acousitc} + \Delta E_{pot.interface}$$

The change in the kentic energy of the gas is must be very small, assuming that the desity of the gas is much less then the liquid. So then $\Delta E_{kin.gas} = 0$. It is left to calculate the potienial energy of the bubble, which can be found by assuming a polytropic gas and integrating the volume from the intial state to the final state as follows:

$$\Delta E_{pot.gas} = \int_{V(0)}^{V(t)} p_g(V)\, dV = \begin{cases} p_{g0}V(0)ln\frac{V(t)}{V(0)}, & \gamma = 1 \\ \frac{p_{g0}V(0)}{\gamma-1}[1-(\frac{V(0)}{V(t)})^{\gamma-1}] & \gamma > 1 \end{cases}$$

where

$$V(0) = \frac{4}{3}\pi R_0^3$$

and γ is the polytropic exponent. The pressure in the gas has a contribution from the surface tension of the bubble and the ambient pressure at infinity so $p_{g0} = p_0^\infty + \frac{2\sigma}{R_0}$ where p_0^∞ is the ambient pressure and σ is the surface tension of the liquid. Thus the left hand side of the energy balance equation has been put in terms of bubble constants and the volume.

For the left hand side we start with the kinetic energy of the liquid around the bubble. This will be equal to

$$\Delta E_{kin.liquid} = \frac{\rho}{2}\int_{S(0)}^{S(t)} \Phi\frac{\partial\Phi}{\partial\mathbf{n}}\, dS$$

where Φ is the velocity potential described in (17). The integral is evaluated over the surface of the bubble and $\mathbf{n}$ is a unit normal vector to the bubble surface. The evaluation of this integral reveals

$$E_{kin.liquid}(t) = 2\pi\rho R^3\dot{R}^2 + \frac{2\pi\rho}{(2n+1)(n+1)}[R^5\dot{\epsilon}^2 + 2(n+4)R^4\dot{R}\epsilon\dot{\epsilon}]$$

Next, the acoustic work is found by integrating the changing pressure at infinity

$$\Delta W_{acoustic} = \int\limits_{V(0)}^{V(t)} p^{\infty}(t)\, dV = p^{\infty}(t)V(t) - p^{\infty}(0)V(0)$$

where the pressure at infinity takes the form

$$p^{\infty}(t) = p_0^{\infty} - p_A sin(\Omega t).$$

Finally, the potenial stored at the surface is equal to the integral of the surface tension over the surface of the bubble.

$$\Delta E_{pot.interface} = \int\limits_{S(0)}^{S(t)} \sigma\, dS = \sigma(S(t) - S(0))$$

The surface area of the bubble is given by

$$S(t) = 4\pi R^2[1 + \frac{(n^2+n+2)\epsilon^2}{2(2n+1)}]$$

The assumption of a slightly viscous fluid then contributes energy loss in the form of dissipation. There is also a vorticity at the boundry of the bubble, however this equation does not consider that in order to simplify analysis. Dissipation is therefore

$$D = \frac{\mu}{2} \int\limits_{S} \frac{\partial(\mathbf{u}\cdot\mathbf{u})}{\partial \mathbf{n}}\, dS$$

evaluation reveals

$$D = 8\pi\mu R\dot{R}^2 + \frac{4\pi\mu(n+2)}{n+1}R^3\dot{\epsilon}^2 + \frac{8\pi\mu(3n^2+10n+4)}{(n+1)(2n+1)}R^2\dot{R}\epsilon\dot{\epsilon}$$

which is correct to order ϵ^2. This is not the only form of dissipation for a gas bubble, but in this model other forms are not considered.

The Lagrangian for the shape-volume bubble is formed from the usuall $L = T - U$ where $T = E_{kin.liquid}$ and $U = W_{acoustic} - E_{pot.gas} + E_{pot.interface}$. Then the Euler-Lagrange equations, where the dissiapation function is included gives

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{R}} - \frac{\partial L}{\partial R} = -\frac{\partial D}{\partial \dot{R}}$$
$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\epsilon}} - \frac{\partial L}{\partial \epsilon} = -\frac{\partial D}{\partial \dot{\epsilon}}$$

Taking the derivatives yeilds the following set of equations.

$$R\ddot{R}(1+N_1\epsilon^2)+\frac{3}{2}\dot{R}^2(1+N_1\epsilon^2)=[\frac{p_f(V)-p^{\infty}(t)}{\rho}](1+N_2\epsilon^2)-\frac{2\sigma}{\rho R}(1+N_3\epsilon^2)$$
$$-\frac{4\mu}{\rho}\frac{\dot{R}}{R}(1+N_4\epsilon^2)-N_5\frac{\mu}{\rho}\epsilon\dot{\epsilon}-N_6R^2\dot{\epsilon}^2-2N_1R\dot{R}\epsilon\dot{\epsilon}-N_7R^2\epsilon\ddot{\epsilon}$$

where

$$N_1=\frac{n+10}{(2n+1)(n+1)},\qquad N_2=\frac{3}{2n+1},\qquad N_3=\frac{n^2+n+2}{2(2n+1)},\qquad N_4=\frac{3(5n+2)}{2(2n+1)(n+1)},$$
$$N_5=\frac{2(3n^2+10n+4)}{(2n+1)(n+1)},\qquad N_6=\frac{2n+3}{(2n+1)(n+1)},\qquad N_7=\frac{n+4}{(2n+1)(n+1)}$$

and the equation

$$\ddot{\epsilon}+A(t)\dot{\epsilon}+B(t)\epsilon=0$$

where

$$A(t)=5\frac{\dot{R}}{R}+2(2n+1)(n+2)\frac{\mu}{\rho R^2}$$

and

$$B(t)=3\frac{\dot{R}^2}{R^2}+(2-n)\frac{\ddot{R}}{R}+(n+1)(n-1)(n+2)\frac{\sigma}{\rho R^3}+6n(n+2)\frac{\mu}{\rho}\frac{\dot{R}}{R^3}.$$

We can observe that the first equation is the Rayleigh-Plesset equation with correction terms of order ϵ^2. The second equation is referred to the shape mode equation that is found in several peices of the literature. These two equations are called the shape volume model and are a set of fully coupled ordinary differential equations.

3 Numerical Work

The singularities in the Rayliegh plesset equation make it hard to numerically solve. For most computer programs, the step size becomes too small as the integrartion approaches the minium radius. In fact the singularity makes it so that no manipulaation of the units will allow the complete equation to be integrated using Mathematica, the program I tried to use. I can however integrate around the singularity and see what the general shape looks like. The following two graph are the numerical integration to the right and to the left of the 5.9, the approxamite point of the first singularity.

Now In the region around the sinluarity we can assume two things. First, the bubble radius is the minumum bubble radius possidble physically. For this

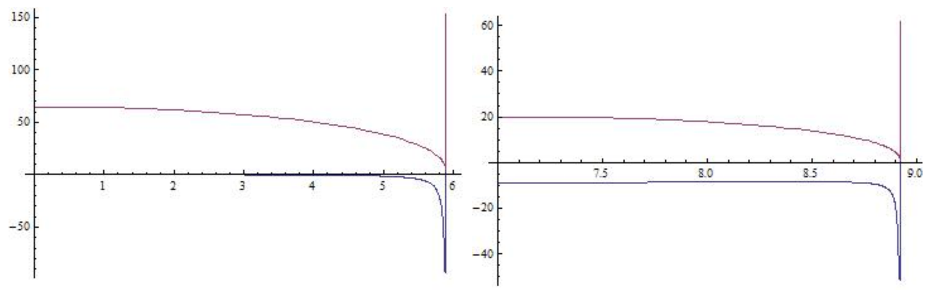


Figure 2: The graphs to the left and right of the first singularity. These are solutions of water and air with a driving amplitude of .15 atm and intial bubble radius of 65 μm. The second graph then inputs the approxamite conditions around t=7 which were $R = 20, \dot{R} = 2, \epsilon = -9, \dot{\epsilon} = 2$.

point there have been several measruments of the minumu bubble radius of air in water and that value can be used to approximate a solution. Secondly, the value of ϵ and its first derivative must approach zero as welll, as the bubble can not flucuate smaller then the minimum radius due to other mechanical reasons. So, takeing the time t=6 to be the moment of minumum bubble radius, we can expand both R and ϵ in a taylor expansion to order 2 and then differentiate to find values of the first and second derivitives of the radius. Now, the first derivative of R must be zero at the bubble minimum radius, R_m, because it is the point at which the radius reverses direction. Plugging a zero for the first derivative into the shape equation and that ϵ is zero gives that $\ddot{\epsilon}$ is zero and the modified Rayliegh Plesset equation becomes

$$R_m \ddot{R}_m = [\frac{p_g(V_m) - p^{\infty}(t)}{\rho}] - \frac{2\sigma}{\rho R_m}$$

where the subscript m denotes a value at the minimum bubble radius. Plugging in the numbers with $R_m = 2$ you get $\ddot{R}_m = 8.47438 * 10^{10}$ which is to be expected as the bubble radius should be expanding quickly at this point. This is an approximate value of the acceleration of the bubble wall at the moment of the the bubble mimimum radius.

This aprroximate solution shows several things. First, the singularty is repeating, as expected with the Rayleigh Plesset equation. Second, the n=3 amplitude is mostly negative and tends to contract the bubble. From this we can conclude that the n=3 solution tends to cause a faster collaspe in non spherical bubbles.

By eliminating all terms of order ϵ^2 the equations become decoupled, with only the shape equation influencing the Rayliegh-Plesset equation. This equation is easier to integrate, however you still run into the problem of the singularity.

From [2] it is shown the that the instabillity of the the n=2 mode increases over several ocillations. The same would most likely happend with the n=3 part.

Analysis of sonoluminessce is very complex and the differential equations invovled are not easy to numerically evalute. The effects of small non-spherical purturbations to the energy concentration could not be determined however a relation between the shape and volume of the bubble was constructed. For futher investigation a better udnerstanding of numerical methods and a better way to implement them is required on the researchers part.

4 Conclusions

The work presented in this paper is a summary of past work and an attempt to implement some orginal anylsis. The numerical anyalsis is unfortunatly very approximate and can only be used for the most general of conclusions. With better numerical methods it might be possible to increase the understanding of each mode, and therefore the understanding of non-spherical effects on the collaspe in general.

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