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Simulation studies of vapor bubble generation by short-pulse lasers


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ABSTRACT

Formation of vapor bubbles is characteristic of many applications of short-pulse lasers in medicine. An understanding of the dynamics of vapor bubble generation is useful for developing and optimizing laser-based medical therapies. To this end, experiments in vapor bubble generation with laser light deposited in an aqueous dye solution near a fiber-optic tip have been performed. Numerical hydrodynamic simulations have been developed to understand and extrapolate results from these experiments. Comparison of two-dimensional simulations with the experiment shows excellent agreement in tracking the bubble evolution.

Another regime of vapor bubble generation is short-pulse laser interactions with melanosomes. Strong shock generation and vapor bubble generation are common physical features of this interaction. A novel effect of discrete absorption by melanin granules within a melanosome is studied as a possible role in previously reported high Mach number shocks [Lin and Kelly, SPIE 2391, 294 (1995)].

Key words: Short-pulse laser, hydrodynamics, bubble, shock wave, melanosome

I. Introduction

The formation of shocks and vapor bubbles is an important physical feature of many applications of pulsed-laser surgery. The efficacy of many treatments depends on the extent to which collateral damage from shocks and expanding vapor bubbles can be limited. On the other hand, laser-induced bubble formation may have beneficial uses in mechanically disrupting occlusions.

There are many examples of collateral bubble formation in pulsed-laser surgery. For example, laser coronary thrombolysis is often accompanied by the formation of vapor bubbles due to selective photo-absorption by arterial thrombi. In transmyocardial laser revascularization, bubbles can form along the laser-generated cylindrical channels and persist for milliseconds.
ophthalmology and dermatology, melanin structures selectively absorb the laser light and may cause damaging bubble formation.4,5

As a result of the prevalence of bubble formation in many applications of short-pulse lasers in surgery, a study of bubble dynamics is warranted. In particular, identifying the threshold for bubble development and understanding the long time-scale evolution can aid in optimizing laser techniques in surgery. To this end, we have embarked on modeling the properties of laser-generated bubbles using two approaches. The first of these methods involves Rayleigh modeling which specifies the bubble radius $R(t)$ as a function of time.6 Here, we use the generic term "Rayleigh model" to also include several extensions made since the original work. Rayleigh models generally assume an almost-incompressible liquid beyond the bubble radius and that the bubble gas is uniformly distributed and obeys a gas equation-of-state (EOS). Rayleigh modeling routinely includes Mach number corrections and a stress-wave source term. The collection of Rayleigh models often used includes the Rayleigh-Plesset equation,7 the Gilmore equation,8 the Herring-Trilling equation,9 and the Kirkwood-Bethe equation.10 However, these models are not valid at two important stages of bubble evolution: (1) during initial bubble expansion and (2) subsequent bubble collapse. During these brief stages, the bubble density approaches liquid density and no longer satisfies the implicit assumption of a low-density gaseous state. Furthermore, the emitted stress wave energy during these transient episodes can appreciably impact the overall bubble energetics.11 One approach toward appropriately considering stress wave emission is to extend the above-described Rayleigh modeling by allowing for high gas density in the bubble interior and properly including shock wave propagation across the bubble boundary.12

The second approach toward properly including stress wave emission is to perform numerical hydrodynamic simulations of the evolving bubble with high spatial and temporal resolution.13 In this Proceeding we describe some of our recent work in simulating bubble experiments in one- and two-dimensions. Two-dimensional effects can be important when the dimension of a fully evolved bubble is comparable to the cylindrical fiber radius. In this case, a significant fraction of the deposited laser energy is converted into nonradial motion which acts to reduce the overall size of the vapor bubble.

Another context in which bubble dynamics is important is the irradiation of individual melanosome particles with a short-pulse laser. Ongoing experiments by Lin and Kelly5 show a persistently high Mach number shock emitted from the melanosome as compared with simulation predictions.14 Possible explanations include an erroneously measured absorption coefficient or perhaps a discreteness effect attributed to substructure of the melanosome which may act to effectively boost the shock strength. We consider and explore this latter scenario in this Proceedings.
initiated vapor bubble near the fiber-optic tip.\textsuperscript{18} We are often interested in knowing how $R_m$ scales with the parameters of the experiments, e.g., deposited laser energy $E_L$, fiber radius $r_f$, laser pulse length $\tau_L$ and absorption coefficient $\mu_a$. The deposited laser energy is assumed to vary exponentially with distance from the end of the fiber, and the absorption length $\mu_a^{-1}$ can be varied experimentally by using different dye concentrations.\textsuperscript{18} In Fig. (2) is shown the results of a series of one-dimensional LATIS simulations for $R_m$ versus absorption length and for two values of fiber radius. As described in reference 13, a meaningful correspondence between the one-dimensional simulations and the experiment requires that the surface area of the simulation sphere match the area of the fiber tip. Using $R_m$ as a measure of bubble generation efficiency, we can conclude from Fig. (2) that larger fiber radii and smaller absorption lengths are conducive to higher bubble efficiency. We have also studied the dependence of bubble efficiency on laser pulse-lengths between 3 ns and 900 ns and found only a very weak variation with pulse length.

![Fig. 2: Simulated maximum bubble radius versus absorption length for two values of fiber radius in water. Laser energy is 0.5 mJ, laser pulse-width is 3 ns, and ambient pressure is 10 bars.](image)

Scaling studies such as that shown in Fig. (2) are useful design tools when two-dimensional effects are not paramount. We expect that two-dimensional effects will become important when $R_m$ is not much larger than $r_f$. This assertion is reasonable because the presence of the fiber tip breaks the spherical symmetry of an evolving vapor bubble and causes nonradial flows around
the end of the fiber. LATIS is well-suited to investigate the role of nonradial motion and the deviations from one-dimensional behavior.

The two-dimensional simulations are run in a Lagrangian mode where the numerical mesh moves with the hydrodynamical flow. A typical simulation involves approximately 5000 quadrilateral zones and nearly 10000 hydrodynamical timesteps. The main challenge of these two-dimensional simulations is to maintain a large numerical timestep while keeping the zonal mesh from becoming too tangled or snarled. Maintaining a quasi-orthogonal mesh requires occasional "rezoning" of the mesh and interpolation of the physical quantities such as mass, momentum and energy. However, excessive rezoning can alter the "mass matching" of adjacent zones over long timescales which can adversely affect the hydrodynamical motion. In addition, excessive rezoning can lead to numerical diffusion of mass, energy and momentum. Interesting long timescale behavior, such as the collapse phase of the vapor bubble, can be difficult to track with simulations if the hydrodynamics is compromised by too much rezoning. For example, Palanker et al have found evidence of forward jetting immediately following collapse of the electric-discharge-induced vapor bubble. Such a hydrodynamic phenomenon

![Mesh plot of simulated vapor bubble at 5 μs.](image)

Fig. 3: Mesh plot of simulated vapor bubble at 5 μs.
may have important ramifications for various laser-assisted vascular therapies, e.g., laser-assisted thrombolysis. To accurately capture this late-time hydrodynamic effect, reliable hydrodynamic simulations are required.

In Fig. (3) is shown a mesh plot at 5 μs from a two-dimensional LATIS simulation of a bubble experiment using a quasi-Lagrangian numerical scheme. The simulated experimental conditions consist of $E_L = 0.317 \text{ mJ}$, $\tau_L = 5 \text{ ns}$, $\mu_a^{-1} = 7 \text{ μm}$, and $r_f = 100 \text{ μm}$. We have improved upon our recent work on two-dimensional vapor bubble simulations with LATIS by (1) implementing a "no-slip" boundary condition on the fiber tip, (2) including 15 μm of cladding surrounding the sides of the fiber as in the experiment, and (3) using the viscosity of liquid water ($1.054 \cdot 10^{-3} \text{ kg/m/sec}$) in the calculation. The no-slip condition is more physically meaningful than a "slip" boundary condition because of the presence, in general, of a viscous boundary layer over the fiber. In addition to the above improvements, we have maintained to a large degree the integrity of the interface separating the vapor bubble and surrounding liquid. Monitoring the

![Graph](image)

**Fig. 4:** Comparison of simulated bubble size in one- and two-dimensions with experiment. Fiber radius is 115 μm, deposited laser energy is 0.317 mJ over 5 ns, and absorption length is 7 μm.
interface is more naturally achieved by running the calculation in a Lagrangian mode where the zonal mesh follows the fluid flow by design.

In Fig. (4) is shown a comparison between the simulated and experimentally observed bubble behavior. The average bubble radius in a cylindrically symmetric geometry is defined as follows: \( R_B(t) = (a^2 - b^2)^{1/3}, \) where \( 2a \) is the maximum extent of the bubble along the symmetry axis (or along the optical fiber) and \( b \) is the maximum bubble radius. The agreement between the two-dimensional simulations and experiment over a complete expansion and collapse phase of the bubble is remarkably good. Also shown are the results of one-dimensional simulations for the same experimental conditions. The significant discrepancy between the one- and two-dimensional simulations is attributable to the substantial component of non-radial motion as the bubble evolves.\(^{13}\)

In brief summary, two-dimensional numerical simulations with LATIS of vapor bubble experiments at LLNL show very good agreement in tracking the detailed evolution of the bubble. With this validation of our modeling capability, a wide variety of problems of interest in laser medicine can now be reliably pursued.

### 3. Melanosome dynamics

In the previous section, we studied the evolution of a vapor bubble at a fiber optic tip in a regime where the speed of the acoustic wave emitted prior to bubble formation is very close to the sound speed. The simulated maximum temperatures are over 300°C, giving pressures typically on the order of a few kbars. Generation of even larger temperatures and pressures is generally not desirable with such a fiber-optic laser delivery system because of the potential for collateral tissue damage, particularly to the vessel wall. By contrast, a strongly supersonic regime of bubble formation is often characteristic of laser-melanosome interactions involving the retina or epidermis where larger energy densities are normally achieved. Typically, peak pressures on the order of several tens of kbars, temperatures of several thousands of degrees [°C], and Mach numbers approaching two can be generated over micron-size scales.

Lin and Kelly have conducted experiments to study sub-nanosecond laser irradiation of bovine melanosomes.\(^5\) Strong shocks were observed to emanate from the melanosomes with average shock speeds approaching 2700 m/sec with inferred pressures of nearly 35 kbars. As previously reported,\(^{14}\) we attempted to understand this strong shock behavior by performing one-dimensional LATIS simulations of a single bovine melanosome absorbing the incident laser light. We assumed a homogeneous absorption over the entire volume of the melanosome which had an average diameter \( d \) of 2.3 μm. For an average absorption coefficient of 2000 cm\(^{-1}\) as described in reference 14 and a laser fluence of 2 J/cm\(^2\), the absorbed energy per melanosome was
estimated to be 24 nJ. The simulated shock pressure at the surface of the melanosome was only 9.5 kbars. We next considered the possibility that the laser absorption coefficient in the melanosome could be higher than reported in the literature by a factor of three. In this case, the absorbed energy was 72 nJ and the peak shock speed increased to nearly 26 kbars, which more closely agreed with the inferred experimental value of 35 kbars.\textsuperscript{14}

Another possibility for explaining the discrepancy between simulations and experiment is that a large number of absorbing sites within the melanosome is responsible for a stronger superposed shock compared to the uniform absorption case. Melanosomes are known to contain thousands of melanin granules with an average radius $r_g=0.015\ \mu m$. We now consider how a large number of discrete absorption sites may possibly provide a collective boost in shock strength at the surface of a melanosome.

In the case of a bovine melanosome, there are about $N_g=2.4\cdot10^4$ melanin granules per melanosome.\textsuperscript{14} Therefore, the average (half) separation between nuggets $r_s$ is 0.04 $\mu m$. Consequently, a uniform absorption of 24 nJ over the entire melanosome is equivalent to depositing 1 pJ of energy into $N_g$ volumes, each of radius $r_g$. We now consider the effect of discrete absorption by individual melanin granules. If the same 1 pJ of energy is absorbed over the volume of the melanin granule with radius $r_g$ instead of $r_s$, then the energy density increases by the factor $(r_s/r_g)^3$. Here, we have assumed stress confinement over the duration of the laser pulse (100 ps) for simplicity. In addition, the amplitude of the (strong) shock at $r=r_s$ is reduced by the factor $(r_g/r_s)^2$ due to the combined effects of shock dissipation and spherical divergence.\textsuperscript{20} Thus, a net enhancement in shock strength at $r=r_s$ by the factor $r_s/r_g$ over the uniform case may result, according to this very simple analysis. For the case at hand, this factor corresponds to a pressure enhancement of nearly 3.

We have performed one-dimensional LATIS simulations to study further this simple scaling behavior and to consider in greater detail the issue of stress confinement. For the expected high temperature conditions, a SESAME two-phase equilibrium equation-of-state was employed.\textsuperscript{21} A stress confinement time $\tau_c$ is defined as an acoustic transit time across an energy-deposition region and is on the order of 20 ps for a melanin granule. For laser pulse-lengths $\tau_L$ less than $\tau_c$, the deposited energy remains mostly localized during the pulse. Figure (5) shows the results of
Fig. 5: Simulated peak pressure enhancement at an inter-granular (half) separation $r_s$ versus laser pulsewidth due to discrete absorbing centers. Enhancement factor is derived from ratio of simulated peak pressures at $r_s=0.04 \, \mu m$ for energy deposition of 1 pJ over two nested volumes: (1) granular volume of radius $r_g=0.015 \, \mu m$ and (2) smoothed volume of radius $r_s$.

A series of simulations for the enhancement in peak pressure at $r_s$ when the energy absorption occurs within the melanin granule radius $r_g$ instead of $r_s$. For very short pulsewidths, the pressure enhancement is less than expected because the pressure increase with deposited energy density is less than linear for very high energy densities, according to SESAME. For laser pulse-lengths on the order of 100 ps as considered in the experiment, a nearly three-fold enhancement in peak pressure at the inter-granular distance $r_s$ is predicted. This level of enhancement persists for even longer pulse-lengths despite poorer stress confinement. Work is in progress to better understand this regime using analytical modeling. We believe that the mechanism for pressure enhancement at longer pulse-lengths is no longer mediated by a shock as in the stress confined case but is determined by the longer timescale dynamics of vapor bubble expansion.
We now consider in more detail how discrete absorbing sites uniformly distributed throughout a melanosome can collectively yield higher shock strengths at the surface of a melanosome compared to the case of homogeneous absorption. First, we require a scaling-law expression which superposes the individual shocks produced by the granular absorption sites. The pressure at the surface of a melanosome $P_m$ can be straightforwardly written in terms of the peak pressure $P_s$ at $r = r_s$ and the number of absorbing sites $N_g$ as follows:

$$P_m(t) = 6FN_gP_s\cdot \left(\frac{r_s}{d}\right)^2 \cdot g(t).$$  \hspace{1cm} (2)$$

Here, $g(t)$ describes the time-dependence of pressure on the melanosome boundary and incorporates transit time effects within the melanosome and the temporal history of energy absorption within $r_s$. Figure (6) displays some examples of $g$ versus normalized time $\tau$. We note from Fig. (6)
that the maximum of $g$ varies little with the absorption history or $v_g$; thus, we take the maximum value of $g$ as 0.38. In Eq. (2) we have assumed the strong shock limit for energy dissipation throughout the melanosome, i.e., $P = r^{-\alpha}$ with $\alpha = 2.20$ because we do not know \textit{a priori} how the myriad shocks precisely interact within the melanosome, we have introduced a form-factor $F$ which will be determined from a LATIS simulation for a uniformly heated melanosome. Note that such a simulation and the analysis based on Eq. (2) with a uniform energy deposition within $r_s$ describe the same model system, i.e., a homogeneously heated melanosome. We determine $F$ by comparing Eq. (2) with a LATIS simulation for the case of a uniformly heated melanosome. We use $N_g = 2.4 \cdot 10^4$, $d = 2.3 \mu m$, and $P(r_s) = 2.2$ kbars from LATIS simulations of a uniformly heated volume of radius $r_s$ and $\tau_L = 100$ ps. A direct LATIS simulation of the peak pressure at the surface of a uniformly heated melanosome gives $P_m = 9.5$ kbars; thus, $F = 0.26$. We now consider the case of discrete absorption over a granular volume of radius $r_g = 0.015 \mu m$. From the calculations used to obtain Fig. (5), we found that $P(r_s) = 6$ kbars. Equation (2) now gives a peak melanosome pressure of nearly 30 kbars which compares favorably with the experimentally inferred value of 35 kbars. Additionally, we point out that the overall dependence of Eq. (1) on the number of granules per melanosome is rather weak, varying only as $N_g^{1/3}$ since $r_s \approx N_g^{-1/3}$.

An implicit assumption made in the above argument is that $F$ changes little for the case of discrete absorption, particularly when $r_s / r_g$ is not too much larger than unity. Determining whether this assumption is valid for the case at hand with $r_s / r_g \approx 2.6$ and whether the scaling predicted by Eq. (2) holds ultimately requires three-dimensional hydrodynamic simulations. Such a computational capability is presently being developed at LLNL.

4. Summary

We are continuing to develop modeling techniques based on the LATIS simulation code for understanding the onset and evolution of vapor bubbles in various medical applications. By successful comparison with experiment, we have demonstrated that a two-dimensional modeling capability is important for understanding the evolution of a laser-initiated vapor bubble in a medically relevant geometry.

We have begun exploring the role of discrete absorbing sites in a laser-irradiated melanosome. A simple model is suggested to aid in explaining a previously reported discrepancy between modeling and experiment concerning the amplitude of shocks exiting the melanosomes. Further work is needed to understand and model the complicated shock interactions intrinsic to a matrix of absorbing sites in biological tissue.

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6. References


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