**Validation of pressure relaxation coefficient in RELAP-7 seven-equation model**

Award Identification Number:

The U.S. Department of Energy, DE-NE0008747

Period of Performance: 01/01/2019 to 03/31/2019

Principal Investigator: Philippe M Bardet

Submitted by

Philippe Bardet

Department of Mechanical and Aerospace Engineering

George Washington University

Science and Engineering Hall, suite 3580  
800 22nd St, NW, Washington, DC 20052

and

Eric Johnsen

Department of Mechanical Engineering

University of Michigan

2043 Walter E. Lay Automotive Laboratory

1231 Beal Ave, Ann Arbor, MI 48109

April 30, 2019



George Washington University

Department of Mechanical and Aerospace Engineering

Thermo-Fluids Laboratory

Quarterly Report: 2019 q2

by

Philippe Bardet

George Washington University

and

Eric Johnsen

University of Michigan

April 30, 2019

Prepared for

Nuclear Energy University Programs

The U.S. Department of Energy

800 22nd St NW

Washington, DC 20052

# ACKNOWLEDGEMENTS

This research is performed using the funding received from the U.S. Department of Energy (DOE) Office of Nuclear Energy’s Nuclear Energy University Program. The authors are grateful for the opportunity to work on this exciting project.

# ABSTRACT

The RELAP-7 code is the next-generation nuclear reactor system safety analysis code being developed at Idaho National Laboratory. The code builds on the Multi-Physics Object Oriented Simulation Environment (MOOSE) framework, enabling massively parallel calculations and coupling to other codes for multiphysics simulation. In RELAP-7, the comprehensive Seven-Equation multiphase model is used to represent quasi-one-dimensional gas-liquid flows for problems with varying cross-sectional areas. For fast transients (such as water hammer or steam explosion) in water, the Seven-Equation model takes into account non-equilibrium processes through relaxation rate terms.

Due to the complex polar and tri-atomic nature of the H2O molecules, the relaxation rate terms in the seven-equation model rely on simplified models and limited data. There is therefore significant empiricism and knowledge gap in those terms that limits the application domain of RELAP-7 for fast transients. This projects aims to acquire validation data of non-equilibrium processes to validate the seven-equation model in R7. This will be accomplished by:

1- Measuring return to equilibrium in fast transients with high-speed non-intrusive and non-perturbative laser diagnostic in canonical experiments;

2- Complementing experimental data with first-principle simulation of energy exchange processes;

3- Validate RELAP-7 with assistance of 3D proprietary direct numerical solver.

**TABLE OF CONTENTS**

[ACKNOWLEDGEMENTS 2](#_Toc10717697)

[ABSTRACT 3](#_Toc10717698)

[PROJECT BACKGROUND 5](#_Toc10717699)

[Chapter 1. Background 7](#_Toc10717700)

[1.1 Background on multiphase model 7](#_Toc10717701)

[1.2 Background on the pressure relaxation coefficient for water vapor and liquid water 7](#_Toc10717702)

[1.3 Background on multi-scale simulations 8](#_Toc10717703)

[1.4 Background on diagnostics for pressure and velocity in multiphase flows 9](#_Toc10717704)

[1.5 Background on ultrafast laser absorption spectroscopy 10](#_Toc10717705)

[Chapter 2. Experimental Progress 12](#_Toc10717706)

[2.1 Compressed air cannon 12](#_Toc10717707)

[2.2 Laser Bubbles in confined channels 14](#_Toc10717708)

[2.3 Diagnostics progress 15](#_Toc10717709)

[2.3.1 MTV in aqueous phase 15](#_Toc10717710)

[2.3.2 MTV in vapor phase 16](#_Toc10717711)

[2.3.3 Ultrafast Absorption Spectroscopy in water vapor 17](#_Toc10717712)

[Chapter 3. Multiscale simulations 19](#_Toc10717713)

[3.1 Direct simulations of laser bubbles 19](#_Toc10717714)

[Chapter 4. Conclusion and Future Works 23](#_Toc10717715)

[4.1 Work Summary and Conclusion 23](#_Toc10717716)

[4.2 Future Work 23](#_Toc10717717)

# PROJECT BACKGROUND

**Project Objectives**

The primary objective of the proposed research is to characterize the pressure relaxation coefficient in RELAP-7 seven-equation model. Due to the complex polar and tri-atomic nature of the H2O molecules, the relaxation rate terms rely on simplified models informed by limited data. Therefore, there is significant empiricism and knowledge gap in those terms that limits the application domain of R7 for fast transients. This project aims to acquire validation data of non-equilibrium processes to validate the Seven-Equation model in R7 by:

(1) Measuring velocity and pressure in each phase and the interface as well as return to equilibrium in fast transients with high-speed non-intrusive laser diagnostics in canonical experiments;

(2) Complementing experimental data with a multiscale computational approach, including a 3D proprietary direct numerical solver;

(3) Validating R7 with a combination of experimental data and first-principle simulations.

**Technical Approach**

These tasks will be performed in close collaboration between an experimental team at Geroge Washington University (PI: Philippe Bardet) and a theoretical team at University of Michigan (Co-PI: Eric Johnsen). The PIs will work closely with a DOE National Laboratory (DOE Lab). Experiments and simulations of two canonical and repeatable problems will be considered: (i) a laser steam explosion in a pipe, and (ii) a water hammer in a pipe (Rich pipe).

By building on several years of instrumentation development by the PI (some with NEUP support), a suite of demonstrated molecular-based non-intrusive optical diagnostics will be deployed to measure velocity in each phase and at the interface. Additionally, a laser absorption spectroscopic technique in the PI’s laboratory will be further advanced to measure pressure in the gas phase. The pressure in the liquid will be measured with high-speed needle hydrophones. From those the pressure and velocity at the interface will be deduced. All measurements will be conducted with repetition rates > 1 MHz and, therefore, will be time-resolved even in these challenging fast transients. All the dynamical quantities in the Seven-Equation model will be measured, enabling direct estimation of the relaxation coefficients entering this model. Additionally, the new laser spectroscopy technique enables very fine measurements that resolve individual vibration and rotation of water vapor molecules: relaxation rates to equilibrium will be measured directly providing a second estimate (first-principle based) of the relaxation terms!

The co-PI will utilize state-of-the-art molecular dynamics to simulate the relaxation processes; such first-principle simulations are necessary due to the complexity of water vapor molecule; it will also enable to gain more confidence in the experimental results and complement the validation domain covered by the experiment. Relaxation rate coefficients and conditions from the MD simulations will then inform Rayleigh-Plesset models that will complement a 3D multiphase direct numerical simulation code. This multi-scale scheme complementing the experiments will provide a complete set of validation data for the Seven-Equation model in R7. Additionally, this collaborative approach will provide new class of diagnostics and theory for complex phase change processes in water. Such tools and fundamental knowledge will be transformative to the thermal-hydraulics phase change community and invaluable for NEAMS effort for R7 and Nek5000 as well as traditional LWRS programs.

**PROJECT SUMMARY**

**Accomplishments this quarter**

* Started assembly of compressed air cannon facility to generate repeatable water hammer events. Shake down testing is expected in the next quarter. The lab in which the system will be mounted has been thoroughly renovated and is now certified for laser use.
* Ordered the laser for the main diagnostics to measure return to equilibrium. We leveraged a DOD DURIP equipment grant to order a custom laser much more capable than initially budgeted in the proposal. Expected delivery date is 06/10/2019.
* First laser bubbles have been obtained in open environment to check laser and optics performance before going to enclosed environments (the second planned experiment for the project).
* Initial simulation of laser bubbles in enclosed have been conducted with 3D Direct Numerical Simulations. The data are still being analyzed and interpreted, but it appears that confinement has a strong effect on bubble growth.

# Background

## Background on multiphase model

In the RELAP-7 code, the Seven-Equation multiphase model is expected to represent interfacial fluid dynamics as well as multiphase mixtures. Assuming no mass, momentum, or energy transfer other than relaxation between the two phases, it is written as follows [1, 2]:

(1), (2),

(5), (6),

where the subscripts 1, 2 and, *I* denote phase 1, phase 2, and the interface, respectively, **is the volume fraction, ***u*** the velocity vector, *p* the pressure, ** the density, *E* the total energy per unit volume, and ***I*** the identity tensor. Here, the acoustic limit is considered, where ** and ** are relaxation coefficients determining the rates at which the velocities and pressures of the two phases reach equilibrium. Although specific expressions have been proposed for these coefficients in various limits, *λ* and ** could be taken as arbitrary parameters to be determined based on experimental measurements. Different expressions for interfacial velocities and pressures have been suggested, one set of which include, in the acoustic limit (*Z=ρc* is the acoustic impedance, *c* is the speed of sound):

Each phase is governed by its own equation of state (not given here), e.g. the stiffened equation of state for liquids or the ideal gas law. Viscous effects and heat transfer can readily be added. Though the equations are written for generalized coordinate systems, the governing equations are implemented in quasi-1D form in R7. From equations (1-7), it can be seen that validate the terms ** and ** it is necessary to resolve pressure and velocity in each phase as well as at the interface.

Different variants of the Seven-Equation model have been proposed, with modifications to the system of equations listed above. In the limit of stiff mechanical relaxation, velocity relaxes to a single value for both phases, as does pressure, and the Seven-Equation model naturally reduces to the   
Five-Equation model [3, 4], and the simple (three-equation) Homogeneous Equilibrium Model, as well as other more or less sophisticated approaches.

## Background on the pressure relaxation coefficient for water vapor and liquid water

The pressure relaxation, or return to mechanical equilibrium, is governed by relaxation of molecular degrees of freedom, in other word, the adiabatic energy exchange between internal energy and translational degrees of freedom. The coefficients are derived from the relaxation times that can be measured experimentally.

In pure liquid water, the two known processes are thermoviscous and structural; the details of these processes can be found in [5]. They are both occurring at picosecond time scales and are negligible at first order for most transients of interest here.

In water vapor, the main dissipative processes are translational, vibrational, and rotational relaxations. For most pressure and temperature conditions, the translational relaxation time is too short to be considered, and only vibrational and rotational relaxation of water vapor molecules must be resolved. Analytical models describe these relaxation times accurately for small diatomic gas molecules and even for simple triatomic molecules such as CO2. Unfortunately, no analytical model describes H2O satisfactorily over the range of parameters considered here because of its complex geometry and polar nature. Therefore, one must rely on a combination of experiments and molecular dynamic simulations (partly calibrated by experimental results) to estimate the relaxation times. To measure return to equilibrium, an experiment should therefore resolve independently rotational and vibrational temperatures, the relaxation time will be the time at which the two temperatures agree [5]. Additionally, the independent measurement of rotational and vibrational temperatures will enable to reconstruct the pressure from the spectroscopy data. Therefore, the thermal and mechanical relaxation times will be determined experimentally. They depend on temperature and pressure and are on the order of 10th of microseconds or longer for the experimental cases that will be considered here. Molecular Dynamics (MD) simulations will enable to expand the experimentally covered parameter range to broader conditions.

## Background on multi-scale simulations

While experimentally measuring non-equilibrium phenomena at the molecular level is beyond the scope of the proposed research, Molecular Dynamics simulation can be leveraged to determine the thermodynamic conditions produced at early time during laser-induced cavitation. The major portion of the lifetime of a laser-induced cavitation bubble is well described by continuum fluid mechanics under thermodynamic equilibrium. However, the laser breakdown phenomenon and possibly the last stages of collapse are governed by thermodynamics far from equilibrium. Furthermore, the spatial and temporal scales may be too small to be well described by continuum mechanics. The LAMMPS code [6] has potentials capable of describing laser deposition in water with acceptable accuracy. Fig. 1 shows preliminary simulations of laser-induced nucleation of a vapor bubble in water. A void forms and grows until a critical temperature is reached, at which point the nucleus stabilizes; this first stage is clearly a manifestation of relaxation effects. Thereafter, the cavity fills with vapor, and eventually grows again. Due to the greater laser power, production simulations for the problems under consideration will require far greater run-times, more molecules, and more sophisticated modeling of water molecules [7]. These MD simulations will provide the thermodynamic state of the bubble during the nucleation phase, which will subsequently be input into continuum approaches for cavitation-bubble dynamics to better represent the thermodynamic state at early time following the laser energy deposition. In particular, the MD simulations will determine the time scales over which non-equilibrium effects are active, and beyond which our continuum approaches are valid.

The computational expense of MD simulations is such that they will be run for nanoseconds, the thermodynamic state (e.g., pressure, temperature, composition of the bubble) will be incorporated into the Rayleigh-Plesset (RP) ordinary differential equation as initial conditions accounting for the laser deposition phenomenon. RP approaches have the advantage of being computationally inexpensive. Despite being homobaric and assuming thermodynamic equilibrium, the RP equation is capable of accurately representing spherical bubble oscillations and collapse, though it is known to fail to represent the early growth of laser-generated vapor bubbles (it can also be modified to take into account non-thermal equilibrium). The MD simulations will thus provide far more representative initial conditions for the RP simulations.

The Rayleigh-Plesset results will be used as initial conditions, as well as compared to the 3D numerical code of University B. The code is currently based on the Five-Equation model and will be expanded to the Seven-equation model. It solves the compressible Navier-Stokes equations in three-dimensions using a high-order accurate, solution-adaptive, finite-difference approach. Time is marched forward using a third-order explicit Strong-Stability-Preserving Runge-Kutta scheme. For the spatial discretization, a discontinuity sensor discriminates between smooth regions, in which explicit fourth-order central differences are used, and discontinuities, where a fifth-order Weighted Essentially Non-Oscillatory (WENO) scheme is applied. Diffusive and sources terms are solved using central differences. The code is parallelized using MPI, with excellent parallel scaling up to over 100,000 CPUs, and has been used for direct numerical simulations of multifluid turbulent flows, in which all scales are resolved with no model. The resulting approach is conservative, high-order accurate and preserves pressure/temperature equilibrium at material interfaces and contact discontinuities. As part of this project, the Seven-Equation models will be incorporated into this code by adding the relaxation terms in the equations, thus providing an approach complementary to R7 and enabling direct code-to-code comparison and benchmarking.

## Background on diagnostics for pressure and velocity in multiphase flows

A progression of optical diagnostics will be deployed in the proposed experiments. The volume fraction and interface velocity will be measured with high-speed shadowgraphy. The PI’s lab has cameras and light sources able of MHz repetition rate and 10 ns pulse length to guarantee that the dynamics of the fast transients is captured. In parallel, velocimetry in both phases will be implemented.

In the fast transients of interest here, measuring velocity and acceleration in the liquid and gas phases is challenging with particle based methods; a slight mismatch in density will result in particle lag and biases, the gas phase will also be challenging to seed and glare at interface will prevent resolving velocity fields. Instead, the PI is proposing to use molecular tracers in both phases: Molecular Tagging Velocimetry (MTV), Fig. 1.1. The PI will be able to leverage existing efforts in the lab to conduct MTV in liquid and gas phases. In the liquid, a small fraction (10-6 molar) of caged fluorescent dye is mixed with the water. A fluorescent pattern is imprinted in the liquid with a first UV laser (Nd:YAG at 355 nm); the pattern is tracked multiple time in a time of flight manner with a high-speed pulse-burst (PB) Nd:YAG laser at 532 nm. The PB laser in the PI’s lab is one of a kind and can operate at repetition rate > 1 MHz. In the gas phase, the PI has recently demonstrated that water vapor was a very efficient tracer for MTV. H2O is photo-dissociated in OH radicals by an ArF laser (193 nm, 10 ns pulse). The OH radical pattern is then tracked with a quad-pulse tunable dye laser (at 283 nm, 10 ns pulse) and OH fluorescence recorded. The quad-pulse of the gas MTV enables to measure acceleration, which is necessary to resolve (eq. 1-7). Finally, it should be pointed out that MTV relies on fluorescence: the signal can be spectrally isolated from the laser, eliminating glares at interfaces that would otherwise limit particle based approaches. If a residual water film coats the tube surface, it will distort the images (and reduce resolution), but will not prevent laser lights to be delivered in the steam bubble. In a repeatable facility, those two diagnostics can be conducted sequentially to facilitate deployment (while being simultaneous with shadowgraphy) and will be attempted simultaneously. Shadowgraphy with and without MTV will enable to assess the effect of the dye and potential (minimal) leaser heating on the dynamics of the flow, enabling optimization and/or corrections.

|  |
| --- |
| Image result for molecular tagging velocimetry inside a  droplet |
| **Fig. 1.1. Sample MTV data. Patterns of fluorescent markers created in-situ, images (a) and (b), are cross-correlated to lead to velocity fields in (c) [8].** |

Pressure in the liquid phase can be measured with high-speed (30 MHz) needle hydrophones. However, there exists no demonstrated approach to measure pressure in the gas phase. Instead, we are proposing to develop a new spectroscopic diagnostic based on an existing technique in the PI’s laboratory. Additionally, this technique will enable to directly measure the relaxation times that will be invaluable for the CFD and to validate the relaxation time coefficients.

## Background on ultrafast laser absorption spectroscopy

The relaxation time in gases is a very challenging quantity to resolve; it has been measured in a variety of manner and with mixed results. To date deployed techniques include scattering and absorption of ultrasound waves or pressure measurements in shock tubes or expansion nozzles. However, the effect of liquids and gases are challenging to isolate in water hammer environments and the results disagree by 200-300% [9]. Laser spectroscopy techniques are more suitable for probing the gases in multiphase flows as liquid phase has a negligible effect on the spectrum. Femtosecond Coherent Anti-Stokes Raman Scattering (fs-CARS) offers a promising approach to resolving vibrational or rotational temperatures in a small probe volume without adding too much energy to the gas [10]. However, this technique is hard to synchronize externally due to the nature of the fs laser amplifier, is prohibitively expensive (>$400k in hardware alone), and is very sensitive to beam steering likely present at the scattering interface between the liquid and gas. Instead, we are proposing to use Ultrafast Absorption Spectroscopy [11], which is an evolution of tunable diode laser spectroscopy (TDLAS), which has been developed by the PI’s group with NEUP support. Absorption spectroscopy is less sensitive to noise introduced by scattering as fs-CARS.

Small gas molecules have discrete spectral absorption features that are related to individual rota-vibrational transitions: light absorption is resonant, i.e. it is wavelength dependent and each absorption feature has a narrow spectral range. Each individual feature is the result of Doppler and collisional broadening. Doppler broadening is described by a Gaussian distribution, which is fully characterized by its half-width (eq.8) and depends only on temperature. Collisional or pressure broadening is best modeled by a Lorentzian distribution, with half-width (eq.9 for pure water) that depends on temperature and pressure. The overall absorption feature is the convolution of a Gaussian and a Lorentzian, which is a Voigt distribution [12]. The Voigt distribution half-width, can be approximated as (eq.10). The propagation of the laser beam through the pure liquid phase, which will be case for some of the tests, will not affect the discrete absorption features mentioned above. Instead, the liquid phase and scattering at the liquid-gas interface will result in a shifted zero-baseline, which will be subtracted from the signal of interest here during data processing step.

(8), (9),

(10)

In ultrafast absorption spectroscopy one takes advantage of the unique properties of short pulse (picosecond to femtosecond) lasers to generate supercontinuum (SC) sources (that cover a large spectral region) to characterize those spectral absorption features [11]. The theory shares similarity with FTIR spectrometry, which is commonly used for characterizing chemical species, but it can operate at much higher acquisition rates, sensitivity, can also resolve pressure, and the fiber delivery simplifies deployment in harsh environments as expected here. The generation of SC light by pumping dispersive nonlinear fibers with ps- or fs-lasers offers very stable pulse to pulse spectrum, enabling low noise and highly sensitive measurements. There now exist a large selection of such SC sources that are optimized in the spectral range of interest here. They are affordable and can operate between 0.5 and 100 MHz.

*Instrument integration:* To simplify detection aspect of the proposed instrument, the pulse from a Mid-IR super continuum source will be stretched from picoseconds to 100s of nanoseconds upon passage through a dispersion-compensating module (DCM) commonly used in telecommunication, and therefore affordable. The stretched pulses will be subsequently recorded in the time domain using an ultrafast photodiode with 20 GHz bandwidth coupled to a 4 GHz oscilloscope. By knowing the dispersion property of the DCM and the viewport used in the experiment, we will reconstruct the absorption spectrum. See Fig. 3 for a sketch of the proposed instrument.

|  |
| --- |
|  |
| **Fig. 1.2. Instrument integration. Gas phase in the test section is probed along the open path red beam. SMF: single mode fiber used for transmitting beam to region of interest.** |

*Vibrational and Rotational Temperature reconstruction from UAS data:* HITRAN (a database of several millions known absorption lines of gas molecules) simulations show that water vapor has a very rich absorbing features near 1.5 µm (Fig. 1.2); by scanning over 300 nm, one will resolve numerous roto-vibrational transitions. By doing a spectral fit of the feature peaks and of the underlying theory, the vibrational and rotational temperatures will be independently resolved at repetition rate of up to 1 MHz. First the zero baseline will be estimated (red curve on fig. 1.3 left) and the resulting absorption spectra calculated (curve on fig. 1.3 right). The peak of each absorption feature depends on the temperature of the gas. Therefore, the vibrational and rotational temperatures will be resolved in an inverse process by minimizing the residuals of the experimental subtracted from the theoretical absorption spectra. To accelerate data processing development, we will reuse the TDLAS codes of the PI’s lab.

|  |  |
| --- | --- |
|  |  |
| **Fig. 1.3. Typical broad scan of water vapor and absorbance reconstruction [11].** | |

*Pressure reconstruction from UAS data:* Once the temperature is known, several schemes exist to reconstruct pressure from the absorption signal of a single transition, the main one is described in [13]. It extracts the pressure from the Lorentzian component of the linewidth. From the temperature, the Doppler component of the linewidth is estimated (eq.8). The Lorentzian (or pressure broadening) component is extracted from the total linewidth given the Doppler width, using (eq.10). The pressure is then determined from the Lorentzian width (eq.9) using pressure broadening coefficient and exponent (*γ* and *n* in eq.9) found in the literature or calibrated in the laboratory. With adequate temporal resolution one will therefore record the rapid evolution of the pressure and therefore estimate its relaxation time.

*Temporal resolution*: As mentioned above, the laser operating frequency will be adjustable, with a nominal operation at 1 MHz. The SC pulse will be stretched to a bit less than 1 µs to increase the resolution of the time-domain acquisition. Published work on this technique indicate that shot noise limits single spectra acquisition and it might be necessary to phase average the measurements over 10-100 pulses to obtain adequate resolution on the spectral reconstruction, Fig. 1.3. Therefore, with a very repeatable and precisely triggerable experimental facility one will be able to resolve the phase average thermal and mechanical relaxation times with a temporal resolution on the order of 1-2 µs. Alternatively, one could perform a moving average on the data to obtain relaxation times over a single event, reducing the temporal resolution to 5-10 µs. A combination of both will be used during the course of the project to assess their accuracy and precision. Thermal relaxation will be obtained once the two temperatures agree and mechanical relaxation once the pressure has converged to sufficient level.

# Experimental Progress

## Compressed air cannon

The main experimental facility is based on the Rich pipe concept. However, instead of using a drop tower, a compressed air cannon is being constructed, Figure 2.1. It consists of a driver and barrel. The projectile will be a pipe filled with water that will go water hammer when the pipe hits a solid obstacle. The final velocity of the projectile is a function of the driver pressure (gas pressure in cylinder) and barrel length. A simple model was derived to predict the projectile velocity (assuming a mass of 2 kg, which provides ample room for designing the projectile) and enable to size the driver and barrel size. Figure 2.2 shows the final design as a function of the driver volume. After iterating with Dr. Martineau’s team at INL, we designed the system such that the projectile has a final speed in excess of 50 m/s.

To save on cost and time, the compressed air cannon is being assembled from standard components. For example, the driver is a large diameter (6”) compressed air cylinder (14” length) with a piston inside. The end walls of the cylinder have been modified to enable loading the cylinder with compressed air on each side of the piston. The side facing the barrel (front) has been modified to seal the driver when a higher pressure is injected on the back side of the piston (Figure 2.3.a). To release the projectile, the back end of the cylinder is depressurized causing the piston to move back and inject high pressure air in the barrel. The flow leaving the back end of the barrel is choked providing a very predictable depressurization rate (and therefore piston speed). This design was adopted as it is possible to control pressure very precisely (0.1% or better) and therefore the experiment will be very repeatable.

The barrel length is currently fixed at 2 m. The barrel is made out of a honed cylinder (surface smoothness better than 0.001”) with inner diameter of 50.8 mm. The projectile will have an outer diameter of 50 mm, providing adequate clearance inside the barrel.

Finally, the compressed air cannon is mounted to a 10” I-beam, itself mounted on a frame to bring the barrel to the height of the laser. The I-beam was necessary to add mass to the overall assembly and minimize recoil of the system. Also it will serve as a support to mount a solid obstacle to intercept the projectile. The main components are shown in Figure 2.3.b).

All the hardware for plumbing the high pressure air into the cylinder have been received and pre-assembled.

|  |
| --- |
| https://lh6.googleusercontent.com/7S7KKbR97Em_vjwjhhN5XTNnFtVWCnDX_88xr_HLQNLYp0GjZE3MNIB8rQSnBxRmX2p_WFDQPTx-4eyVDG9v0IJ2iZ5sTp67afuG-VrwLA0tk9YIQlkJgyT8WHBVN1UpyP46Nxm6 |
| **Figure 2.1: sketch of compressed air cannon.** |

|  |
| --- |
|  |
| **Figure 2.2: speed of projectile at the barrel exit with current parameters.** |

|  |  |
| --- | --- |
|  |  |
| **a) Modified piston. The black front plate sits against the barrel end and seals it when the piston is pressurized on its back.** | **b) Components being ready for assembly** |
| **Figure 2.3. Main components of the compressed air cannon.** | |

To monitor the projectile speed exiting the barrel, a series of 3 fast photodiode are positioned at the exit of the barrel. They have a rise time of less than 1 ns and will capture precisely the front of the projectile. They will be connected a to a 2 Gsamples/s oscilloscope to measure the velocity. Once the air cannon has been well characterized, the photodiodes will serve as a trigger signal to start the acquisition of the instruments that will be deployed in the water pipe.

Next steps: we are finalizing a couple of components for the driver and plan on assembling the final system in the coming weeks with shake down testing and characterization of the air cannon repeatability to follow shortly after.

## Laser Bubbles in confined channels

This second experiment is being informed by simulations presented in section 3. Currently, we are generating laser bubbles in an unconfined environment to validate our optical system to generate the bubbles against published data in the literature. A frequency doubled Nd:YAG laser (532 nm) with 6 ns-pulse is used to generate the bubbles. Bubbles are created where the laser beam is focused. From literature review, it appears that the shape of the laser beam at the focal point is very important. We are currently assessing this effect by varying our optical arrangement and laser power to try and recover values published in the literature. Figure 2.4 shows a sample laser bubble.

While this setup is significantly easier to instrument than the air cannon, its main limitation might be the minimal repeatability. The laser has a variance of +/- 2% of pulse energy from pulse to pulse by design. We are also working on determining the sensitivity of the bubble size on pulse energy to better understand this effect and assess the overall repeatability of the system.

|  |
| --- |
| E:\Users\cfort\Documents\Charles\8_MTV_cageddye\051618_test_08\051618_test_08_1127_-1145.tif |
| **Figure 2.4. Sample laser bubble.** |

## Diagnostics progress

Several diagnostics will be deployed in this project. Update on them are provided here. It should be noted that some diagnostics development are driven by other sponsored projects: this is acknowledged, but still reported as we will rely on them for this project.

### 2.3.1 MTV in aqueous phase

To measure liquid velocity, PIV will not be the most appropriate diagnostic as particles will not follow the flow faithfully and will contaminate the liquid-vapor interface. While we will still use PIV in a first phase, thanks to simplicity in deploying it, we will focus on using time-resolved MTV here. Under support from DOD – Office of Naval Research, we have improved MTV in water in two very significant manner that will enable us to successfully complete this task. 1- We have identified a series of tracers that can be used in water using traditional PIV (green) lasers (Fort and Bardet, Experiments in Fluids, 2019). 2- We have improved the spatial resolution of MTV by nearly 2 order of magnitude, we are now able to resolve beamlets less than 30 µm in diameter compared to 1000 µm in Figure 1.1 (Fort et al, Experiments in Fluids, 2019). 2D MTV data are very small scale are illustrated on Figure 2.5. We are also in the process of upgrading our pulse burst laser to generate long pulses (100 ns). Based on a simple analytical model (Fort and Bardet, Optics Express, 2019), we will be able to significantly increase our signal to noise ratio from the process.

|  |  |
| --- | --- |
| **E:\Users\cfort\Documents\Charles\10_MTV_2018\030819_GRID\NICE FRAMES\fluorescence_grid\denoise_032819_MTV_grid2 - frames 1-270_000146.png** | **E:\Users\cfort\Documents\Charles\10_MTV_2018\030819_GRID\NICE FRAMES\fluorescence_grid\denoise_032819_MTV_grid2 - frames 1-270_000147.png** |
| **Figure 2.5. µ-MTV data. The lines are 30 µm-Ø with a spacing of 300 µm. This is the highest resolution achieved with MTV to date by factor of 15…** | |

Next steps: We hope to deploy MTV in water in this project within 1 or 2 quarters. All the instruments are now there or being upgraded thanks to other grants to enable us to acquire velocity data at more than 100 kHz and therefore reconstructing pressure from the time resolved velocity data.

### 2.3.2 MTV in vapor phase

Here we will rely on development conducted during a previous NEUP grant to Dr. Bardet. We will photo-dissociate H2O gas molecules with an ArF excimer laser and follow the OH radicals with a tunable dye laser. This variant of MTV is commonly called hydroxyl tagging velocimetry or HTV. Currently the system operates at 2×10 Hz, but we plan on going to higher repetition rates (time-resolved) by pumping the dye laser with the pulse burst laser. We will need to first demonstrate that the µ-MTV pattern presented in section 2.3.1 can also be generated in the gas phase.

So far we have conducted an analytical study of absorbance of ArF excimer laser (193 nm) in pure water. Because this beam will travel in water and water absorbs significantly photons in the UV (see Figure 2.6 for the real and imaginary part of the refractive index of water) we estimated how much. The linear refractive index can be expressed as a complex number, . The real part is the traditional refractive index used in diffraction, *n*, while the imaginary part is the extinction coefficient, *κ*:

(11)

The extinction coefficient is related to the absorption coefficient, *ka*, through the equation below. The energy of the electric field decreases by *1/e* after a distance *1/ka* in water.

(12)

At *λ* = 193 nm, *κ* ~ 2.5 × 10-7, so *ka* = 16.3 m-1. So in pure water, the laser energy will be attenuated by 37% after traveling 6 cm in water. In all the tests envisioned at this stage, it is not anticipated that laser beams will travel more than 1 cm in pure water (we are working in confined environments) and thus laser light will be delivered effectively in our tests.

|  |
| --- |
|  |
| **Figure 2.6. Linear refractive index of water (real and imaginary part).** |

Next Steps: We have confirmed that HTV can be successfully deployed in our configuration. We will work on validating the small patterns of µ-MTV in gases first before deploying it to bubbles. We anticipate to conduct the tests during the summer.

### 2.3.3 Ultrafast Absorption Spectroscopy in water vapor

Since the proposal has been submitted we have been fortunate enough to have received an equipment grant: DURIP grant from DOD – Office of Naval Research to explore nonlinear optics based diagnostics for multiphase flows. As part of this grant, we had proposed to acquire an ultrafast laser amplifier (Coherent Astrella, Figure 2.7). We have therefore decided to use portion of funds allocated to acquire a small fs laser for the current project with the DOD funds and customize the laser to have a more capable system. The customization took several months of back and forth with the engineering team at Coherent. In the end the seeder of the laser has been customized to a larger power system, which can be used independently of the amplifier. Furthermore, the amplifier has been built with synchronization actuators to enable to synchronize it the future, which might be required for the tests proposed here. In the end, we have a significantly more powerful and capable system. The laser amplifier is expected to ship on 05/31/2019. Once we are trained by Coherent’s engineers we will start development of the technique with many of the data processing code already pre-existing thanks to an effort on Tunable Diode Laser Absorption Spectroscopy in the lab.

|  |
| --- |
| https://proxy.duckduckgo.com/iu/?u=https%3A%2F%2Ftse2.mm.bing.net%2Fth%3Fid%3DOIP.DkWZerUNu1ZRrjxt3kB0pwAAAA%26pid%3DApi&f=1 |
| **Figure 2.7. Image of Coherent Astrella femtosecond power amplifier.** |

# Multiscale simulations

## Direct simulations of laser bubbles

It has been conducted a 3D simulation using a high-order, solution-adaptive numerical method, using the five-equation multiphase model (Beig, Rodriguez, & Johnsen) to model bubble growth and collapse in a 2.5 mm wide square channel. This is one of the proposed geometries for the laser bubble in confined channels.

Using novel approach to model bubble growth and collapse as a small volume, high-pressure bubble (nidus) using the Keller-Miksis equations (Mancia & Johnsen, in preparation):

* Determines the initial bubble (nidus) size, pressure, and temperature to match maximum bubble radius and approximate growth and collapse behavior
* These parameters are then set as initial conditions for 3D simulations

The initial conditions for the simulation are provided in Figure 3.1. The parameters are summarized in Table 1. Fluids properties are provided in Table 2.



**Figure 3.1: Initial conditions for 3D bubble growth in confined channel. Bottom and front planes are planes of symmetry.**

|  |  |
| --- | --- |
| Table 1: initial conditions for direct simulations | |
| *Rnidus* (initial radius) | 0.392 mm |
| *Rmax* (max radius) | 1.25 mm |
| *P∞* | 0.1 MPa |
| *Pnidus* | 74 MPa |
| *δ0 = H/Rmax* | 1 |
| resolution | 128 per Rmax ~ 0.05 billion points |
| Stress unit | 5.2 kPa |
| Initial temperature | 300 K |
| Time unit | 1.1 µs |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Table 2: Fluid properties | | | | | |
| Medium | *ρ* (kg/m3) | *a* (m/s) | *n* | *B* (MPa) | *b* (m3/kg) |
| Water, vapor | 0.027 | 439.6 | 1.47 | 0 | 0 |
| Water, liquid | 1051 | 1613 | 1.19 | 702.8 | 6.61×10-4 |

Figure 3.2 shows the evolution of pressure waves and temperature in the confined channel. The view is a 2D cross-section of the 3D simulation. The walls are at the top and left (for pressure, right for temperature) boundaries. In frame a) the shock wave is propagating outward from the high pressure nidus bubble. The shock wave amplitude drops as 1/r. In frame b) the shock wave is reflected from the channel walls towards the bubble and doubles in strength. Then the shock waves interact with each other further strengthening the pressure field surrounding the growing nidus bubble, frame c). The gas temperature drops as the bubble starts expanding. Finally, the reflected shock waves interact with the growing nidus bubble, constraining its growth (frame d)).

|  |
| --- |
|  |
|  |
|  |
|  |
| **Figure 3.2: time history of contours of pressure (left) and temperature (right). Dotted lines denotes *Rmax* and *Rnidus*, solid line is instantaneous bubble radius.** |

The reflection of shockwaves inhibit the bubble growth. In fact the bubble will asymptotically reach a finite diameter, figure 3.3. Bubble growth in a channel can be simulated in 1D with 1D Keller-Miksis equations. This is employed next. In this model, the long-time pressure is assumed to reach *2pnidus/(Rmax-Rnidus – 1)*. This long-term pressure takes into account the *1/r* expanding shock waves and doubling of pressure from reflections. The results of the 1D Keller-Miksis model are compared with 3D direct simulations in figure 3.3.

|  |
| --- |
|  |
| **Figure 3.4: 1D Keller-Miksis model vs 3D direct simulations.** |

Key result: Bubble growth is inhibited by the pressurized liquid in the channel relative to the bubble growth in a free-field; however, the bubble growth in a channel can be modeled using 1D Keller-Miksis equations

Next steps: Refining 3D simulation initial conditions and 1D Keller-Miksis modeling

# Conclusion and Future Works

## Work Summary and Conclusion

We have made significant progress in setting the two proposed experiments and 3D simulations. We have been working closely with the numerical team (bi-monthly phone calls + 2 face to face meeting this quarter) to advance the design of the experiments.

The main instrument has been ordered and should be delivered in the next quarter. We leveraged other funds to also advance purchasing of equipment and development of tools that will be uniquely deployed in this project providing new application domains for them.

## Future Work

In the next reporting period, we anticipate to have the air cannon operational as well as the projectile designed and being fabricated. µ-MTV will be started in the gas phase. First time resolved velocimetry measurements will also be conducted in the liquid phase, once our pulse burst laser has been upgraded (due in mid-June-mid-July). On the simulation front, we will refine the direct simulation conditions and domains to keep on informing experiment design.