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TRANSIENT FLOW DYNAMICS IN OPTICAL MICRO WELL INVOLVING GAS BUBBLES

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ABSTRACT

The Lab-On-a-Chip Application Development (LOCAD) team at NASA's Marshall Space Flight Center is utilizing Lab-On-a-Chip to support technology development specifically for Space Exploration. In this paper, we investigate the transient two-phase flow patterns in an optic well configuration with an entrapped bubble through numerical simulation. Specifically, the filling processes of a liquid inside an expanded chamber that has bubbles entrapped. Due to the back flow created by channel expansion, the entrapped bubbles tend to stay stationary at the immediate downstream of the expansion. Due to the huge difference between the gas and liquid densities, mass conservation issues associated with numerical diffusion need to be specially addressed. The results are presented in terms of the movement of the bubble through the optic well. Bubble removal strategies are developed that involve only pressure gradients across the optic well. Results show that for the bubble to be moved through the well, pressure pulsations must be utilized in order to create pressure gradients across the bubble itself.

INTRODUCTION

The Lab-On-a-Chip Application Development (LOCAD) team at NASA's Marshall Space Flight Center is utilizing Lab-On-a-Chip to support technology development specifically for Space Exploration. Controlling bubble movement in microfluidic channels has been an active topic in micro total analysis system (micro-TAS) [1,2]. Bubble formation in microdevices can come from various sources. Inside the microgravity realm, bubbles are detrimental to the operation of microfluidics chips due to their unpredictable behavior. In our design of the pressure-driven MAPOC chip for space exploration [3], bubbles may be formed due to the electrolysis of aqueous solution at the upstream electro-lysis operation [4]. Initial filling processes may also entrap gas bubbles [5]. As long as they do not serve specific purposes, such as a virtual valve for flow control and/or blockage purpose, bubbles should be avoided or removed. Bubble removal can be achieved by modifying interfacial tension through surfactants, thermal effect or electric field [6]. Other removal methods using traps and passive venting [7, 8], or active methods such as membranes [9] are available. These methods, however, require modification of existing operating conditions or channel geometries. Detailed description of a moving bubble in a fluid conduit is a very complicated problem as it involves interaction of the free surface (gas-liquid interface) with driving forces such as pressure, viscous and buoyancy forces. For microfluidic systems, scaling law indicated that both the Bond number ($Bo = \frac{\rho g l^2}{\sigma}$) and Capillary number ($Ca = \frac{\mu U}{\sigma}$) are very small. Thus, the surface tension related phenomena dominate the dynamics of bubble movement, when compared with other forces such as viscous and gravity. As the surface tension effects are directly related to the geometry of the fluidic channels, bubble movement (or lack of movement) would affect the functionality of Lab-On-a-Chip operation since microfluidic networks composed of various shapes and sizes of channels and wells. Of specific concern is the situation of entrapment and removal of bubbles in the optical well within the MAPOC chip. In this paper, we investigate numerically the transient two-phase flow patterns in an optic well configuration with an entrapped bubble. The purpose is to study the possibility of using the existing pumping mechanism for bubble removal.

NUMERICAL MODELING APPROACH

Due to the difficulty of obtaining close-form analytical solutions in multi-dimensional flows, utilizing CFD (computational fluid dynamics) enables systematic investigations of operating parameters involved. Over the last decade, several numerical techniques have been developed for complex multiphase problems [see ref. 10]. Among the available methods, the PLIC-VOF (piecewise linear interface construction-volume of fluid) method has been shown to be capable of the capture gas-liquid interfacial phenomena with the enhancement of Continuous Surface Force (CSF) modeling for surface tension treatment. This method, incorporated in the CFD-ACE+ code [11], is utilized in this study. The micro-well configuration is shown in Figure 1. To obtain increased optical path, thus a better signal detection, a double 45 degree-expansion configuration with total length of 800 micro-meters is utilized. Of specific interest in study is to investigate the filling processes of a liquid inside the expanded chamber that has bubbles entrapped. Detailed implementation of the CFD can be found in ref. 12.

RESULTS AND DISCUSSION

We first investigate the bubble movement at the entrance region of the micro-well. Several inlet bubble/liquid boundary conditions were investigated. Shown in figure 2.a is the case starting a single bubble placed at the center of the channel at the inlet plane. In figure 2.b, the inlet involves one half bubble attached to the wall. Under the initial pressure drop of 5 psi across the well, for both cases, the bubble migrates to the center of the channel and enters the second expansion. Due to the micro back flow created by channel expansion, the entrapped bubbles tend to stay stationary at the immediate downstream of the expansion. The x-direction velocity component distributions are also shown in Figures 2.a and 2.b. Several pressure drops across the micro-well were applied and the bubble was found to be trapped at the expansion juncture. At this stationary position, depending on the pressure drop across the well, the geometry of the bubble also changes. However, further increases of pressure drops fail to move the bubble towards the exit plane.

Numerical simulations are performed for the movement of a bubble inside the microchannel and the optic well. Due to the huge difference between the gas and liquid densities, mass conservation issues associated with numerical diffusion need to be specially addressed. These issues can be resolved by utilizing the Mass Conservation VOF Flux Correction within CFD-ACE+. This numerical treatment provides higher order accuracy in terms of mass flux calculations. The VOF is a volume tracking code, therefore the volume is always conserved and the normalized mass imbalance must meet the specified tolerance on residuals of 10^{-4}. The implementation of the mass conservation correction, the mass must be conserved for each time step, eliminating the mass conservation issues.

The results are presented in terms of the movement of the bubble through the optic well. Bubble removal strategies are developed that involve only pressure gradients across the optic well. Many techniques can be utilized for bubble removal, but in this paper the use of pressure oscillation is of primary interest. This allows for bubble removal strategies without further modifications of the existing design. It is shown that once the bubble becomes lodged at the expansion juncture that a simple increase in the pressurized driving force is unsuccessful at removal. The introduction of pulses in the pressure proves to be the key at successfully removing the bubble from the well.

The first study shown is for the pulses to be set by a cosine wave with a magnitude of 43.1 kPa (6.25 psi) at a frequency of 1000 Hz. This is essentially an mild acoustic wave [13]. The results for this case are shown in Figure 3. In Figure 3, the bubble's position in the well is shown as well as the position of the pressure profile. It can be seen as the pressure decreases to approximately 27.6 kPa (4 psi) that the bubble will once again be lodged in the well. As the pressure increases on the next pulse to a value of approximately 37.9 kPa (5.5 psi), the bubble once again can be forced to exit the well. Any pressure magnitude below 6.25 at 1000 Hz proved to be futile at removing the bubble. At lower pressure magnitudes, the pulse is insufficient at dislodging the bubble once it has stopped. As shown the bubble is easily removed within approximately two pulses. The pulsations create pressure gradients across the well as well as the bubble itself creating bubble movement.

The last study completed, shows the behavior of the bubble for 36.2 kPa (5.25 psi) at a frequency of 100 Hz. These results are shown in Figure 4. These results prove that the magnitude of the pulse is directly proportional to the frequency at which the pulses are supplied. The decrease in the frequency corresponds to a decrease in the magnitude of the pressure that must be supplied to the incoming fluid. Once again, any magnitude below 36.2 kPa (5.25 psi) is unsuccessful at bubble removal.

A preliminary study at a frequency of 10 Hz has shown interesting results. At the lower frequency, rotational velocities develop within the bubble itself, resulting in the breakup and discharge of the bubble from the well.

An experimental study of the bubble movement in the micro optical well is currently underway. Comparisons of the current numerical results with the test data will be reported in the near future.

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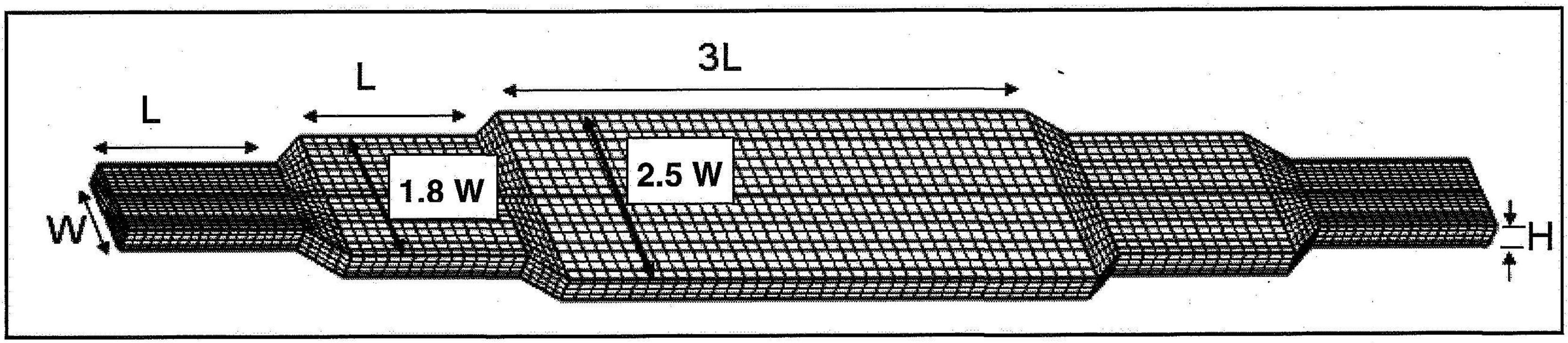

Figure 1 – Layout of Optic Well Showing Computational Grid and Well Dimensions

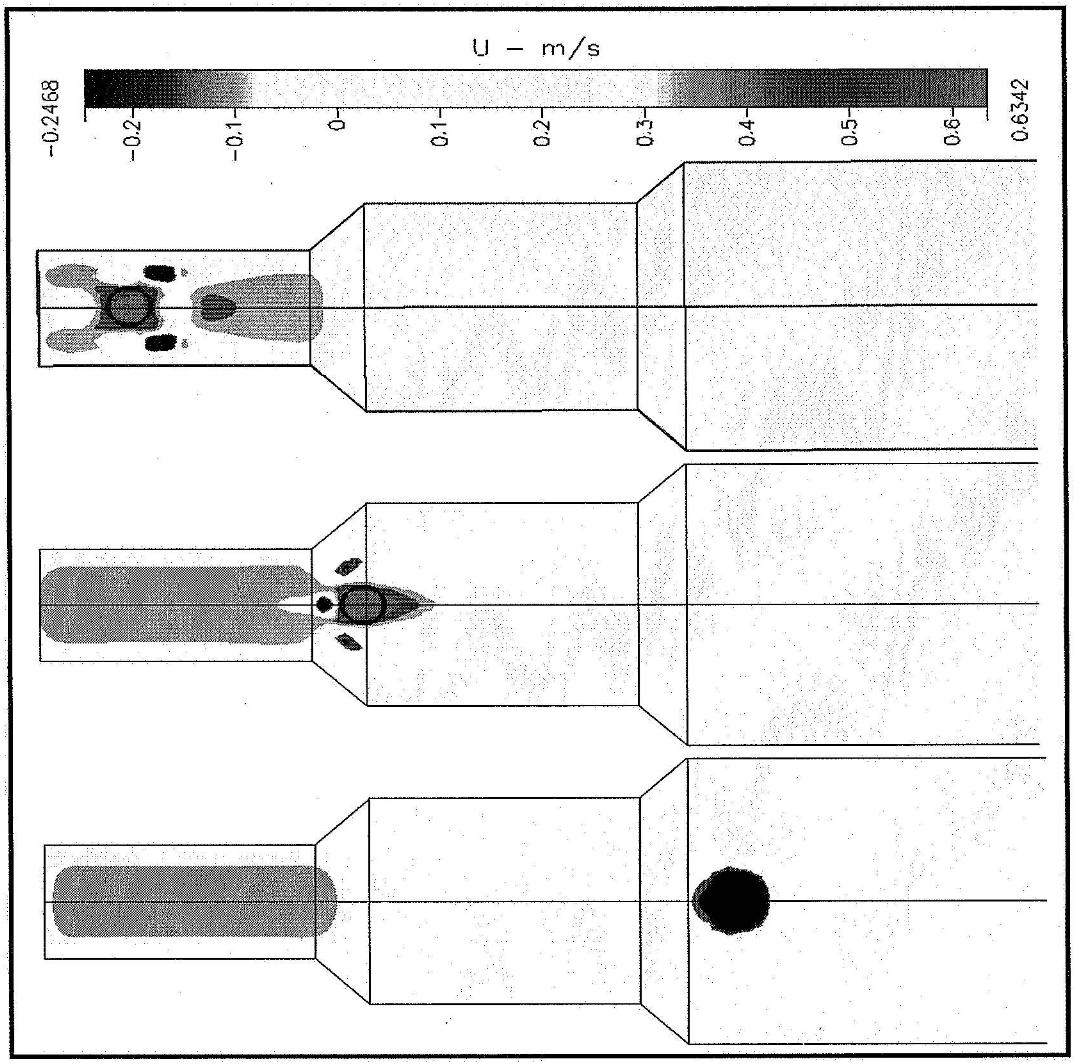

Figure 2.a – Fluid Velocity and Bubble Position for a Single Bubble

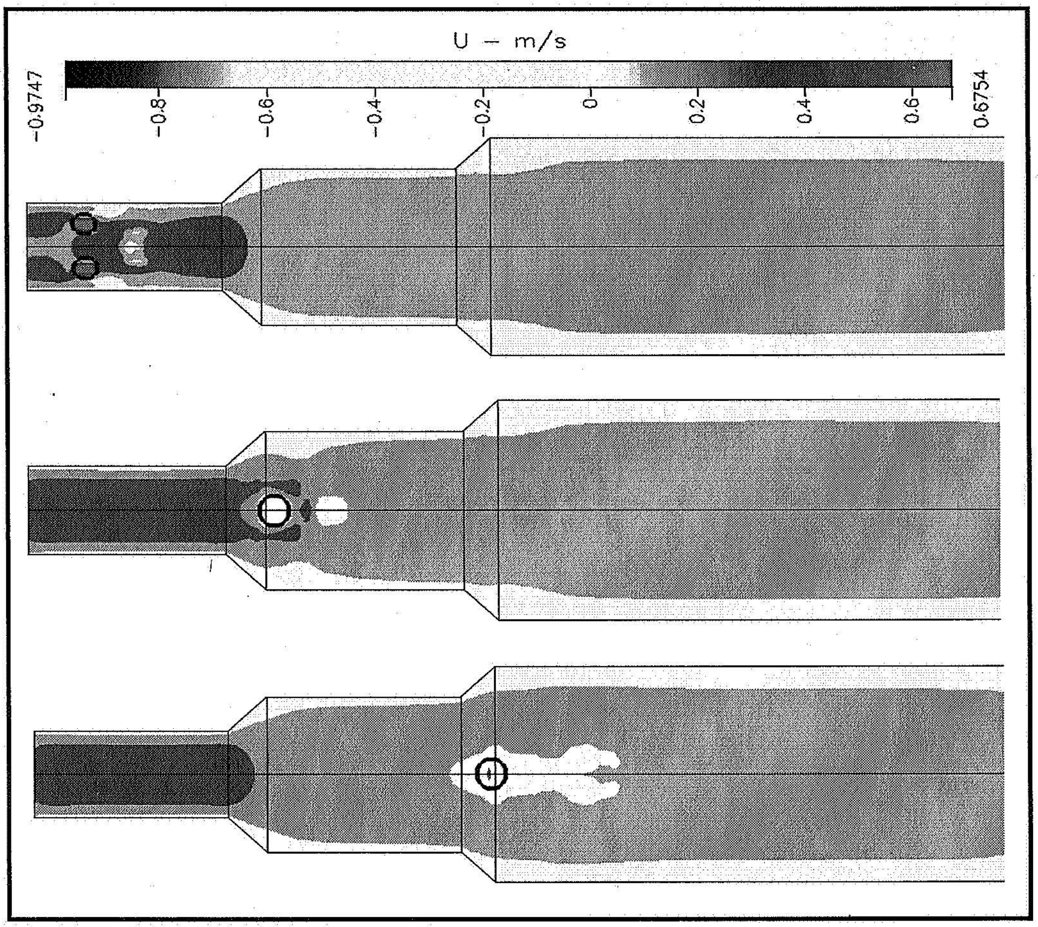

Figure 2.b – Fluid Velocity and Bubble Position for Half Bubbles

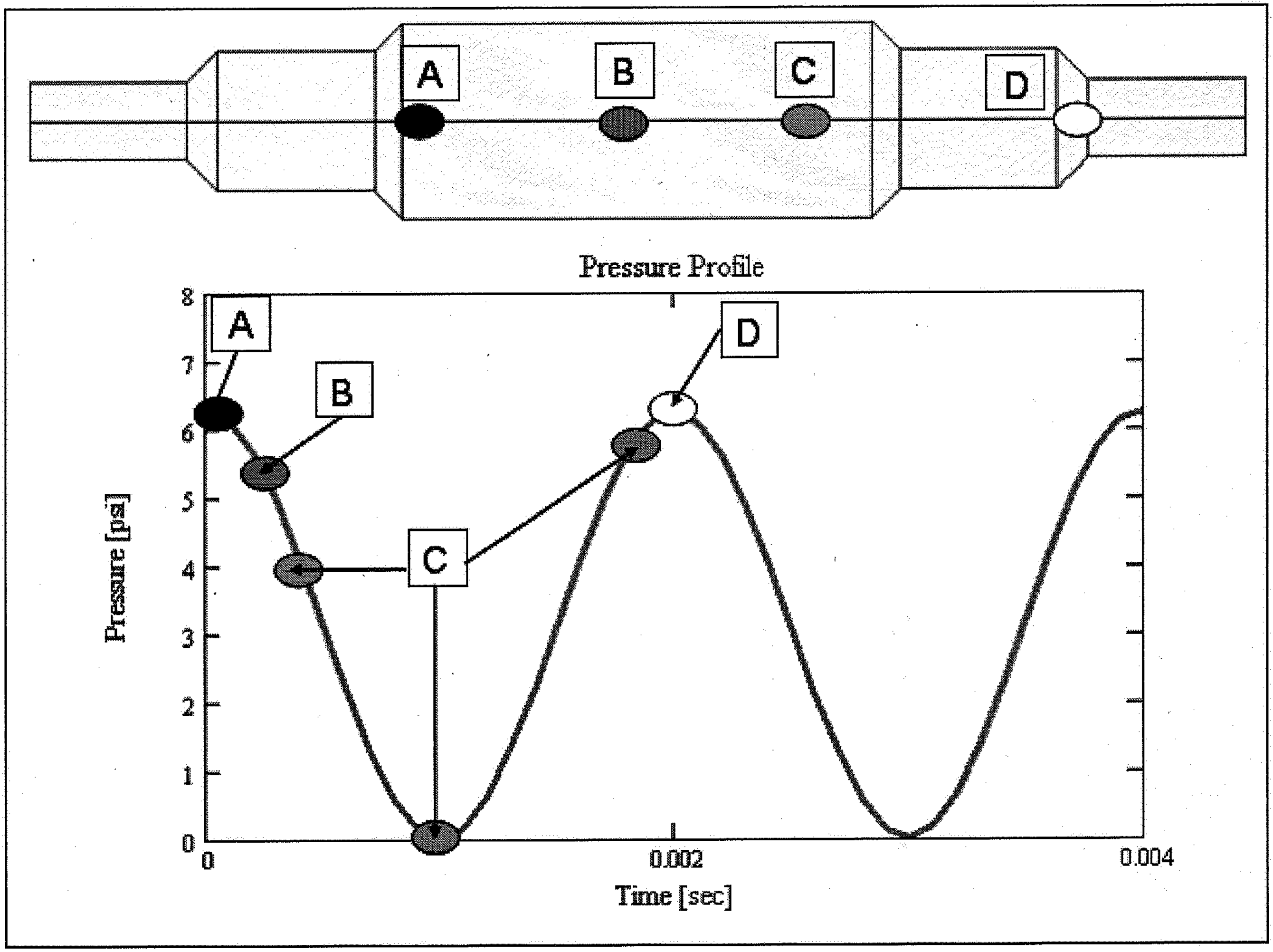

Figure 3 - Progress of the Bubble with Respect to the Pressure Profile for 6.25 psi @ 1000 Hz

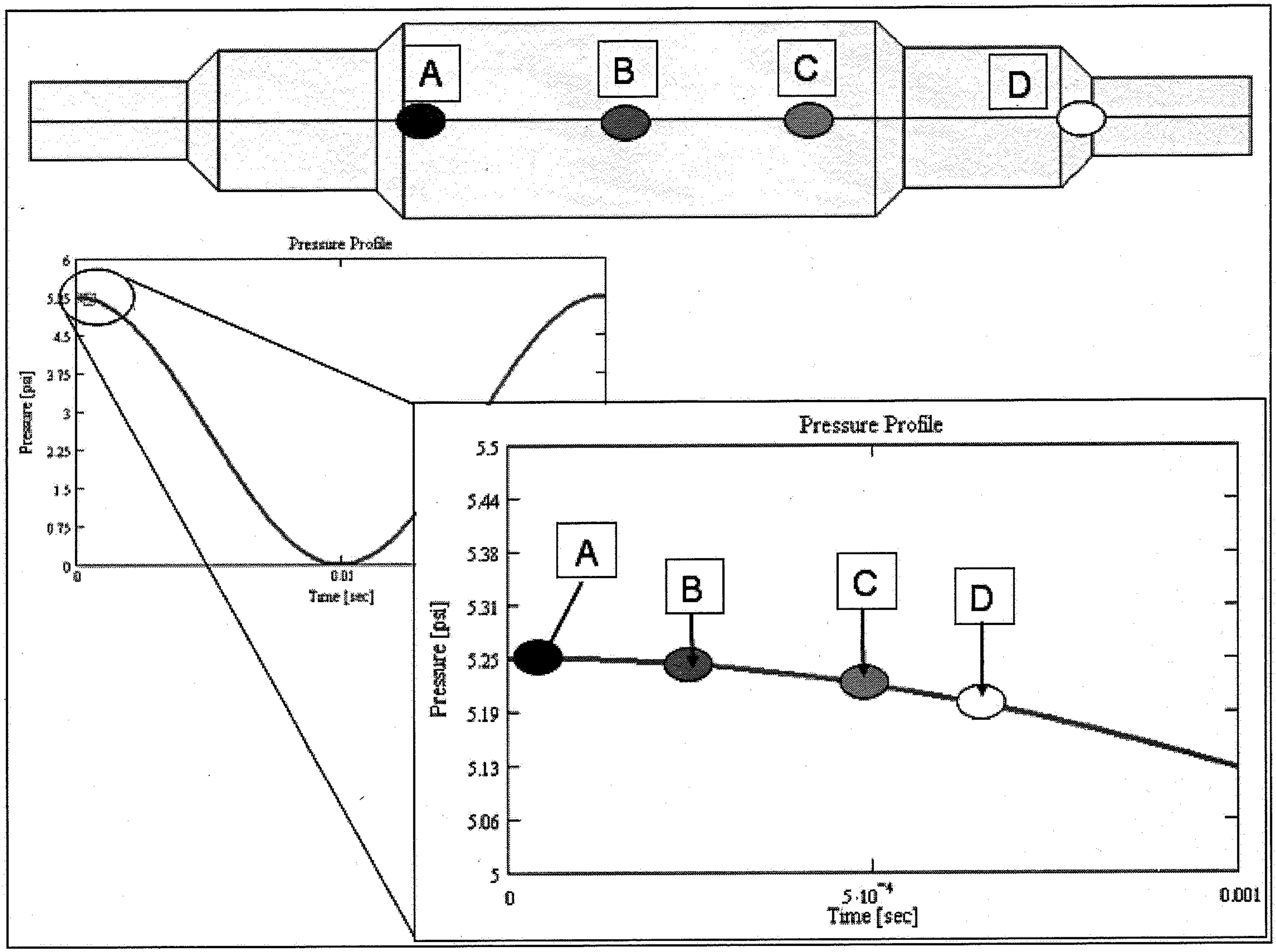

Figure 4 – Progress of Bubble with Respect to Pressure Profile for 5.25 psi @ 100 Hz