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Experimental and Numerical Investigation of Shock Wave Propagation
Through Complex Geometry, Gas Continuous, Two-Phase Media

by

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Abstract

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The work presented here investigates the phenomenon of shock wave propagation in gas continuous, two-phase media. The motivation for this work stems from the need to understand blast venting consequences in the HYLIFE inertial confinement fusion (ICF) reactor. The HYLIFE concept utilizes lasers or heavy ion beams to rapidly heat and compress D-T targets injected into the center of a reactor chamber. A segmented blanket of falling molten lithium or Li_2BeF_4 (Flibe) jets encircles the reactor's central cavity, shielding the reactor structure from radiation damage, absorbing the fusion energy, and breeding more tritium fuel.

Xrays from the fusion microexplosion will ablate a thin layer of blanket material from the surfaces which face toward the fusion site. This generates a highly energetic vapor, which mostly coalesces in the central cavity. The blast expansion from the central cavity generates a shock which propagates through the segmented blanket - a complex geometry, gas-continuous two-phase medium. The impulse that the blast gives to the liquid as it vents past, the gas shock on the chamber wall, and ultimately the liquid impact on the wall are all important quantities to the HYLIFE structural designers.

The work here presents a numerical method called the Transient Shockwave Upwind Numerical Analysis Method for ICF (TSUNAMI). It is a tool for analyzing two-dimensional blast venting in the HYLIFE reactor. TSUNAMI relies on the assumptions of

adiabatic and ideal gas behavior by the vapor and immobile liquid to simplify the problem of two-phase shock propagation to a problem of single phase gas dynamics in a fixed, complex geometry.

To validate the accuracy of the numerical method, experimental data for comparison was obtained from the Liquid Jet Array Shock Tube (LJAST). The experiment provided transient pressure data for gas shocks impacting an array of solid cylinders and an array of liquid jets with similar geometry to the HYLIFE blanket. The comparisons showed that the numerical method accurately predicts shock propagation through a cylindrical array. Furthermore, the experiment provided liquid impact data indicating that liquid jets striking the wall impart only Bernoulli stagnation pressures and not waterhammer pressures.

The application of TSUNAMI to the HYLIFE reactor calculations revealed that venting is very dependent on the blanket geometry. Calculations were performed using two types of blanket geometries, one with a hexagonally pack array of cylindrical jets and the other with a slab array. Both geometries resulted in asymmetric wall loading by the blast, but the slab jets received much less impulse than the liquid jets due to less form drag.

The work here also investigated the effect of condensation on shock reflection. A method of integrating the kinetic theory of condensation with transient gas dynamics is presented. The method was applied to the HYLIFE reactor with slab geometry which revealed a negligible effect of condensation due to the lack of condensing surface area.

Dedication

*To My Sister, Doming
Your Love, Hope and Dreams - That These May Always Live On*

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Nomenclature

A	cross-sectional area
C	Lagrangian sound speed = ρc
c	sound speed
c_p	constant pressure specific heat
c_v	constant volume specific heat
D	net form drag
E	total energy
e	internal energy
F	flux tensor of mass, momentum and energy
G	mass flux
h	enthalpy
h_{fg}	heat of vaporization
I	impulse given to the liquid by the gas
I	photon energy fluence
I_0	photon energy fluence at the liquid surface
i	photon energy density in the liquid
k	thermal conductivity
k_b	Boltzmann's constant
L	the Law-Wendrof operator
M	Mach number
m	mass of molecule
N	total number of molecules in a Maxwellian distribution
n_0	average particle density in a distribution
p	pressure
q	a scalar gas dynamics quantity, usually ρ , u , v or p
q''	heat flux
R	molecular weight based gas constant
R_0	universal gas constant
Re	Reynolds number
r	shock retardation coefficient
S	an arbitrary combination of linear operators
s	entropy, ratio of average bulk flow velocity to most probably molecular speed, shock speed
T	temperature

t	time
U	vector of conserved quantities, density, momentum, and total energy
u	x-direction velocity
V	vector of non-conserved quantities (i.e. primitive variables) - (ρ, u, v, p)
V	volume
v	specific volume, velocity, y-direction velocity
w	mass flux behind a shock
x	linear horizontal position
y	linear vertical position
Z	slope $ dp/du $

Symbols

α	thermal diffusivity
α	void fraction
β	2nd-order Godunov extrapolation terms
δ	penetration depth of the x-rays
Δ	the difference
ϕ	particle flux across an interface
Γ	Shrage correction factor for mass motion into interface
γ	ratio of specific heats c_p/c_v
λ	eigenvalue representing the slope dx/dt of a characteristic, also a wave speed
μ	dynamic viscosity
ρ	density
Σ	macroscopic photon attenuation cross-section (units of inverse length)
τ	specific volume

Superscripts and Subscripts

$\sim$	interpolated or intermediate value
$\cdot$	relative to a frame of reference moving with the shock
$*$	pertaining to the interior state inside the Riemann centered wave solution, the solution along the $x/t = 0$ characteristic
$+$	right traveling $u+c$ wave
$-$	left traveling $u-c$ wave
0	stagnation state, boundary value, value at an interface, density u-wave
1	in the undisturbed test gas
2	between the contact surface and shock

3	upstream of the contact surface
4	the undisturbed driver gas
<i>A,B,C,etc</i>	pertaining to transducer A,B,C, etc.
<i>cond</i>	condensation
<i>evap</i>	evaporation
<i>g</i>	gas or vapor
<i>high</i>	upper bounding value in a Newton-Raphson iteration
<i>i + 1/2</i>	at the cell edge
<i>i</i>	integer index of x-direction cell on a finite difference grid
<i>j</i>	integer index of y-direction cell on a finite difference grid
<i>k</i>	net amount based on kinetic theory
<i>L</i>	left state
<i>l</i>	liquid
<i>low</i>	lower bounding value in a Newton-Raphson iteration
<i>ls</i>	liquid side of the interface
<i>max</i>	maximum
<i>min</i>	minimum
<i>N</i>	pertaining to a particle distribution
<i>n</i>	integer index of the discrete time
<i>n+1/2</i>	at the half time step
<i>norm</i>	the normal component into a surface
<i>R</i>	right state, reflected state
<i>ref</i>	reference state
<i>s</i>	taken at constant entropy
<i>sat</i>	saturated condition
<i>surf</i>	surface
<i>tan</i>	the tangential component
<i>v</i>	vapor
<i>vs</i>	vapor side of the interface
<i>W</i>	wall value
<i>x</i>	pertaining to the x-direction, derivative with respect to x
<i>y</i>	pertaining to the y-direction, derivative with respect to y
∞	infinitely deep into the liquid

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1. INTRODUCTION

1.1 Background and Motivation

Research into Fusion Energy holds the great promise of developing an abundant, economical, reliable and ecologically sound energy source for the future. One often compares fusion research to the process of trying to simulate in small scale, the thermonuclear processes in our own sun. However, unlike our sun and most other stars which fuse four hydrogen atoms to produce helium, the reaction which is likely to be used in commercial applications is that of deuterium (D or ^2H) and tritium (T or ^3H), heavy isotopes of hydrogen.

Deuterium can be found abundantly in sea water while tritium can be produced from the absorption of a neutron by lithium.

Einstein's Law, $E = mc^2$, applies equally to fission and fusion. However, DT fusion, producing 17.6 MeV from 5 atomic mass units (amu) yields about 3.5 MeV/amu versus fission which produces about 200 MeV from about 236 amu, about 0.85 MeV/amu. Hence, fusion has a higher efficiency in converting mass into energy than fission. A similar comparison can be made for chemical fuels which release energy many orders of magnitude smaller than fission.

For fusion to occur, the positively-charged deuterium and tritium nuclei must be given sufficient energy to overcome their Coulomb repulsion. This requires heating the fuel to very high temperatures where it becomes a completely ionized plasma, and then confining it long enough for collisions to take place. Achieving this goal has typically taken two paths, one of Magnetic Confinement Fusion (MCF) and one of Inertial Confinement Fusion (ICF). In the MCF concept, fusion energy production is relatively

constant as strong magnetic fields confine the hot plasma and provide a continuous thermal barrier between the reactor vessel wall and the edge of the plasma. The key technological issues which must be overcome in MCF are magnetic field stability and strength, radiation control and heat extraction for commercial use.

The ICF concept makes use of a series of thermonuclear microexplosions. Laser or ion beam irradiation of small pellets or targets ablates an outer layer and by shock compression, drive the core D-T reactants to 1000 times normal density and temperatures of 10^6 K, where thermonuclear ignition occurs. For several nanoseconds, the fuel confines itself due to its own inertia, hence the term inertial confinement. For ICF to work, research must demonstrate commercially usable driver beams and targets, and long term vessel survivability under the stress of repetitive microexplosions.

Radiation exposure on structural components in fusion systems is a major concern, especially in ICF. The DT fusion reaction releases 17.6 MeV of energy which appears as a 14.1 MeV neutron and 3.5 MeV alpha particle. In ICF, the fusion neutrons travel away from the micro-explosion and can cause neutron embrittlement if they are allowed to deposit in the reactor structure. The alpha particles have only very short deposition lengths and do not travel beyond the micro-explosion's fireball. However, the alpha particles, along with a small fraction of the neutrons, interact quickly with debris in the fusion micro-explosion and convert some of their energy into x-rays and transfer some to target debris kinetic energy. Because ICF is a pulsed concept, this will produce intense pulses of x-rays which are expected to ablate any nearby exposed surfaces. Roughly two-thirds (68%) of the total fusion yield is expected to be emitted from the fireball as neutron energy, one-sixth (16%) as x-rays, and one-sixth (16%) as debris kinetic energy.

The High-Yield Lithium-Injection Fusion Energy (HYLIFE) reactor [Blink et. al., 1985; Moir et. al. 1992] is one ICF concept which mitigates the radiation exposure problem and provides a possible method of extracting heat from the fusion for commercial power production. Research for this design is a joint effort sponsored by the U.S. Department of

Energy through the Lawrence Livermore National Laboratory. The concept employs lasers (HYLIFE-I) or heavy ion beams (HYLIFE-II) to repetitively heat DT fuel pellets injected into the center of a reactor vessel. The center of the vessel is surrounded by a continuously falling annular blanket of molten metal or molten salt, which forms a central cavity where the fusion takes place. The first design concept, HYLIFE-I [Blink, et al. 1985], utilized liquid lithium for the blanket material, incorporated laser drivers, used 1800 MJ yield targets and had a 1.5 Hz repetition rate (figure 1.1). HYLIFE-II [Moir et al., 1991] proposes to use a lithium fluoride and beryllium difluoride (Li_2BeF_4 - "Flibe") molten salt, 350 MJ yield targets, a heavy ion beam driver and a 6 to 8 Hz repetition rate. Lithium is an essential component in the blanket because it must be used to capture fusion neutrons to breed tritium fuel, which has only a 12.26 year half-life and is not available in significant quantity on earth. HYLIFE-II uses Flibe rather than pure lithium to eliminate the lithium fire hazard. (See Fig. 1.2). In this case, breeding is aided by the (n,2n) reactions on beryllium, a component in Flibe.

The geometry of the blanket in HYLIFE incorporates a segmented, discrete jet array which superimposes 0.5 m of molten salt along all lines-of-sight out for neutrons and x-rays, except at the beam ports, which will incorporate other shielding techniques because the beams require direct line-of-sight to the target. The blanket is segmented to allow the blast, which is comprised of x-ray ablated blanket material and debris, to vent quickly through the blanket. The presence of this protective blanket, although beneficial in terms of radiation damage to structural components and tritium fuel production, is expected to generate a new set of hydrodynamic phenomena, each of which requires a detailed understanding in order to verify the soundness of the concept.

A brief chronology of events following a shot is given in Table 1.1. The sequence of phenomena in HYLIFE can be separated into three time categories: early, intermediate, and late. At early times, the first nanoseconds to 50 to 100 microseconds after fusion, x-rays are deposited in a thin layer of the exposed liquid surfaces and the neutrons deposited

deeper and more uniformly in the blanket and debris expanding outward toward the blanket. (See also figure 1.3). During this period, the energy deposition by the x-rays and neutrons is expected to initiate the phenomena of x-ray ablation and neutron isochoric heating [Chen 1992].

The spectrum of x-rays emitted in ICF is approximately that of a black body at 350 eV. For this spectrum, the liquid lithium will absorb the majority of the x-ray energy in just tens of microns, and Flibe in just several microns. [Orth 1989, Chen 1992]. Because the deposition of most of the x-ray energy mostly occurs in such a small volume, the energy per unit mass is sufficient to vaporize, dissociate, and partially ionize the thin layer, which subsequently explodes off the blanket surface. This sends a shock into the liquid and may cause spalling off the rear of the inner jets. The ablation blow-off also imparts a small outward momentum to the inner jets. Furthermore, because the geometry of the blanket is roughly annular, the inner exposed surfaces will re-direct most of the ablated mass back into the central cavity where it will collide with the oncoming target debris. The imploded ablation material and debris will stagnate and mix in the central cavity, a process known as thermalization. The ablated material which is not directed into the central cavity expands into the voids in the blanket. The combined vapor mass in the central cavity radiates at sufficient intensity to evaporate even more vapor off the inner jet surfaces. The combined vapor mass, or blast material, then explodes outward and must vent through the blanket. The central-cavity processes are analyzed by Chen et al. [1992b].

Also occurring as an early time phenomenon is isochoric heating of the blanket (i.e. heating at constant volume) by neutrons. The neutrons deposit their energy more uniformly in the blanket. Although traveling at a lower velocity than the x rays, they still deposit their energy in a time too short for the blanket to relax volumetrically. Thus, the blanket suddenly possesses a pressure much greater than the pressure in the surrounding void, which is near zero. The pressure relaxation in the liquid blanket begins from the surface of each liquid jet or slab in the form of a relief or rarefaction wave propagating in

toward the center of the jet. As the rarefaction wave moves inward, the liquid it passes through accelerates in the outward direction. Chen [1992] showed that for cylindrical jets, this creates tension in the liquid due to the divergent geometry, and if the neutron deposition imparts sufficient energy density to the blanket, the tension may be great enough to cause the disassembly of the blanket in the form of annuli expanding away from each cylindrical jet core. For slabs there is no tension until the two plane waves meet on the midplane. Within the first several microseconds, the disassembly is underway, and may completely close off the flow channels in several hundred microseconds. However, most of the ablated material which makes up the blast is expected to reach the inner jets at around 50 microseconds [Chen et al. 1992b] and pass from the inner cavity beyond the first row of jets before they completely close off.

Disassembly is not a uniform process because the liquid which is closer to (i.e. has a shorter stand-off distance away from) the fusion micro-explosion encounters a higher intensity of neutrons than liquid situated farther away. The other jets will disassemble with lower velocities and the jets or slabs farther away from the center may not even absorb enough neutron energy to fracture. The gradient in absorbed neutron energy density therefore causes the inner liquid to disassemble more violently than the outer liquid. Momentum is conserved so there is negligible momentum contribution by the neutrons. However, a small mass of liquid is accelerated at high velocity toward the center of the cavity resulting in a net outward momentum contribution to the remaining liquid.

At intermediate times, 50 microseconds to 1 millisecond, the majority of the ablated material reaches the inner surface of the jets and then vents through. The rebounding ablated vapor forms blast wave which moves into a lower pressure (probably sub-atmospheric pressure or vacuum but possibly or likely a higher pressure than at shot time) vapor emanating from the liquid at lower energy. The less energetic vapor will tend to expand in all directions including into the vent channels. The approaching blast therefore encounters an atmosphere between the jets which consists of the smaller fraction of ablated

material which did not get directed into the central cavity. Because of the main inner cavity blast material possesses a large portion of the ablation energy, its venting is expected to occur at an outward velocity which exceeds the sound speed of the atmosphere ahead of it. The atmosphere ahead of the blast will therefore undergo compression by the supersonic blast and a compressive wave, that is, a shock wave will propagate ahead of the blast into the atmosphere. Within one millisecond, the primary blast front impacts the first structural wall (FSW) and delivers an impulse to the wall. In addition, form and viscous drag by the blast flowing around the cylinders or slabs contributes more outward momentum to the liquid.

Condensation momentum flux also contributes to the liquid radial momentum away from the microexplosion site. Mass transfers occur simultaneously with all other processes, from early to late times. At early times, x-ray ablation, followed by re-radiation from the imploded ablated layer, cause net evaporation of material from the inner exposed surfaces. At intermediate times, as the blast vents between the channels in the blanket, the very hot vapor will encounter much colder liquid surfaces and undergo a rapid energy exchange with the liquid. At first, the stagnation of the vapor against the cold surfaces generates high temperatures and pressures in the vapor which drives net condensation into the liquid. But as the venting progresses and the pressure drops in the wake of the blast, evaporation may occur off of surfaces which have been heated by the prior condensation. Later, at times greater than 1 millisecond, most of the vapor has passed beyond the blanket and occupies the void between the blanket and FSW. The chamber vapor must be condensed prior to the next fusion cycle (667 ms in HYLIFE-I or 125 ms in HYLIFE-II) to bring the particle density to below 10^{22} for HYLIFE-I or 3×10^{19} per m^3 for HYLIFE-II [Blink et al. 1985, Moir 1991]. In the HYLIFE-II concept, a proposed droplet spray performs this condensation function by providing an adequate amount of cold liquid surfaces for the vapor to condense on.

1.2 Objectives

The objectives of the research presented in the following chapters are to investigate the gas dynamics phenomenon of shock wave propagation through a gas continuous, two-phase medium as it applies to the blanket geometry in HYLIFE, and then to apply the knowledge to obtain estimates of the final wall loads in the reactor. Specifically, the work focuses on how the shock speed and pressure ratio change upon traversing the jet array, what impact this has on the shock loading on the FSW, and what impact it has on the momentum exchange with the blanket. The work takes two approaches, experimental and numerical. The objective of the experiment is to simulate in small scale shock wave propagation in a jet geometry similar to that in the HYLIFE reactor, while the objective of the numerical work is to develop a computational method which can then be verified by comparison with the experimental data. The numerical work which follows is limited only to gas dynamics effects and assumes ideal gas behavior. This simplification provides only a qualitative assessment of the real situation in ICF, because, as outlined above, the actual fusion process is followed by many other simultaneously occurring phenomena such as radiation heat transfer, real gas effects, isochoric heating, condensation, and liquid jet disassembly, all of which will have some affect on the blast venting. However, the consideration of only ideal gas dynamics with neglect of energy transfer mechanisms like radiation and condensation provides a conservative estimate of the FSW pressure loading, because the adiabatic ideal gas assumption maximizes the energy available in the gas to do $p dv$ work. Lastly, the combined simultaneous occurrence of all the phenomena outlined above requires actual ignition of a large yield fusion pellet, which is still beyond the state-of-the-art.

The specific goals of the experiment are to provide pressure trace data of shocks propagating through arrays of discrete solid and liquid jets which are similar in geometry proposed in the HYLIFE reactor. In addition, another goal is to provide wall loading data due to the impacts first by the attenuated shock followed by (in tests using liquid jets) the

accelerated liquid. The use of both solid and liquid cylinders permits the comparison between shocks propagating in a rigid geometry versus a deformable geometry. The experiment uses room-temperature (295K) non-condensable air and helium as the gaseous medium and therefore prohibits the possibility of mass transfer through condensation or evaporation.

The numerical investigation portion of the research applies the theories of gas dynamics to develop a finite difference method for tracking shock waves in complex but fixed two-dimensional geometries. We chose to implement a finite difference method known as the Godunov method [Godunov et al., 1961] in combination with an ideal gas Riemann [1860] solver [Colella and Glaz, 1985]. One particular task in the development of the numerical method is the generation of boundary conditions which accurately model the complex geometry found in the HYLIFE reactor blanket, which may consist of plane as well as curved surfaces. After development of the numerical method, the next goal is to reproduce the experimental results obtained in the experiment, and then second, to apply the method to provide an estimate of blast venting consequences for various proposed blanket geometries in the HYLIFE reactor design. It is intended that this research will lay the groundwork for a method, which will later incorporate models for the simultaneous interaction of the other phenomena in ICF reactors. In this regard, Chen's work [1992b] has already introduced radiant energy transport and real gas effects for the central cavity gas dynamics. In addition, here, the last chapter of this thesis develops a method for assessing condensation in shock wave gas dynamics. Both Chen's work and the work on condensation are limited to simple geometries. Chen [1992] has performed simple geometry 2-D (r,z) calculation for real gases, however, currently available computing speed and cost have limited the complex two-dimensional calculations to ideal gases only.

1.3 Previous Work

One can argue that the concept of ICF has existed as long as thermonuclear devices

have been around, but the actual engineering and design of pulsed ICF reactors has only gained attention in the late 1970's and '80's [Dolan 1982]. Much of this progress in ICF reactor design stems from the progress in laser or heavy-ion beam technology which can be eventually used to drive the fusion. As such, little research exists in the literature on the investigation of shock wave propagation in gas-continuous, two-phase media for the coarsely separated flow geometry of an ICF reactor blanket. Most of the previous work done in predicting blast venting consequences in ICF comes from the HYLIFE-I study.

Glenn [1980] was the first to actually model the lithium vapor blast venting in the HYLIFE-I reactor (see figure 1.4). His model predicted the divergent and impulsive cross flow of lithium vapor over a packed columnar array of cylinders. His analysis considered gas dynamics in a one-dimensional diverging channel in the radial direction of varying cross section with steady-state drag coefficients for supersonic flow. His work was also extended to include two-dimensional, radial-axial (r-z) calculations. In addition, he also included simple diffusive radiation transport and gas/liquid heat transfer models. Glenn's work provided extensive, and at the time, the best available parametric predictions on wall loading and liquid impulse for 200 to 4000 MJ yield targets at 1 to 20 Hz repetition rates. His work produced comparisons of gas-to-liquid impulse and wall loading for varying cases of adiabatic vapor and non-adiabatic vapor. He also showed that drag due to viscous skin friction was negligible compared to form or profile drag. However, Glenn recognized deficiencies in using drag coefficients based on steady state Reynolds as well as Mach numbers and also modeling of the blanket flow passages as one-dimensional in the radial direction. His model was incapable of predicting important multi-dimensional effects such as shock reflection, oblique shocks, and the phenomenon of supersonic flow separation. Glenn's predictions lacked experimental verification and as such he concluded that any further analyses should also be accompanied by experimental verification.

Table 1.1 Chronology of Physics Events in HYLIFE-II [Moir 1991]

Time Realm	Physics event Description
-60×10^{-3} s	Fuel pellet enters 3-m radius chamber at 50 m/s
-15×10^{-9} s	Driver beams begin contacting the target.
0×10^{-12} s	Fusion burn begins.
10×10^{-12} s	Fusion burn ends, having released up to 350 MJ.
2×10^{-9} s	X-rays begin vaporizing inner surfaces of inside row of jets at radius 50 cm
10×10^{-9} s	Neutrons (traveling at 5 cm/ns) begin volumetrically heating inner jets.
20×10^{-9} s	Neutron volumetric heating of all jets is complete.
11×10^{-6} s	Neutron generated isochoric heating tension in inner most row of jets causes cylindrical fracture to begin.
$20-30 \times 10^{-6}$ s	Vaporized and partially dissociated and ionized) jet material reaches chamber center, thermalizes, radiates to the first row of jets (causing a second wave of ablation)
$10-30 \times 10^{-6}$ s	Vapor expanding from center of chamber reaches vicinity of jets, re-thermalizes as it impacts the slower vapor near the jets and beings two-phase shock propagation through jet structure.
0.1×10^{-3} s	Major vapor propagation through jet fragments is well under way, imparting an outward momentum that adds to outward momentum created by the gradient in neutron isochoric heating and to the x-ray ablating momentum.
$0.1-0.2 \times 10^{-3}$ s	First vapor blast penetrates jet curtain.
0.3×10^{-3} s	Vapor impacts FSW after fragmenting the existing condensation spray jets and accelerating the small droplets toward the vessel wall. This impulse stresses the FSW.
$1-2 \times 10^{-3}$ s	Uniform vapor pressure established within chamber. Massive transient condensation is initiated.
2.5×10^{-3} s	Uninhibited condensation jet spray begins to enter chamber.
20×10^{-3} s	Jet fragments consolidate to form a thick annular two-phase region.
0.065 s	Clearing is completed along the path for the next pellet to enter the 3-m radius chamber at 50 m/s.
0.1 s	Enough vapor has condensed to permit another driver pulse.
0.125 s	New Flibe jets are established for next chamber pulse (assuming 16 m/s over 2 m). Driver beam path clearing is completed and next fusion burn begins.

1.4 Brief Review of 1-D Gas Dynamics

In the design of the experiment as well as numerical computations, we make a number of references to shock propagation in shock tubes and the generalized Riemann shock problem [Riemann 1860]. For example, to design the experiment with sufficient length and strength, one needs prior knowledge of the range of shock speeds in a gas, pressure rises across the face of shock waves and the pressures resulting from the impact of these shocks on a rigid surface. One can obtain quantitative design estimates from Riemann's analytical solution to the general shock tube problem. Riemann's solution is also the kernel for the computational scheme. It is instructive at this point to present a basic review of one-dimensional gas dynamics as it pertains to the shock tube problem.

The generalized shock tube problem begins with the premise that initially, an interface separates a long tube into two sections, a left and a right side (see figure 1.5). The gases on each side of the interface possess uniform states (i.e. density, velocity and pressure) which are different from each other. In a laboratory shock tube, both left and right velocities are usually zero, but in the general Riemann problem, the velocities need not be zero, (i.e. the gases need not be stationary). At time equal to zero, the two gases are allowed to interact. Riemann's model assumes that the gas is inviscid and ideal. An ideal gas is one whose pressure, density and temperature are related by the ideal gas law:

$$p = \rho RT \quad (1.4)$$

where p is the pressure, ρ the density, R the ideal gas constant (i.e. ratio of universal gas constant with molecular weight), and T the temperature. The enthalpy is the sum of internal energy and pressure volume product ($h \equiv e + pv$). In differential form it may be related to the temperature by:

$$dh = c_p dT \quad (1.5)$$

where c_p is the isobaric specific heat. Assuming that the specific heat is relatively constant,

the enthalpy can be rewritten as:

$$h = c_p (T - T_{ref}) \quad (1.6)$$

where T_{ref} is a reference temperature. The internal energy, e , of an ideal gas can be given by an expression similar to the enthalpy:

$$e = c_v (T - T_{ref}) \quad (1.7)$$

where c_v is the constant volume specific heat. For the ideal gas, the specific heats are related by the expression:

$$c_p - c_v = R \quad (1.8)$$

A useful constant is the ratio of specific heats γ given by:

$$\gamma = \frac{c_p}{c_v} \quad (1.9)$$

The subject of one-dimensional gas dynamics has been extensively developed for the model of ideal gas with constant specific heats (therefore constant γ). The specific heats of all real gases have significant temperature dependence even when the gases conform closely to the ideal gas law. The fact that γ is less sensitive to temperature than are c_p and c_v gives justification for the simple theory. Many closed form results are obtainable with this simplification. They are not exact, but the error is often acceptable for practical application.

Referring back to the shock tube and figure 1.5, Riemann determined that for any arbitrary combination of initial left and right states there is a unique solution which must fit one of four categories. He showed for any possible combination of initial density, velocity and pressure on either side of the interface, the solution must be one of the following types: 1.) a right-traveling compression wave (i.e. shock) and left-traveling expansion wave (i.e. rarefaction), 2.) a left-traveling shock and right-traveling rarefaction, 3.) left- and right-traveling rarefactions, or 4.) left- and right-traveling shocks. (See figure 1.6). Cases 3 and 4 occur when initially the velocities are non-zero and either away from either at the interface or toward each other. Case 3 is the problem of two rarefactions colliding and

reflecting, and case 4 is the case of two shocks colliding and reflecting.

To further clarify Riemann's statement, one can examine the classic ideal shock tube problem which is a special case of the first type. In this example, a diaphragm divides two regions initially at rest (i.e. velocity is zero in the lab frame in both gases). The left state initially has higher pressure than the right state. At time equal to zero, the diaphragm is removed and the higher pressure material expands into the lower pressure region. The expanding gas from the left compresses the material to the right and sends a right-traveling shock wave ahead. At the same time, a rarefaction wave travels to the left, setting the higher pressure gas into motion toward the right (figure 1.7). The rarefaction is not an abrupt discontinuity, but is a fan because it tends to spread for reasons which are explained in section 1.4.3. As long as the higher pressure gas continues to expand, it will continue to drive the shock into the lower pressure medium and thus the higher pressure gas is often referred to as the driver gas. The low pressure side is often referred to as the driven or test gas.

1.4.1 Isentropic and Non-isentropic Processes

Reversible adiabatic processes occur at constant entropy (independent of the EOS) and are called isentropic. For the isentropic process:

$$pv^\gamma = \frac{p}{\rho^\gamma} = \text{constant} \quad (1.10)$$

where v is the specific volume and γ is given by:

$$\gamma = -\left[\frac{\partial \ln p}{\partial \ln v}\right]_s = -\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_s = -\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_T \frac{c_p}{c_v} \quad (1.11)$$

When $pv = RT$, as in an ideal gas, the product of specific volume to pressure ratio and the derivative of term:

$$-\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_T \Big|_{\text{ideal gas}} = -\frac{v^2}{RT}\left[\frac{\partial}{\partial v}\left(\frac{RT}{v}\right)\right] = 1$$

and therefore, $\gamma = c_p/c_v$.

Shock waves are an irreversible, adiabatic compression phenomenon. Entropy increases in accordance with the conservation of mass, momentum and energy across the plane wave (discontinuity).

1.4.2 Sound Speed

The sound speed is defined as the rate at which infinitesimally small isentropic, adiabatic compression or expansion waves travel in a gas. Since these waves are small their passage does not induce any net motion in the medium they travel through. For any fluid, the sound speed is defined as [Liepmann and Roshko, 1957]:

$$c = \left(\frac{\partial p}{\partial \rho}\right)_s^{1/2} \quad (1.12)$$

where c is the sound speed and the subscript s implies that the derivative is evaluated for isentropic conditions. Substituting equation (1.10) into the sound speed and evaluating results in:

$$c = \left(\frac{\gamma p}{\rho}\right)^{1/2} \quad (1.13)$$

Combining with the ideal gas law gives:

$$c = (\gamma RT)^{1/2} \quad (1.14)$$

1.4.3 Formation of (Finite Amplitude) Shock and Rarefaction Waves

Both shocks and rarefactions can be considered the superposition of many

infinitesimally small amplitude compression waves or expansion waves. In the example shock tube, the diaphragm removal immediately initiates the propagation of these many waves, the compression waves move downstream while the expansion waves move upstream. Each wave travels at the sound speed local to its surroundings relative to the gas. Thus, for the many weak compression waves that form the shock, the lead wave will always compress and heat, however slightly, the material it traverses, thus leaving behind it a medium with a higher local sound speed. The compression waves which follow at the local sound speed, therefore travel at a higher speed than the lead wave. As a result, in a superposition of many small compression waves, any trailing waves will always overtake and merge with the lead wave. This process continues until all the compression waves merge into a single steep shock front, which for most analytical purposes may be considered a discontinuity (figure 1.8).

Rarefaction waves, for the same reason, will spread as they propagate. The leading expansion wave travels upstream at the sound speed of the material it moves into. The material which has been traversed by the lead wave is expanded slightly and cooled so the local sound speed just behind the lead wave is slower. The passage of successive expansion waves imparts an ever increasing downstream velocity to the expanded medium. Therefore each following wave travels at an ever slower sound speed and must also travel upstream against a downstream flowing gas. A rarefaction wave therefore spreads as it propagates in a gas (figure 1.9)

1.4.4 The Euler Equation of Gas Dynamics

The conservation of mass in an Eulerian frame for a one-dimensional compressible flow with no area change [Liepmann and Roshko, 1957], can be expressed by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0, \quad (1.15)$$

Similarly the conservation of energy can be written as:

$$\frac{\partial}{\partial t} \rho \left(e + \frac{u^2}{2} \right) + \frac{\partial}{\partial x} \rho u \left(e + \frac{u^2}{2} \right) + \frac{\partial}{\partial x} u p = 0. \quad (1.16)$$

where e is the internal energy. The Euler equation is the conservation of momentum for an inviscid fluid. Here, it is applied to the compressible medium:

$$\rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) + \frac{\partial p}{\partial x} = 0, \quad (1.17)$$

In both the energy and momentum equations, viscosity and heat conduction are neglected. All real gases are viscous and heat conducting, but in gas dynamics analysis, these diffusive terms can often be neglected because they are small compared to inertial or convective terms [Liepmann and Roshko 1957, pp.305-6]. Often the three equations are expressed in vector form which is convenient for numerical solution methods presented in chapter 3. Using a little algebraic manipulation yields the expression:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0. \quad (1.18)$$

where U is the matrix of conserved properties:

$$U = (\rho, \rho u, \rho E)^T. \quad (1.19)$$

and $F(U)$ is the flux tensor,

$$F(U) = (\rho u, p + \rho u^2, \rho u E + u p)^T. \quad (1.20)$$

The variable, $E = (e + u^2/2)$ is defined as the sum of internal and kinetic energies within the gas.

An important gas dynamics concept that will be mentioned repeatedly is the characteristic. Characteristics represent solution curves in the $x-t$ plane that trace the

progress of waves in the system. In the gas dynamics to be discussed here, these waves represent solutions of constant U , which satisfy equation (1.18). To determine these characteristics, equation (1.18) can be written in non-conservative form [LeVeque, 1990] as:

$$\frac{\partial V}{\partial t} + A \frac{\partial V}{\partial x} = 0. \quad (1.21)$$

where

$$V = \begin{pmatrix} \tau \\ u \\ p \end{pmatrix}, \text{ and } A = \begin{pmatrix} u & -\tau & 0 \\ 0 & u & \tau \\ 0 & \rho c^2 & u \end{pmatrix} \quad (1.22)$$

The quantity $\tau = 1/\rho$ is the specific volume. The eigenvalues for matrix A define the slope of the characteristics in x - t space and their corresponding eigenvectors define the gas dynamics quantities which are constant along the characteristics. The eigenvalues for A are $u-c$, u , and $u+c$ where c is the sound speed as defined in equation (1.12) [Leveque 1991]. These indicate that in gas dynamics, the velocity of the waves travel at either the gas velocity or at the sound speed relative to the gas velocity.

The characteristics define a path in x - t space where some functional quantities remain constant. The constant value functions are found by taking the dot product of each eigenvector corresponding to each eigenvalue with $\partial V/\partial t + \lambda_k \partial V/\partial x$ and setting equal to zero, where λ_k is the eigenvalue and the subscript k represents either the + wave ($u+c$), the - wave ($u-c$) or the 0 wave (u). Colella and Glaz [1985] give the constant value functions as:

$$dp - \frac{1}{c^2} dp = 0. \quad \lambda_k = u \quad (1.23)$$

$$\rho c du + dp = 0. \quad \lambda_k = u+c \quad (1.24)$$

$$\rho c du - dp = 0. \quad \lambda_k = u - c \quad (1.25)$$

1.4.5 Shock Waves - the Rankine-Hugoniot Equations

One can consider the problem of a long tube with a constant cross-section within which propagates a shock discontinuity (figure 1.7). The shock moves into the undisturbed medium ahead of it with some shock speed s and in doing so compresses, heats and accelerates the gas to some velocity u_p . The use of a discontinuity to represent the shock front is a good assumption as shocks fronts tend to have thicknesses of only several molecular mean free paths thick. [Zel'dovich and Razier 1966, pp. 73, 244]. The consideration of the shock as a discontinuity however excludes the application of Euler's equations in differential form. Instead, one must apply the "jump" relationships which represent conservation of mass, momentum and energy across a sudden finite jump in states.

The first step in applying the conservation relations is to perform a change of reference frames from that of a fixed observer in the laboratory frame to one moving with the shock front (figure 1.10). In the moving frame of reference, gas appears to be entering and leaving the shock front at speeds:

$$u'_1 = u_1 - s \quad (1.26)$$

$$u'_2 = u_2 - s \quad (1.27)$$

respectively. For gas initially at rest, $u_1 = 0$ and so $u'_1 = -s$, the shock speed.

Then for a constant cross section shock tube, one can write the conservation of mass, momentum and energy respectively:

$$\rho_1 u'_1 = \rho_2 u'_2 \quad (1.28)$$

$$p_1 + \rho_1 u_1'^2 = p_2 + \rho_2 u_2'^2 \quad (1.29)$$

$$h_1 + \frac{u_1'^2}{2} = h_2 + \frac{u_2'^2}{2} \quad (1.30)$$

where h_1 and h_2 are entering and exiting enthalpies of the gas, which for an ideal gas with constant specific heats can be expressed:

$$\begin{aligned} h_1 - h_2 &= c_p(T_1 - T_2) \\ &= \left(\frac{\gamma}{\gamma - 1} \right) R(T_1 - T_2) \\ &= \left(\frac{\gamma}{\gamma - 1} \right) \left(\frac{p_1}{\rho_1} - \frac{p_2}{\rho_2} \right) \end{aligned} \quad (1.31)$$

Substituting this expression for enthalpy into equation (1.31) yields:

$$\left(\frac{\gamma}{\gamma - 1} \right) \frac{p_1}{\rho_1} + \frac{u_1'^2}{2} = \left(\frac{\gamma}{\gamma - 1} \right) \frac{p_2}{\rho_2} + \frac{u_2'^2}{2} \quad (1.32)$$

The goal of this analysis is to produce a set of governing relations between the initial undisturbed gas properties and the shocked gas. These relationships include the ratio of pressures, densities and velocities across the shock front. To obtain the pressure ratio across the shock front, the first step is to apply the conservation of mass and momentum from equations (1.28 and 1.29) to eliminate u_1 and u_2 from the energy equation.

$$\begin{aligned} \rho_1 u_1' &= \rho_2 u_2' \rightarrow u_1' = \frac{\rho_2}{\rho_1} u_2' \\ &\rightarrow u_1'^2 = \frac{\rho_2^2}{\rho_1^2} u_2'^2 \end{aligned} \quad (1.33)$$

$$\begin{aligned} p_1 + \rho_1 u_1'^2 &= p_2 + \rho_2 u_2'^2 \\ \rightarrow u_1'^2 &= \frac{(p_2 - p_1)}{\rho_1} + \frac{\rho_2}{\rho_1} u_2'^2 = \frac{\rho_2^2}{\rho_1^2} u_2'^2 \\ \rightarrow u_2'^2 &= \frac{(p_1 - p_2)}{\rho_2 \left(1 - \frac{\rho_2}{\rho_1} \right)} \end{aligned} \quad (1.34)$$

applying to the energy equation gives:

$$\left(\frac{\gamma}{\gamma-1}\right)\frac{p_1}{\rho_1} + \frac{1}{2}\left(\frac{\rho_2}{\rho_1}\right)\left(\frac{p_1-p_2}{\rho_1-\rho_2}\right) = \left(\frac{\gamma}{\gamma-1}\right)\frac{p_2}{\rho_2} + \frac{1}{2}\left(\frac{\rho_1}{\rho_2}\right)\left(\frac{p_1-p_2}{\rho_1-\rho_2}\right). \quad (1.35)$$

A little algebraic manipulation yields:

$$\frac{p_2}{p_1} = \frac{\left(\frac{\gamma}{\gamma-1}\right)\rho_2 - \left(\frac{\rho_1+\rho_2}{2}\right)}{\left(\frac{\gamma}{\gamma-1}\right)\rho_1 - \left(\frac{\rho_1+\rho_2}{2}\right)}. \quad (1.36)$$

One can substitute the identity:

$$\left(\frac{2\gamma}{\gamma-1}\right) = \left(\frac{(\gamma+1)+(\gamma-1)}{\gamma-1}\right) = \left(\frac{\gamma+1}{\gamma-1}\right) + 1 \quad (1.37)$$

into equation (1.36) and obtain the expression:

$$\frac{p_2}{p_1} = \frac{1 - \left(\frac{\rho_1}{\rho_2}\right)\left(\frac{\gamma-1}{\gamma+1}\right)}{\frac{\rho_1}{\rho_2} - \left(\frac{\gamma-1}{\gamma+1}\right)} \quad (1.38)$$

One can re-write this equation in terms of the ratio of densities or velocity to obtain:

$$\frac{\rho_2}{\rho_1} = \frac{\frac{\gamma-1}{\gamma+1} + \frac{p_2}{p_1}}{\left(\frac{\gamma-1}{\gamma+1}\right)\frac{p_2}{p_1} + 1} = \frac{u_1}{u_2} \quad (1.39a,b)$$

Equations (1.38) and (1.39) are known as the Rankine-Hugoniot Equations. [Rankine 1870, Hugoniot 1887].

Shock strength, meaning the pressure ratio across a shock, can be expressed as a function of Mach number and γ . Since γ is assumed constant, the shock strength varies only with Mach number for a given gas. The Mach number of a shock moving into a gas initially at rest is defined as:

$$M_s = M_1 = \frac{u'_1}{c_1} = \frac{|s|}{c_1} \quad (1.40)$$

where u'_1 is shock speed and c_1 the local sound speed ahead of the shock. Note that M depends on the coordinate system. M is greater than 1 entering the plane of the shock and M is less than one leaving. The momentum equation (1.29) can be rewritten as:

$$\frac{p_2}{p_1} = 1 + \frac{\rho_1 u'^2_1}{p_1} \left(1 - \frac{\rho_1}{\rho_2} \right) \quad (1.41)$$

The sound speed in the undisturbed medium of region 1 is given by equation (1.13):

$$c_1 = \left(\frac{\gamma p_1}{\rho_1} \right)^{1/2}. \quad (1.42)$$

Hence, one can re-write M_1 as:

$$M_1 = u'_1 \left(\frac{\rho_1}{\gamma p_1} \right)^{1/2}. \quad (1.43)$$

The equation for Mach number (1.43) and density ratio (1.39a) can be substituted into (1.41) and (1.39b) to obtain the familiar equations for pressure ratio and density ratios across a shock as a function of Mach number:

$$\frac{p_2}{p_1} = \frac{2\gamma M_1^2 - (\gamma - 1)}{\gamma + 1}, \quad (1.44)$$

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)M_1^2}{(\gamma - 1)M_1^2 + 2}. \quad (1.45)$$

1.4.6 Rarefaction Waves - Riemann Invariants

As explained above, a rarefaction wave reversibly and adiabatically expands gas and is thus an isentropic expansion. This is an approximation whose validity is based on empirical observation. Riemann showed mathematically that for an isentropic wave of finite amplitude, the application of Euler's equations to a packet of mass undergoing an

isentropic change of state would yield two quantities which would remain constant throughout the process. These constants are known as Riemann Invariants. For small variations in pressure in an isentropic change of state, Riemann showed that the particle velocity of the flow changes locally according to:

$$du = \pm c \left(\frac{dp}{\rho} \right) \quad (1.46)$$

He obtained (1.46) by first defining the *condensation* $\bar{s}$ induced in a small amplitude compression according:

$$\rho = \rho_1 (1 + \bar{s}) \quad (1.47)$$

where $\bar{s}$ is some function $F = F(x - c_1 t)$, and then linearizing the sound speed according to the Taylor series expansion:

$$a^2 = \frac{\partial p}{\partial \rho} = \left(\frac{\partial p}{\partial \rho} \right)_1 + \left(\frac{\partial^2 p}{\partial \rho^2} \right) (\rho - \rho_1) = a_1^2 + \rho_1 \bar{s} \left(\frac{\partial^2 p}{\partial \rho^2} \right)_1. \quad (1.48)$$

The state denoted by the subscript 1 represents the gas state initially at rest. By replacing the pressure gradient term in Euler's momentum equation with:

$$\frac{\partial p}{\partial x} = \left(\frac{\partial p}{\partial \rho} \right) \left(\frac{\partial \rho}{\partial x} \right) = a^2 \left(\frac{\partial \rho}{\partial x} \right), \quad (1.49)$$

Riemann derived the *acoustic* equations:

$$\frac{\partial \bar{s}}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad (1.50)$$

$$\frac{\partial u}{\partial t} + a_1^2 \frac{\partial \bar{s}}{\partial x} = 0. \quad (1.51)$$

Riemann cross-differentiated (1.50) and (1.51) and solved for $dx/dt = c_1$. Combining this result with (1.47) and (1.51) yields (1.46). Liepmann and Roshko [1957, pp. 65-75] provide a more in-depth derivation.

In equation (1.46), the sound speed c is taken locally, and by substituting the isentropic relationships (equation 1.10) into the relationship for sound speed, one then

obtains:

$$c = c_1 \left(\frac{\rho}{\rho_1} \right)^{(\gamma-1)/2} \quad (1.52)$$

where c_1 is the sound speed in the initial unexpanded material. For a packet of gas, initially at rest, which under goes an isentropic change of state, the total change in velocity of the particle will then be the integration of du from the beginning to final state. This can be expressed:

$$u = \pm \int_{\rho_1}^{\rho} c \frac{d\rho}{\rho} = \pm \frac{2c_1}{\gamma-1} \left[\left(\frac{\rho}{\rho_1} \right)^{(\gamma-1)/2} - 1 \right] = \pm \frac{2}{\gamma-1} (c - c_1). \quad (1.53)$$

Equation (1.48) implies that:

$$u \pm \frac{2}{\gamma-1} c = \frac{2}{\gamma-1} c_1, \quad (1.54)$$

and since c_1 is a constant, the quantity $u \pm 2c/(\gamma-1)$ is *invariant* in undergoing an isentropic change of state. The dual sign indicates the possibility that the passage of the rarefaction wave can set gas into motion with either positive or negative direction. What the Riemann Invariants represent physically, are in essence conservation of momentum held in the form of directed kinetic energy (represented by the velocity u) and internal energy (represented by the sound speed or pressure and temperature). As gas becomes more rarefied, its directed velocity increases but its sound speed decreases (i.e. pressure and temperature decrease). The conversion of directed energy into more random internal energy is observed to alter the sound speed in the medium by a ratio of $2/(\gamma-1)$.

1.4.7 Analytical Solution to Classic Shock Tube Problem

From our original definition of the classic shock tube problem, the tube is initially separated into two uniform regions at rest, the left side having higher density and pressure than the right. (See figure 1.7). When one removes the diaphragm, a shock propagates to

the right and a rarefaction to the left. The undisturbed gas to the right of the shock is denoted region 1. The region immediately to the left is the region of gas which has been compressed and accelerated by the traversing shock. This region is denoted region 2. A moving interface separates the shocked gas from the expanding gas and is known as the contact surface. Because the gas is assumed inviscid, diffusion is not permitted across the shock interface. By definition, the pressure and velocity on either side of the contact surface must be the same because no gas flows across the interface. The expanded driver gas just to the left of the interface is denoted region 3. Gas in region 3 achieves its state upon isentropic expansion through the rarefaction fan. The head of the rarefaction fan moves into the undisturbed high pressure gas which is denoted region 4.

The combination of Riemann invariants and the Rankine-Hugoniot equations permits one to solve analytically for the emerging shock and rarefaction waves as a function of diaphragm pressure ratio (p_4/p_1) . Between regions 1 and 2, the pressure ratio across the shock is given as a function of Mach number by equation (1.44):

$$\frac{p_2}{p_1} = \frac{2\gamma_1 M_1^2 - (\gamma_1 - 1)}{\gamma_1 + 1},$$

The equation written here includes a subscript for the isentropic constant γ . In this notation, γ is assumed to be constant on both sides of the shock, but may vary across the contact surface, whose purpose will become apparent further on.

The absolute velocity of material just behind the shock is given by equations (1.27) and (1.44) as:

$$\begin{aligned} u_2 &= s - u'_2 = u'_1 - u'_2 \\ &= u'_1 - u'_1 \frac{\left(\frac{\gamma - 1}{\gamma + 1} \right) \frac{p_2}{p_1} + 1}{\frac{\gamma - 1}{\gamma + 1} + \frac{p_2}{p_1}}, \\ &= \frac{2c_1}{\gamma + 1} \left(M_1 - \frac{1}{M_1} \right) \end{aligned} \tag{1.55}$$

The Riemann invariant applied to the expansion of region 4 gas to region 3 states that:

$$u_4 + \frac{2}{\gamma - 1} c_4 = u_3 + \frac{2}{\gamma - 1} c_3. \quad (1.56)$$

Since the gas in region 4 is initially at rest, $u_4 = 0$. Hence, solving equation (1.56) for sound speed c_3 gives:

$$c_3 = c_4 - \frac{\gamma_4 - 1}{2} u_3. \quad (1.57)$$

From the isentropic relation $p / \rho^\gamma = \text{constant}$ and the definition of sound speed, one can arrive at the expression:

$$\frac{p_4}{p_3} = \left(\frac{c_4}{c_3} \right)^{\frac{2\gamma_4}{\gamma_4 - 1}} \quad (1.58)$$

Combining equations (1.50), (1.51), and (1.52) with the fact that velocity and pressure are equal across the contact surface (i.e. $u_2 = u_3$, $p_2 = p_3$) yields the dependence of shock strength on the original diaphragm pressure ratio.

$$\frac{p_4}{p_1} = \frac{2\gamma_1 M_1^2 - (\gamma_1 - 1)}{\gamma + 1} \left[1 - \frac{\gamma_4 - 1}{\gamma_1 + 1} \left(\frac{c_1}{c_4} \right) \left(M_1 - \frac{1}{M_1} \right) \right]^{\left(\frac{2\gamma_4}{\gamma_4 - 1} \right)}. \quad (1.59)$$

Equation (1.56) determines a limit on the highest Mach number shock which can be achieved in a shock tube. In the limit that $p_4 / p_1 \rightarrow \infty$, then:

$$\left[1 - \frac{\gamma_4 - 1}{\gamma_1 + 1} \left(\frac{c_1}{c_4} \right) \left(M_1 - \frac{1}{M_1} \right) \right] \rightarrow 0. \quad (1.60)$$

For Mach numbers much larger than unity, the inverse Mach number is small, and so the maximum Mach number approaches:

$$M \rightarrow \frac{\gamma_1 + 1}{\gamma_4 - 1} \left(\frac{c_4}{c_1} \right). \quad (1.61)$$

From this expression, one observes that the strongest or highest Mach number shocks are achieved using a driver gas which either has a low specific heat ratio and/or a high sound

speed. Monatomic gases have the highest specific heat ratio while multi-atomic gases have progressively lower specific heat ratio. Also, the sound speed is inversely proportional to the squareroot of the molecular weight. Hence, a light gas like hydrogen or helium is preferred as a driver gas, while nitrogen, air, or heavy noble gases are used for the test gas. The sound speed is also proportional to the square root of the temperature in the gas, so another method of improving shock strength is to heat the driver gas.

Figure 1.1. HYLIFE-I Reactor Chamber

Fig. 1.2. HYLIFE-II Reactor Vessel

Figure 1.3 HYLIFE ICF Phenomenology

Figure 1.4 Proposed blanket geometries for the HYLIFE-I and -II ICF Reactors.

Figure 1.5 The initial condition in a Generalized Riemann Problem. Density (ρ), velocity (u), pressure(p) and Temperature(T) are arbitrary of what the values are on the opposite side of the diaphragm, except, ρ , p , and T must be physically real (i.e. greater than or equal to zero).

Figure 1.6. Four Possible Solutions to the Generalized Riemann Shock Tube Problem

Figure 1.7 Typical density, velocity, pressure and temperature profiles in a classic shock tube problem at some time t_1 after the diaphragm removal. [Gaydon and Hurle 1963].

Figure 1.8 Shock front formation. The formation of a shock front in a shock tube due to expanding driver gas is analogous to accelerating a piston in a tube shaft. As the piston accelerates to its final velocity v , it sends infinitesimal compression waves ahead at ever higher velocities, which in turn propagate in a medium with ever higher sound speed c . Finally, all the small compression waves must overtake and merge at the front. [Becker 1922].

Figure 1.9 Rarefaction wave formation. The formation of a rarefaction wave which propagates into a gas is analogous to withdrawing a piston in a tube shaft. As the piston accelerates to its final velocity v , it sends infinitesimal expansion waves back into the gas. The gas however, travels at ever higher downstream velocities, and the trailing expansion waves must in turn propagate in a medium with ever slower sound speed c . The result is that a rarefaction spreads as in propagates.

Figure 1.10 Motion of gas in the laboratory frame or reference and in frame relative to the shock front.

2. EXPERIMENTAL DESIGN AND APPARATUS

2.1 Introduction

To study shock attenuation in jet arrays with geometry similar to that found in the actual HYLIFE ICF design, the experimental apparatus named the Liquid Jet Array Shock Tube (LJAST) was built. The experiment provides quantitative shock attenuation data which will be compared to the numerical predictions (chapter 4) to partially validate the computational method for predicting the gas dynamics in HYLIFE (chapter 3). Because only a fusion detonation can cause x-ray ablation and neutron isochoric heating, simulating these processes was impractical and not attempted. This chapter has two main parts. Because the design of the experiment considered a number of geometric and hydrodynamic parameters expected to exist during the HYLIFE blast venting, the first part discusses methodology for performing scoping calculations in the HYLIFE reactor. The second part discusses the design of the experiment.

2.1.1 HYLIFE Geometric and Hydrodynamic Parameters

Both the HYLIFE-I and the early HYLIFE-II designs incorporate cylindrical jets for the blanket geometry. The later HYLIFE-II design incorporates slab jets. Because the design and construction of the LJAST experiment began prior to the decision to use the slab geometry in the HYLIFE-II design, the jet geometry for the experiment was based only on the cylindrical geometry cases. Both the HYLIFE-I and -II cylinder blankets consist of a 50% packing fraction of liquid jets at the midplane. In HYLIFE-I, the jets are 20 cm in diameter. In HYLIFE-II, the jets are 5 cm in diameter. By inspection, a hexagonally-packed geometry provides the greatest packing fraction for any pitch-to-diameter ratio. Table 2.1 provides a listing of the HYLIFE-I and -II parameters.

Table 2.1 HYLIFE-I and -II Geometric and Hydrodynamic Parameters [Moir 1991]

	HYLIFE-I	HYLIFE-2 (cylin.)
Vessel Radius	5 m	3 m
Inner Cavity Height	6 m	2 m
Pellet Yield	1800 MJ	350 MJ
Blanket Liquid	Lithium	Flibe (Li_2BeF_4)
Packing Fraction	50%	50%
Jet Diameter	20 cm	5 cm
Repetition Rate	1.5 Hz	8.1 Hz
Operating Temperature	770 K	923 K
Blanket Inner Radius	0.5 m	0.5 m
Blanket Outer Radius	2.1 m	1.5 m

As discussed previously, prior to the fusion pellet injection, the pressure within the vessel must be less than 1 Pa to allow for laser beam propagation or 0.01 Pa for heavy ion beam propagation. Shortly after the fusion, the x-ray ablated material will blow off the inner surfaces of the jets. In the original HYLIFE-I study [Blink, et al., 1985], there was the belief that all the ablated material would implode on the central cavity where it thermalizes and then re-explodes as a blast. Blast venting was assumed to occur into a relative vacuum. This over-estimates the mass and energy in the blast because, while most of the material will be directed toward the central cavity, a smaller fraction will remain which expands and fills the void among the jets. Figure 2.1 shows an approximate schematic of the inner cavity geometry and the surfaces which will be ablated. The determination of the fraction of mass directed toward the central cavity used the numerical method to be described in chapter 3. Figure 2.2 shows the geometry used for the calculation. Assuming symmetry and neglecting the curvature in the jet positioning simplified the computational grid to 75 nodes by 26 nodes. Based on data

from Chen [1992], a fluence of 9.2 MJ/m² was assumed to be entirely deposited in 15 micron thick layer of Flibe on the first row cylinders, and a fluence of 7.6 MJ/m² was assumed to be entirely deposited in 12.3 micron thick layer on part of the second row (figure 2.1). The Flibe vapor generated in the ablation process was assumed to be an ideal gas. An interface (figure 2.2) divides the inner cavity from the jet array region. By tracking the mass flux across this interface, the numerical method is able to determine the mass fraction ejected into the central cavity. Figure 2.3 shows the percentage of mass into the central cavity. The calculation predicts that 84% of the ablation mass is directed into the central cavity and 16% remains in the jet array region.

Table 2.2 Properties of Lithium and Flibe Liquid [Chen, 1992]

	Lithium (770 K)	Flibe (923 K)
Liquid Density	485 kg/m ³	1992 kg/m ³
Specific Heat Ratio	1.67	1.2
X-ray Attenuation Coeff.	1.8 x 10 ⁵ m ⁻¹ (~1 keV)	9.9 x 10 ⁶ m ⁻¹ (~1 keV)
X-ray Mean Free Path	41.5 x 10 ⁻⁶ m	1.14 x 10 ⁻⁶ m
Heat Capacity	4200 J/kg-C	2350 J/kg-C
Heat of Vaporization	1.96 x 10 ⁷ J/kg	7.91 x 10 ⁶ J/kg
Sound Speed	4500 m/s	3200 m/s
Molecular Weight	6.92 g/mole	33 g/mole

If one assumes that the mass not ejected into the central cavity carries a proportional amount of energy which is then uniformly distributed among the jets then the average pressure of the ablated vapor if expanded to fill the void in the jet array would be given approximately by the ideal gas law in energy form as:

$$p = \frac{E(\gamma - 1)}{V} \quad (2.1)$$

where E is the internal energy in the ablated vapor, V the void volume between the jets, and γ the specific heat ratio. One can derive equation (2.1) from equation (1.4) and applying equations (1.7) through (1.9). For the HYLIFE-I and -II parameters, if one assumes that approximately 16% of the x-ray energy (x-ray energy comprises ~16% of the total yield) is allowed to remain among the jets, and the volume is assumed to be the void among the jets, then from the values in Table 2.1, the pressures would be on the order of:

$$p = \frac{(1800 \times 10^6 J)(16\%)(16\%)(1.67 - 1)}{\pi(2.1^2 - 0.5^2 m^2)(6m)(1-.5 p.f.)} = 7.9 \times 10^5 Pa$$

for HYLIFE-I and

$$p = \frac{(350 \times 10^6 J)(16\%)(16\%)(1.2 - 1)}{\pi(1.5^2 - 0.5^2 m^2)(2m)(1-.5 p.f.)} = 2.9 \times 10^5 Pa$$

for HYLIFE-II. The assumption of adiabatic expansion of an ideal gas neglects immediate condensation on cold jets and radiative losses which would lower the density, internal energy and pressure in the ambient vapor. Also, the assumption of the ablated mass carrying with it a proportional amount of energy neglects the non-uniformity of the x-ray energy deposition which may direct more energetic vapor into the central cavity and keep less energetic vapor among the jet void. Hence, the calculated pressures represent an upper bound.

One can obtain a lower bounding estimate of the pressure based on an assumption of an ideal gas at the liquid saturation temperature. This assumes that the mass which is not ejected into the central cavity expands to fill the void among the jets but in doing so its temperature is lowered to approximately the liquid surface temperature, T_L . The calculation requires some estimate of T_L and the mass ablated. There is a question as to what the liquid surface temperature is following ablation. T_L will depend on position and time, especially whether the surface was ablated or not. Unablated surfaces, which make

up the majority of the surfaces in the jets will have a temperature which is $T_{l\infty}$, the original liquid temperature, plus some ΔT due to neutron heating. By inspection, assuming ΔT is zero, i.e. T_b is equal to $T_{l\infty}$, yields the lowest pressure for bounding estimate.

Estimating the amount of mass ablated requires knowledge of the thickness of the x-ray ablated layer. Assuming that a mono-directional x-ray attenuation relationship governs the x-ray deposition, then the fluence is given by [Chen, 1992]:

$$I(x) = I_0 \exp(-\Sigma x) \quad (2.2)$$

where $I(x)$ is the photon energy fluence in (J/m²) as a function of penetration distance into a material, I_0 the surface photon energy fluence, and Σ the total macroscopic photon attenuation cross-section (m⁻¹). The local energy density due to the x-ray deposition is then just the gradient of the fluence divided by the material density, or:

$$i(x) = -\frac{1}{\rho} \frac{d}{dx} [I_0 \exp(-\Sigma x)] = \frac{\Sigma}{\rho} I_0 \exp(-\Sigma x). \quad (2.3)$$

Equation (2.3) provides a method of determining the penetration depth at which vaporization of material will begin. Two significant depths now become important. The first, δ_1 , is the penetration depth to which the energy deposition is equal to or exceeds the required cohesive energy (i.e. the heat of vaporization plus sensible heat) needed to completely vaporize the liquid, and the second, δ_2 is the depth to which the energy just exceeds that of saturated liquid. Both δ_1 and δ_2 are dependent on the saturation conditions which are pressure dependent. Moreover, the pressure itself will be a function of time and position. The pressure rise caused by x-ray heating takes the first several microns of the liquid to beyond the supercritical pressure. However, once the ablated material blows off, the pressure in the wake drops to approximately the order of 1 atmosphere [Chen 1992]. The blowoff of ablated material is assumed to be controlled by

the lower pressure, and therefore, the heat of vaporization for these calculations is assumed to correspond to 1 atmosphere pressure. At this pressure, the heat of vaporization will not vary much from the values given in Table 2.2, which permits their use for the calculation. A smaller mass evaporated and cooled to T_{∞} will result in a lower bounding pressure. Hence, for conservatism, only the mass of the fully vaporized layer (δ_I) is considered. From properties in Table 2.2, the thickness δ_I as given by equation (2.3) is:

$$i(\delta_I) = h_{fg} = \frac{\Sigma}{\rho} I_o \exp(-\Sigma \delta_I). \quad (2.4)$$

where h_{fg} is the heat of vaporization. The fluence, I_o , is given by the x-ray fraction of the yield divided the surface area for a sphere at the inner blanket radius. Solving for δ_I gives:

$$\delta_I(\text{HYLIFE} - I) = 41 \mu\text{m}.$$

$$\delta_I(\text{HYLIFE} - II) = 7.1 \mu\text{m}.$$

Then an order of magnitude approximation of the mass is just the product of the thickness and the projected surface area for a sphere. This gives:

$$\begin{aligned} 4\pi R_o^2 \rho \delta_I &\approx 0.062 \text{ kg (HYLIFE} - I) \\ &\approx 0.045 \text{ kg (HYLIFE} - II) \end{aligned}$$

Assuming that 16% of the mass expands and cools to near saturation temperature gives a lower bound estimate on the ambient pressure inside the jet array void which the blast will encounter. From the ideal gas law,

$$\begin{aligned} p &= \frac{nRT}{V} \approx \left(\frac{16\% \text{ mass}}{\text{mol. wt}} \right) \left(8.3144 \frac{\text{Pa} \cdot \text{m}^3}{\text{mole} \cdot \text{K}} \right) \left(\frac{T}{V} \right) \\ &\approx 234 \text{ Pa (HYLIFE} - I) \\ &\approx 266 \text{ Pa (HYLIFE} - II) \end{aligned}$$

Hence the pressure that the blast will encounter inside the jet array will be equal to or greater than the order of 2×10^2 Pa or approximately 2 torr (mm Hg) and may be as high as several atmospheres to 10 atmospheres. It is important to note here that the estimates for bounding vapor pressure in the ambient volume around the jet array are single values for pressure. In fact, the actual pressure will be a function of space and time.

2.1.2 HYLIFE Shock Strength and Pressure Ratio

One of the most important factors in estimating the shock strength and the propagation time of a shock through a medium is the Mach number, defined in equation (1.35) as ratio of shock wave speed to the sound speed of medium the wave is moving into. For large pressure ratios which are expected in the ICF environment, one can use equation (1.56) to obtain an estimate of the maximum Mach number. Strictly speaking, equation (1.56) applies only to the 1-D plane flow case of initially quiescent vapor on either side of a diaphragm (i.e. a shock tube). However, by assuming that the thermalized vapor in the inner cavity represents the high pressure driver gas and the ambient vapor which fills the void between the jets in the blanket represents the test gas, equation (1.56) can be applied as a method of scaling the shock strength in ICF.

One obtains the pressure ratio between the vapor inside the central cavity and the ambient atmosphere around the blanket by the applying equation (2.1) to the central cavity and then dividing by the expected pressures in the ambient atmosphere.

$$p_4 = \frac{(1800 \text{ MJ})[16\% + .8(16\%)](1.67 - 1)}{\pi(.5^2 \text{ m})(6 \text{ m})} = 7.4 \times 10^7 \text{ Pa (HYLIFE - I)}$$

$$= \frac{(350 \text{ MJ})[16\% + .8(16\%)](1.2 - 1)}{\pi(.5^2 \text{ m})(2 \text{ m})} = 1.3 \times 10^7 \text{ Pa (HYLIFE - II)}$$

Using the higher of pressures computed in section 2.1.1 yields pressure ratios of:

$$\begin{aligned}\frac{p_4}{p_1} &= \frac{7.4 \times 10^7 \text{ Pa}}{1.0 \times 10^6 \text{ Pa}} = 74 \quad (\text{HYLIFE-I}) \\ &= \frac{1.3 \times 10^7 \text{ Pa}}{3.6 \times 10^5 \text{ Pa}} = 36 \quad (\text{HYLIFE-II})\end{aligned}$$

From equation (1.15), one can express the sound speed ratio c_1/c_4 in equation (1.51) as the ratio of temperatures to the one-half power. Assuming the constant volume specific heat remains constant, then the ratio of temperature scales as the ratio of gas internal energies. Of course this assumption is quite crude since vaporization, dissociation and ionization all are involved for the Flibe ablation. From the geometric argument in section 2.1.1, the ratio of inner cavity energy to that in the ambient atmosphere around the blanket is given by:

$$\begin{aligned}\frac{c_1}{c_4} &\approx \sqrt{\frac{T_1}{T_4}} \approx \sqrt{\frac{E_1}{E_4}} \\ &\approx \sqrt{\frac{.2(16\%E_{\text{yield-xrays}})}{16\%E_{\text{yield-debris}} + 0.8(16\%E_{\text{yield-xrays}})}} = 0.33\end{aligned}\tag{2.5}$$

which applies for both the HYLIFE-I and -II since each is assumed to share the similar geometries. Inserting the sound speed ratio and the pressure ratios into equation (1.56) and solving for Mach number gives:

$$\begin{aligned}M &= 5.0 \quad (\text{HYLIFE-I}) \\ &= 5.0 \quad (\text{HYLIFE-II})\end{aligned}$$

These Mach numbers assume relatively high pressure and sound speed in the ambient atmosphere which surrounds the blanket. By inspection, if the amount of energy which the mass carries varies such that the partitioning of the total vapor energy favors more deposition in the central cavity, then the Mach number will be higher.

2.2 Experimental Apparatus

Figure 2.4 provides a general overview of the experimental apparatus. The main components are the shock tube, diaphragm assembly, pressure vessel, test section, liquid delivery system, and instrumentation. The system is designed to be pressurized on the shock tube side to 6.9 MPa (1000 psi) and evacuated in the low pressure side to 1 Pa (10^{-2} torr). A system of diaphragms separates the two regions until the time of the burst. The pressure vessel houses the test section whose sides are constructed of a clear polycarbonate material and instrumented with fast response piezo-electric pressure transducers located on the test section sides and the end of the vessel wall. Data acquisition is done by a PC with a digital oscilloscope board. The vessel has four round glass ports for visual observation and illumination of the test section.

Shock Tube

The goal of the shock tube is to produce strong shocks followed by a sustained period of relatively steady supersonic flow. Based on considerations in section 2.1, the design considers a range of Mach numbers from 1 to 5. For simplicity, the design does not utilize gas heating, combustion or detonation, and the tube is long enough so that the shock which is initially sent into the test section, has ample time to interact with the jet array before any pressure waves due to effects from the opposite end of the shock tube propagate into the test section. Helium and air serve as the driver gas, but helium into air is preferred because it provides a higher Mach number for the same pressure ratio, according to equation (1.56). The driver and test gases are allowed to equilibrate to room temperature before the shock is initiated. The maximum operating pressure on the high pressure side is set at 6.9 MPa (1000 psi).

The shock tube section is made from 4 inch Iron Pipe Size (IPS), 9.3 cm (3.66")

inner diameter schedule 40 carbon steel pipe. A schedule 40, carbon steel cap is butt welded onto one end. A standard schedule 40 flange, approximately 28 cm (11") in outside diameter with a 4 inch IPS inside diameter, is butt welded to the other end. The shock tube's length is 122 cm (48") and determined by the flow duration. In any shock tube, the region between the downstream heading shock front and contact surface is relatively constant until the originally, upstream heading rarefaction reaches the end cap of the shock tube, reflects and catches up downstream with the contact surface. Once the reflected rarefaction catches up with the contact surface, the pressure and velocity in the region between the shock front and the contact surface will become non-uniform. To insure that the primary flow behind the shock front maintains its uniformity when it interacts with the jet array, the shock tube length must be made sufficiently long to delay the reflected rarefaction. The rarefaction travels at the sound speed in the local medium while the shock travels at the Mach number multiple of the sound speed in the local medium. Equation (2.6) defines a conservative criteria for the shock tube length; the time for the rarefaction to travel the length of the shock tube is greater than twice the time for the shock tube to traverse the distance to the end of the test section, i.e.

$$\text{flow time in shock tube} \geq \frac{\text{tube length}}{c_4} \geq 2 \frac{\text{test length}}{M_1 c_1} \quad (2.6)$$

For this relationship to hold for weak shocks, (i.e. $M = 1$) and when the species driver and test gas are the same (i.e. $c_4 = c_1$), the tube length relationship becomes:

$$\text{tube length} \geq 2 \frac{c_4}{M_1 c_1} \text{test length} = 2 \times \text{test length} \quad (2.7)$$

To reach its maximum speed and form a planar front, a shock wave must travel some distance downstream which varies with the diaphragm opening time, Mach number, and sound speed [Gaydon and Hurle 1963]. Therefore, to produce a planar shock close to the maximum possible speed for the given diaphragm ratio, the length of the tube leading

to the test section must provide this formation distance. With no real method of accurately measuring the LJUST diaphragm opening times, the length for the test section tube relies on the experimental data of White [1958]. Extrapolation of White's data indicates that the formation distance for a 9 cm diameter tube, is less than 30 cm (1 foot). Hence, the LJUST experiment includes a 30 cm section of pipe just downstream from the diaphragm. For a test section which is also 30 cm in the length, the conservative criterion given in equation (2.6) a shock tube length of 1.2 m.

As mentioned above, the shock tube has two ends. One end is capped and the other has a flange. The flanged end is designed as part of the diaphragm assembly, and its surface must seal against pressure. Therefore, the flange's face is machined with a 12.7 cm (5.5") diameter $\times$ 0.3175 cm (0.125") deep square O-ring groove. When the shock is released, the diaphragm petals open and a shock will travel down stream. The shock, however, may reflect back upstream before the rarefaction reflects back from the butt cap. This may generate a blow back strong enough to blow the diaphragm petals from a downstream pointing position to an upstream pointing position. To allow for stress relief during possible blow back, the inner lip on the flange is given a radial curvature of 0.48 cm (3/16"). Finally, to allow for a connection to a high pressure gas supply, the end cap is machined with a pipe threaded hole and fitted with a Swagelok™ connector (figure 2.5). The shock tube has been hydrostatically tested for 30 minutes with water pumped to 34 MPa (5000 psi). This provides a known safety factor of at least 5 times the designed maximum operating pressure of 6.9 MPa (1000 psi).

Diaphragm Assembly

The diaphragm assembly (figure 2.6) is designed to operate with either one diaphragm or two diaphragms. The assembly consists of two butt-welded, schedule 40, 4 " IPS flanges and a third, equivalent-sized solid blind flange which has had its inside

machined out to 4 " IPS. One each of the two schedule 40, 4" IPS flanges is welded onto either the end of the shock tube or the end of the pipe leading to the vessel. The flange on the shock tube is aligned facing the flange on the vessel. The third, or intermediate flange rests between the two. By inspection, the third flange provides an intermediate, pressurizable volume when two diaphragms are sandwiched around it. The third flange also has machined pipe thread hole leading from the edge into the intermediate volume. The hole is fitted with another Swagelok fitting with tubing connections that allow for pressurization and depressurization control of the intermediate volume.

When only one diaphragm is used, the mechanism for bursting the single diaphragm is a simple, rapid overpressure brought on by driver gas addition. The single diaphragm is usually placed between the flanges closest to the vessel. Each diaphragm is machined with a uniform-depth, X-shaped groove (figure 2.6). At the grooves, the material is thinner, and therefore, under pressure, the diaphragm is most likely to fail along these grooves, resulting in four relatively uniform petals (figure 2.7). The vessel is evacuated and then the shock tube is slowly pressurized until the diaphragm is within 10% of the predicted burst pressure. Driver gas is then suddenly added to the shock tube until the pressure bursts the diaphragm. The advantage of the single diaphragm operation is that the burst will always be assured because the diaphragm will eventually fail if the pressure continues to increase. However, the disadvantages are that the timing and pressure at which the diaphragm ultimately breaks will depend on the consistency in the diaphragm manufacturing.

Using two diaphragms instead of one, can improve the timing and the burst pressure's uniformity . The first diaphragm is inserted between the shock tube flange and the intermediate flange, and the second diaphragm is inserted between the intermediate flange and the flange on the vessel. With two diaphragms in place, an intermediate volume is formed inside the diaphragm assembly. This intermediate volume is kept filled

to approximately half the pressure in the driver section. By inspection, this configuration causes the total pressure differential to be shared equally between the two diaphragms, and permits the driver pressure to be increased to twice the single diaphragm pressure. Because neither diaphragm is able to hold back the driver pressure by itself, a shock can be instantly generated by a rapid depressurization of the intermediate volume which places the entire differential across the first diaphragm. To depressurize the intermediate volume, a solenoid valve (EV2) is connected to the intermediate flange, which opens and relieves the pressure into an accumulator reservoir (figure 2.6). The differential between the driver and vessel pressures need not be fixed at twice the burst limit of a single diaphragm. As long as the total differential between driver and vessel pressures is greater than the ability of either single diaphragm to withstand, then the double-diaphragm configuration works. However, care must be taken to maintain the manufacturing tolerances to assure breakage of the diaphragms at a uniform and known pressure.

The three flanges are clamped together by means of eight, 2.86 cm (1.125") diameter threaded studs and nuts. Alignment of flanges and diaphragms is by means of guide pins protruding from the downstream-side flange faces which are also used as diaphragm retainer pins (figure 2.6). The upstream-side flange faces have precisely aligned holes which accept the pins. The diaphragms themselves are made from either of two materials. Low pressure runs up to 60 psi use a 0.13 mm (0.005") thick mylar plastic sheet. Higher pressure runs use 0.020" to 0.050" thick 6061-T6 aluminum sheet. To facilitate proper petalling, the mylar diaphragms are hand-scribed with a razor in a cross pattern and the aluminum machined with the same pattern using a 0.8 mm (1/32") diameter mill bit. The hand-scribing of the mylar is not sufficiently consistent to produce a uniform and predictable burst pressure, and so the mylar can only be used singly. Most of the aluminum diaphragms are made from 0.813 mm (0.032") thick 6061-T6 aluminum sheet. The machining process work hardens the metal near the groove which may cause

non-uniform petalling. To relieve the work hardening, the machined aluminum diaphragms are annealed at about 800°C for 5 minutes. Some trial and error experiments were performed on the machined aluminum diaphragms to determine the burst pressure as a function of groove depth. The experiments determined the approximately linear relationship:

$$\text{burst pressure}(\text{psi}) \approx 532 - 25500x \quad (2.8)$$

where x is the depth of the machined scribe marks in inches (figure 2.8).

Vessel

A pressure vessel houses the test section for three purposes. The first is to provide a low pressure environment which closely approximates the initial ICF environment just prior to the blast arrival. The second is to act as a pressure vessel to contain the shock which is sent down the tube. The third is as a reservoir to store the fluid delivered into the system as liquid jets (figure 2.9).

The vessel is made from schedule 40 fittings and has three basic sections, the lid, the mid-section and the base. The lid is made from a cast 30 cm (12" IPS) diameter end cap with an 8.9 cm (3 1/2") diameter hole machined on top. A 30 cm (12") long section of 8.9 cm (3 1/2" IPS) diameter pipe is welded over this hole for fluid delivery. A 2" diameter pneumatically actuated ball valve (BV1) caps the pipe. To attach the lid to the vessel, a 5 cm x 1.27 cm (2" x 1/2") thick ring of steel with a 30 cm (12" IPS) inside diameter is welded to the lid's base. The ring serves as a flange. A similar flange is welded onto the top of the vessel's midsection. Thirty-two 0.794 cm (5/16") nuts and bolts secure the lid to the vessel.

The midsection of the vessel is made from a schedule 40, 12" to 6" IPS reducing tee. The 12" section is part of the vessel while the 6" opening connects to the shock tube. Inside the midsection, at mid-level, two welded braces provide a support and anchor for the test section. A 6" to 4" IPS schedule 40 concentric reducer is butt welded on to the 6"

opening of the midsection which is then welded to the 30 cm of pipe leading to the diaphragm assembly. At the diaphragm assembly, the vessel-side flange has a 1/2" pipe threaded fitting which allows for gas evacuation.

Three welded-on stainless steel window fittings for thick quartz blanks are provided at the normal and two opposing 45 degree positions on one side of the vessel. Another window is located on the opposite side of the vessel also normal to the test section. This provides back lighting during photography (figure 2.9).

The base of the vessel expands to 24" diameter IPS. A 24" to 12" diameter IPS concentric reducer welded to both the midsection and base, connects the 12" IPS midsection to the 24" IPS base. The majority of the base is made from a 61 cm (24") long section of 24" diameter IPS pipe. The base is capped by a 24" IPS end cap with a machined 3/4" pipe fitting at the center for fluid extraction. The vessel, with its cap secured and schedule 80 PVC fittings mounted above the lid, was hydrostatically tested for 30 minutes at 0.34 MPa (500 psi). The volume of the vessel, 0.42 m³ (15 ft³), is 10 times the volume of a standard helium cylinder (0.042 m³, 1.5 ft³). This assures safety because, should the entire contents of a single standard cylinder originally at 2500 psi empty into the vessel half filled with liquid, the final pressure in the vessel will be still less than 0.34 MPa (500 psia).

Test Section

Figure 2.10 shows the test section assembly. The assembly consists of the test section and the conical diffuser. The test section is a rectangular box having dimensions 8.26 cm (3.25") wide by 8.26 cm (3.25") high by 26.67 cm (10 1/2") long. Its top is a 1/2" thick aluminum orifice plate with an array of 48 holes each 0.95 cm (0.375") in diameter. The holes are hexagonally-packed at a 50% packing fraction. The conical diffuser, mounted above the orifice plate and connected to the fluid delivery pipe entering

from the vessel's lid, directs liquid down to the orifice plate. The bottom support plate is a 3.81 cm (1.50") thick aluminum plate with its center machined out in the area just under the jet array orifices. This opening exists so that the liquid jets can fall unimpeded out of the test section. To run the experiment with a solid cylindrical array rather than a liquid jet array, an optional lower orifice plate can be inserted into this opening and then solid polycarbonate rods press fit into holes to make an array of solid rods (figure 2.11). The side plates of the test section are made of 1/2" thick Tuffak™ polycarbonate which is impact rated against .22 caliber projectiles at 3000 fps. This provides a suitable transparent medium for observation and photography. One of the side plates is left clear while the other side has 5 mounts for the pressure transducers. Seven 6" long bolts clamp the test section together. The front and back of the test section are open.

The test section entrance has an inside recessed lip which fits around a square metal fitting. The fitting is cast inside acrylic plastic, which fills the inside of the 6" section of the reducing tee that makes up the midsection of the vessel (figure 2.12). The shock tube leading to the vessel has a circular cross-section but the test section is square. Therefore, prior to entering the test section, the cross sectional shape of the acrylic casting, must change from round to square. Chisnell [1957] gives the relationship from one-dimensional analysis for shock wave Mach number change for a change in cross sectional area as:

$$\frac{\delta A}{A} = \frac{2M\delta M}{K(M^2 - 1)} \quad (2.9)$$

where A is the cross-sectional area, δA the change in area, M the Mach number, and K a weak function of Mach number which varies between 0.5 for weak shocks and decreases to 0.394 as M becomes large. From equation (2.9) it becomes clear that a change in cross-sectional area will change the Mach number originally determined by the diaphragm pressure ratio. Additionally, work by Bird [1958] on shock strength increase

in converging channels indicates that the theoretical Mach number increase in converging channels is most closely approached in gradually varying channels. Therefore, to maintain a constant Mach number in the approaching shock, the acrylic casting is designed to preserve the cross-sectional area and change shape gradually. The manufacturing of the acrylic casting begins with a wax plug shaped to create a gradual round-to-square transition of constant cross sectional area. That is, the wax transition piece is round on one end and square on the other end such that the cross-sectional areas on either end follow the simple relationship:

$$\frac{\pi D^2}{4} = s^2. \quad (2.10)$$

The wax plug is made from a special high temperature paraffin which is able to withstand the exothermic reaction of the uncured acrylic resin when it is poured around the plug. However, the paraffin possesses a lower melting point than the cured acrylic and is easily liquefied by a heat gun after the curing is complete.

Liquid Delivery system

As mentioned above, one can fit the LJUST test section with either an array of solid cylinders or deliver liquid past the orifice plate to establish the jets. When jets are desired, liquid can be drawn from a 55 gallon drum through a 3 1/2" IPS schedule 80 PVC pipe (figure 2.4). The specific liquid used here is either water, or more preferably standard mechanical vacuum pump oil (because water is conductive and is able to short out the pressure transducer cabling while the oil is electrically inert and has lower vapor pressure). Flow is controlled with a 2" diameter, pneumatically actuated PVC ball valve. The valve assembly connects the steel pipe emerging from the lid to the PVC pipe leading to the 55 gallon drum (figure 2.4). Inside the vessel, a diffuser cone connects the lid opening to the orifice plate. The differential driving pressure needed to deliver the

liquid was provided by pumping the vessel down to the vacuum condition for the test.

One of the difficulties in using liquid is establishing smooth jets. Jet downward velocity, packing fraction of the jets, orifice plate design, and jet Reynolds numbers are factors which determine whether or not the exiting jets will be smooth. The first factor, jet velocity, affects the Reynolds number and therefore the degree of turbulence in the jet. A slower and therefore more laminar jet is desirable, however, if the jet velocity is too slow it may suffer from *necking down*, and therefore the packing fraction will decrease. A jet necks down as it falls according to a relationship dictated by gravitational acceleration and conservation of mass. One can show that for any distance z , through which a jet falls, the void fraction in a hexagonally-packed array as a function of distance away from some orifice plate is given by:

$$\alpha(z) = 1 - \frac{v_{top}}{\sqrt{v_{top}^2 + 2gz}} \left(\frac{\pi}{2\sqrt{3}} \frac{D^2}{P^2} \right) \quad (2.11)$$

where v_{top} is the velocity of a jet just exiting the orifice plate, g the gravitational constant, and P/D the pitch to diameter ratio. For a 50% packing fraction (i.e. 50% void fraction) it is straight forward to show that the corresponding P/D is 1.35. The goal is to use the minimum initial jet velocity which produces a relatively uniform jet array that varies by less than 10% in void fraction as it falls through the vertical dimension of the test section. Using equation (2.11), a fall height of 10 cm in the test section, and P/D of 1.35, the jet velocity must greater or equal to 2.9 m/s.

Another factor in jet smoothness is the design of the top orifice plate. Because of the relatively high packing fraction, the jets are close to each other. The main flow coming down the conical diffuser strikes the orifice plate and encounters a myriad of holes (figure 2.13). To facilitate the funneling of liquid through the holes, a countersinking bit was used to machine the upper lip on each hole and therefore produce a smoothly rounded entrance. This improves the jet smoothness over that produced by a

simple flat plate with non-countersunk holes. For the oil, this modified plate is sufficient to produce smooth jets at 3 m/s, but for water this was not achieved.

Turbulence in the water jet was considered as one possible cause. For water, the diameter based Reynolds number at 3 m/s is:

$$\begin{aligned} \text{Re} &= \frac{\rho u D}{\mu} & (2.12) \\ &= \frac{(1000 \text{ kg/m}^3)(3 \text{ m/s})(.01 \text{ m})}{(0.001 \text{ Pa-s})} = 30,000 \text{ (water)} \\ &= \frac{(900 \text{ kg/m}^3)(3 \text{ m/s})(.01 \text{ m})}{(0.2 \text{ Pa-s})} = 135 \text{ (pump oil)} \end{aligned}$$

which is turbulent for water but laminar for the oil. This is due mostly to the large difference in viscosities which are 0.001 Pa-sec. for water and 0.2 Pa-sec for oil. For water, decreasing the velocity to 2.5 m/s and inserting a short conical wedge of aluminum honeycomb on top of the orifice plate to provide upstream flow straightening improved the jet smoothness.

Homogeneous nucleation was a concern for the water because the water, originally at room temperature (295 K) was being delivered into a low pressure environment corresponding to approximate 275 K saturation temperature. However, it could not be concluded absolutely from photographic data whether some jets underwent homogeneous nucleation or if the apparent bubbles carried remaining gas trapped in the elbows or above the ball valve not evacuated in the original priming of the piping system. Figures 2.14(a) through 2.14(c) show three typical views of smooth jets, partially smooth and turbulent jets, respectively. Figure 2.14(a) shows smooth jets for water at about 2.5 m/s flow velocity. The jets are typical of the smooth jets formed with both oil and water, except an aluminum honeycomb is used in the water cases for flow straightening prior to the orifice plate. Figure 2.14(b) shows relatively smooth jets at about 2.5 m/s formed with water and a tube bank above the orifice plate. Although the jets appear smooth, they

are not as smooth as those in figure 2.14(a) due to very minute surface roughness which isn't apparent in the photograph, but is inferred by in the change in light transmission intensity. It was observed qualitatively that the smoother the jets, the greater the light transmission. Figure 2.14(c) shows a turbulent jet flow, which results when no upstream flow straightening is used with water.

The maximum driving head available for fluid delivery is one atmosphere assuming negligible pressure inside the vessel. This must equal the sum of all the pressure losses the fluid encounters, which consists of the dynamic pressure component of the jets, the gravitational head, the loss in the 2" pneumatically actuated ball valve and any losses due to friction and pipe elbows i.e.:

$$\Delta p_{total} = \frac{\rho u^2}{2} + \rho g \Delta z + \Delta p_{valve} + \Delta p_{pipe} + \Delta p_{elbows} + \Delta p_{entrance \text{ and exit}} \quad (2.13)$$

Using loss coefficients from a standard fluid mechanics handbook [Crane, 1988], it was determined with the ball valve completely open, the total pressure loss as computed according to equation (2.13) was below one atmosphere for a flow velocity of 3 m/s. Also, tests of the liquid delivery system showed that the system is able to deliver 150 liters (40 gallons) of water in approximately 6 seconds, and the same quantity of oil in about 9 seconds. These volumetric flow rates can be converted to jet velocities by dividing by the total orifice plate flow area, which gives an average velocity of 7.3 m/s for the water and 4.9 m/s for the oil. Therefore the one atmosphere driving head is more than sufficient to produce 3 m/s jets for both water and oil. The task is to control the fluid delivery to the desired velocity. This is achieved by adjusting the opening of the valve to increase or decrease the pressure drop across the valve. The initiation of the flow introduces transient aspects into the jet establishment. However, sufficient liquid was held in the barrel for the jets to obtain steady flow.

Instrumentation

There are a total of eight Kistler 601B piezo-electric pressure transducers used in the experiment. Five are located on the sides of the test section housed inside the vessel to record the pressure transients along the test section. (See Fig. 2.10) Three are located along the vessel wall that the gas from the test section impacts. (See Fig. 2.9) These record the wall impact pressures. Figure 2.15 shows a typical fitting and mounting assembly for a miniature piezo-electric pressure transducer. The transducers output a charge signal whose quantity varies linearly with the pressure on the crystal. The transducers can resolve sudden pressure changes to within 2 microseconds (500 kHz frequency response). The charge signals are amplified and converted to transient voltages by Kistler charge amplifiers, and then the data are recorded by a PC-based data acquisition system which samples analog data at 500 kHz. The data acquisition system is a Rapid Systems™ R1000 4x4 PC-based digital oscilloscope (figure 2.16) which consists of a input box and separate memory boards installed into the slots inside a standard color graphics PC. The input box has 8 total analog input channels, each channel with its own BNC coaxial input plug and a switch which can be set to accept either direct current or alternating current inputs. The box basically serves as an analog-to-digital signal converter, that is, the it converts the DC charge amplifier output voltages into digital information understandable by the PC. The digital data are then delivered to the memory boards inside the PC which store up to 32 kilobytes of data per run for each channel.

Because the transducers only produce small amounts of charge relative to the compression placed on the piezo-electric crystals (approx. 1.0 pCb/psi), they must use high impedance coaxial cabling. Moisture degradation of the impedance (i.e. short circuiting) during the liquid runs with water was a constant problem. To enhance the moisture barrier, the cabling was double sealed with heat shrinkable tubing, and dried in a kiln overnight after every run. Fortunately, the vacuum pump oil exhibited no conducting

qualities and was the fluid of choice.

Another proposed method of data collection was through high speed motion picture photography with a 8000 max. pps (full frame) HYCAM movie camera. The high speed camera could have been used in the study of jet stability. To capture the consequences of the shock passage through the liquid jet array required very exact timing of the camera, lighting and shock initiation systems. Due to inabilities to manufacture the diaphragms to a sufficient tolerance, the initiation of the shock at the desired time using the two diaphragms was not achieved, and high speed photography was not accomplished. The allowable uncertainty in the time of shock initiation was approximately 0.5 seconds. The primary difficulty was in bursting the diaphragms which often did not burst at all.

2.3 Operational Procedures and Precautions

The use of high pressure gases and shock waves in experimentation requires adherence to operational procedures and precautionary measures to insure the safety of the personnel in the laboratory. The hazards in the LJAST experiment include the use of high pressure helium gas bottles, the threat of projectiles from experimental fragments and serious concussion and hearing loss if a shock is permitted to exit into the laboratory because of inadequate containment by the vessel. To avoid these dangers, three sets of procedures were used, one for preparations, one for operations, and one for shut down. Tables 2.3 through 2.5 list these procedures in detail.

Table 2.3. Procedures for LJUST preparation (cf. figure 2.4).

Step	Description
1	Opening the diaphragm assembly. This is achieved by loosening the large nuts on the diaphragm assembly flange studs, then pushing the shock tube, which is supported on rollers, away from the vessel about 10 cm. A pair of the studs must be removed to permit access to the space between the flanges, however, the 2 studs on top must remain in place to support the intermediate flange from falling.
2	Inserting the diaphragm(s). Either one or two diaphragms can be inserted between the flanges. If two diaphragms are being used, they are inserted one on either side of the intermediate flange. If only one diaphragm is being used, it is inserted in the space closer to the vessel. The diaphragms are placed on the small alignment pins (figure 2.6). The flanges are brought slowly together by tightening the nuts on the diaphragm flange studs. Some minor lifting of the intermediate flange is sometimes necessary for the alignment pins to match with their corresponding holes. The nuts require tightening to about 40 N-m (30 ft-lb _f) of torque.
3	Checking the security of the vessel lid and windows. Thirty-two bolts secure the pressure vessel lid to the vessel and eight bolts each secure the view ports.. The bolts should be tightened using 13.5 N-m (10 ft-lb _f) of torque.
4	Checking to see that drain valve (DV1) is closed. The valve at the bottom of the vessel should be closed. If it is not, then the valve handle is tightened until the valve is shut.
5	Checking the valve position indicator on the 2" pneumatic ball valve (BV1). The degree to which the ball valve is open when high pressure air is supplied to the pneumatic actuator can be preset by adjusting the limiter screws. A dial indicator on the valve face tells the angle to which the valve is open. Zero degrees (horizontal) indicates that the valve is closed and 90 degrees indicates a full open valve. For one atmosphere of driving head, the maximum open position should be about 50 degrees for water, and 70 degrees for oil. The valve can tested for the correct setting by supplying high pressure air to the actuator.
6	Evacuating the system. Both the vessel and the shock tube are usually evacuated together. Therefore to connect all the volumes, valves SV1 and SV2 are opened, and SV3 turned to the right so that the it connects with the vacuum line instead of the high pressure gas supply. Also VV2 must be opened. Using the mechanical vacuum pump to evacuate air at atmospheric pressure is a strain on the pump. To reduce the strain, VV1 (a 3-way valve) is switched over to the house vacuum which can evacuate the vessel to about 3 psia. When the house vacuum can no longer lower the vessel pressure, VV1 is switched over to the vacuum pump and the vacuum pump turned on.

Table 2.3. Procedures for LJUST preparation (continued).

7	Priming the pipe (Liquid runs only). If liquid jets are to be used, the 3" main PVC line must be primed in order to minimize the air trapped inside the pipe which is delivered into the vessel with the liquid. This is accomplished by applying suction to the priming line (figure 2.4). The most convenient method is to connect the priming line to the drain valve DV1 and then open DV1 for a brief period of time and then shut it when the 3" main line is primed. A small amount (< 4 liters) of liquid can be inadvertently sucked into the vessel with no concern.
8	Flushing and re-evacuating (Helium runs only) . The goal of evacuating the air in the shock tube is to lower the remaining air partial pressure such that it represents a negligible fraction of the total gas and therefore has negligible impact on the gas dynamics. (For air-to-air shocks, simply evacuate the vessel and shock tube to the desired level.) For helium-to-air shocks, both the shock tube and intermediate volume must be evacuated before the helium is added. To insure that the vessel also has a negligible fraction of impurity gas, the vessel must be evacuated, flushed with helium or water vapor (i.e. water) and then re-evacuated (sometimes more than once) to insure that the air partial pressure is less than 0.1%.
9	Closing valves. After the completion of evacuation, valves VV1, VV2, SV1 and SV2 are closed.

Table 2.4. Procedures for LJUST Operations.

Step	Description
1	Initializing the data acquisition system. The data acquisition system includes the PC, transducer amplifiers and control box. The transducer amplifiers require 5 to 10 minutes to warm up to a completely steady output and are therefore activated in advance. The software program on the PC which controls the R1000 unit is called "scope." It has a windowing graphical user interface with pull-down menus accessed by a mouse. The program is initiated by typing "scope" and then the data acquisition system configured to single-shot mode and 500 kHz sampling rate. The data acquisition system constantly samples data at the user specified sampling rate, but it does not store these data into the memory board until the system is triggered by a detected voltage spike (i.e. a shock). The trigger is user definable and the number of pre-trigger as well as post-trigger data points can be specified as long as the data stream is continuous and does not exceed 32,000 data points. For the experiments done here, the trigger was set to digital mode and the discrimination voltage set to 130 mV which is a reasonable level above noise. 5,000 pre-trigger data points and 27,000 post-trigger data were stored. Once these parameters are set, hitting the space bar causes the system to begin waiting for a trigger. Once an event is detected which triggers the system, the system stores the data until the memory boards are full and then terminates storage.

Table 2.4. Procedures for LJAST Operations (continued).

- 2 Activating the control timer (liquid runs only). A control timer box activates the valves and camera power and lighting in the following order: EV1 for the air supply on BV1; delay 2.4 seconds; high speed camera power (high speed movies only); no delay; activate camera lighting; delay 0.4 seconds and then open EV2 (double diaphragm runs only). If using liquid, the necessary electric solenoid valves (EV1 and EV2) as well as any photographic cameras and lighting must be plugged into the appropriately labeled sockets behind the control box.
 - 3 Pressurizing the shock tube. To gradually stress the diaphragms, the shock tube pressurization occurs at no more than 100psi/min. Two pressure regulators determine the maximum pressures in both the intermediate section and the main shock tube. If running with only one diaphragm, the primary regulator from the main driver gas source will need to have a higher pressure setting than the burst pressure of the diaphragm. In double-diaphragm mode, the regulator for shock tube is set to the driver pressure and the regulator on the intermediate section is set to half the driver pressure. Before pressurization begins, some piece of shielding about the size of one square meter (e.g. a sheet of metal or a wood board) must be found to protect against the unlikely event of projectiles. The shielding is placed between the head/body and the vessel glass ports. In both single diaphragm mode and double diaphragm mode, SV1 and SV2 are opened. Then the driver gas supply is opened and SV3 is switched over just enough to the left so that driver gas begins to pressurize the system slowly. In single diaphragm mode, the pressurization is stopped (turning SV3 vertical) 10% before the expected burst pressure. For double-diaphragm mode, pressurization is stopped when the pressure reaches the desired level. Then, the driver gas supply should be closed and valves (SV1 and SV2) need to be shut off.
 - 4 Starting the shock. In single diaphragm mode, two people are needed, one person to press the actuator button on the control box which begins the liquid flow (liquid runs only) and one person to open SV3 all the way to the left. The second person should wait about 3 seconds before turning SV3's knob all the way to the left to allow smooth jet formation. For double diaphragm runs, pressing the start button on the control timer is all that is needed.
 - 5 Saving the data to disk. Once the shock has passed, and the data stored on the memory boards, they must be transferred to the disk. The file is saved in binary or ASCII. The ASCII format requires more disk space but permits the file to be transferred to other computer platforms such as a Sun workstation or a Macintosh computer.
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Table 2.5. Procedures for LJUST Shutdown.

Step	Description
1	Draining liquid from the vessel. (Liquid runs only) By pressurizing the vessel to approximately 10 psi above atmosphere (if the pressure is not already in excess of the this level), the liquid in the vessel can be quickly pumped out of the drain valve (DV1) and back into the 55 gallon drum. BV1 should be in the closed position. A high pressure air hose is attached at VV1. Air is added to the system until the pressure in the vessel is about 10 psi above atmosphere. This requires that the BV1 be closed. Then DV1 is opened and the liquid returned to the drum.
2	Removing the old diaphragms. When the draining is complete, open the diaphragm assembly and remove the old diaphragms which should now have petalled back. The 10 cm extent to which the shock tube can be moved back should be sufficient to remove a single diaphragm at a time.
3	Transducer maintenance. If using water as the liquid medium, the cables may require removal and baking after several runs because of impedance degradation. Oil does not cause this degradation. One can observe degradation when the voltage output signals drift quickly away from ground even though no signal is being measured. To remove the cables, one must first remove the 32 lid bolts and un-couple the union fitting above the ball valve (BV1). Re-installing is just the reverse of removal. Baking the cables at 150°C overnight is usually sufficient to return the impedance back to its original value.
4	Removing Debris. While the lid is off, there is opportunity to remove small pieces of aluminum and other diaphragm material which will inevitably break-off, be blown down the shock tube and fall to the bottom of the vessel. A wet-dry shop grade vacuum cleaner with a long extension is usually effective in removing these small pieces.
5	Inspecting the test section. The transparent sides of the test section should be inspected for evidence of fatigue, especially on the side where the transducers are mounted. A failure of the polycarbonate may result in major damage to cabling and the transducers.

Figure 2.1 Ablated surfaces of the first and second row of liquid jets in HYLIFE.

Figure 2.2. Computational grid used to estimate fraction of ablated mass remaining in the central cavity. All boundaries are impermeable unless specified otherwise.

Figure 2.3. Plot of mass fraction into and out of the central cavity as a function of time.

Figure 2.4. LJAST Overall Schematic.

Figure 2.5. LJAAT shock tube cross section.

Figure 2.6. LJAST Diaphragm Assembly.

Figure 2.7. Typical diaphragm petalled after being burst.

Figure 2.8. Diaphragm burst pressure vs. scribe depth for 0.032" thick 6061-T6 aluminum

Figure 2.9. LJUST Pressure Vessel.

Figure 2.10. LJUST Test Section.

Figure 2.11. Vertical cross-section view of the test section with press fit 0.95 cm (3/8") polycarbonate rods.

Figure 2.12. Round-to-square transition piece.

Figure 2.13. Liquid flow just above the orifice plate.

Figure 2.14a. Water jets at 2.5 m/s initial downward velocity after first flowing through a vertically aligned piece of aluminum honeycomb. Note that backlighting transmits brightly through jets. Shutter speed 1/1000sec.

Figure 2.14b. Water jets at 2.5 m/s initial downward velocity after first flowing through a vertically aligned tube bank. Note that surfaces of jets do not transmit as much light as in case (a). Shutter speed 1/1000sec.

Figure 2.14c. Water jets at 2.5 m/s initial downward velocity with no upstream flow straightening. Note the completely turbulent jets. Shutter speed 1/1000sec.

Note: A particle moving at 2.5 m/s moves 2.5 mm during a frame exposure thus blurring the image.

Figure 2.15. Miniature Piezo-electric Pressure Transducer and flush mount fittings.

3. NUMERICAL METHODS

3.1 Introduction

Most of the vapor which is ablated off of the HYLIFE reactor's inner jet surfaces in the first several tens of microseconds after fusion will combine in the central cavity, thermalize and then rebound toward the jet array. The rebounding blast will eventually vent through the blanket and then impact the first structural wall, delivering some stress to the wall. The liquid jets will also have some momentum imparted to them due to drag from the blast venting process. Since the blast vents from the central cavity out to the vessel wall, the momentum imparted to the liquid will give the liquid jets a net outward velocity. If the velocity of the jets is sufficiently large, they may impact the wall, delivering a second stress. To estimate the magnitudes of these stresses, ICF reactor designers need a method of predicting the gas dynamics behavior, first in the central cavity, then in the blast venting process.

Others have recognized the importance of gas dynamics in ICF reactors. Glenn [1980, 1982] investigated blast venting in the HYLIFE-I reactor using the AFTON-CF code. Peterson et al. [1988] investigated gas dynamics and radiation in ICF reactor chambers using the CONRAD code. Glenn [1980] and Peterson et al. [1988] used 1-D calculations for their estimates. One expects the flow during ICF blast venting reactor to be highly geometry-dependent, and hence, one cannot expect one-dimensional analysis for gas dynamics to be adequate. Recognizing this, Glenn [1982] performed a 2-D calculation. However, his calculation still did not consider the complex boundaries presented by specific jet geometry inside the HYLIFE reactor. His use of the quasi-steady channel flow approximation for the effect of viscosity is not appropriate for such rapid transients.

This chapter discusses in detail the numerical method known as the second-order Godunov [1961] finite difference method. The method incorporates a number of features such as van Leer limiting [1979] to discern numerically between shocks (i.e. discontinuities) and smooth regions of flow (i.e. continuous first derivatives); operator splitting [Strang, 1968] to permit the use of one-dimensional operators in a two-dimensional scheme, and the Riemann shock tube solution outlined in chapter 1. The same numerical method is used by Chen [1992]. The method presented here also uses a straightforward technique for implementing complex boundary geometries in two dimensions. The goal of this work is to provide a tool for ICF blast venting analysis. Comparison with the LJAST experiments data (chapter 4) provides a partial validation of the computational method.

3.2 Simplifying Assumptions

The actual problem in ICF is very complex in both the phenomena involved and the multidimensional behavior. This investigation studies the blast venting as a separate effect (i.e. some important phenomena of the ICF case are omitted from consideration). The basic assumption is that the gas may be assumed to experience isentropic state changes everywhere except in shock waves, which are treated as discontinuities. The work here makes other several simplifying assumptions. First, it is assumed that the gas behaves as an ideal gas with a constant ratio of specific heats (γ). For the comparisons with the LJAST experiment, this assumption is acceptable since it uses helium and air as the driver gases to produce the shocks at modest temperatures and pressures. One does not expect the gas behavior to deviate far from ideal. In ICF, the gas will consist of ablated, partially ionized vapor from the surface of the jet blanket, and therefore, the equation of state of the vapor will vary from that of an ideal gas. Chen et al. [1992] used a real gas equation of state for the HYLIFE inner cavity calculations, and the same technique used by Chen can be used here. However, the combination of extremely

complex geometries and a real gas equation of state used for these computations makes the numerical method computationally too demanding for the current generation of computer hardware. The deviation from ideal gas due to real gas effects is difficult to assess without implementing the real gas equation of state for the HYLIFE problem. This is left for future work.

The second assumption is that the blast venting occurs on a time scale too short for liquid motion, and any objects such as liquid jets or slabs are rigid in the flow field. This assumes that the liquid jets have sufficient inertia which prevents the liquid from either moving or deforming significantly at the early times of the venting process, hence no work is done on the liquid (i.e. the gas loses no energy to the liquid).

The third assumption is that the gas is adiabatic, and therefore there are no energy sinks in the system. In gas dynamics the main phenomena are the motion of compression waves and mass convection. The characteristic times scales for this to occur defined by L/c where L is the characteristic dimension of the system and c is the characteristic speed of travel of compression waves, which is roughly the sound speed. Diffusive processes as caused by thermal diffusivity have characteristic times scales of L^2/α . The thermal diffusivity of gases in SI units are usually much less than unity ($\sim 10^{-7}$) while the sound speed is roughly ($10^2 \sim 10^3$ m/s). By inspection, for a characteristic system length of roughly 0.01 meter, the time scales for heat diffusion effects are about 7 orders of magnitude greater than compressive processes. Hence, the time for heat transfer effects to take place is much longer than for gas dynamic effects. For this reason, we neglect diffusive processes such as heat conduction. One case where the scaling above may be flawed is at the vapor-liquid interface where the characteristic length scale (distance to the surface) is very small. Chapter 6 presents a method of assessing the effect of condensation and also an estimate of its effect in HYLIFE.

The last assumption is that the gas is inviscid. A similar argument can be presented as in the previous paragraph. The characteristic time scale for viscous effects is L^2/ν . For most gases, the kinematic viscosity is $\sim 10^{-4}$ in SI units. Hence viscous effects occur over times scales at least 3 orders of magnitude longer than time scales for gas dynamics. Although the scaling indicates that viscous effects are small in the vapor, the effect again at the vapor-liquid interface may be significant in causing boundary layer stripping. The process of stripping is assumed negligible by the assumption of immobile boundaries, but may in fact be an important effect in altering the boundary geometry and the surface area available for condensation. These effects are neglected here, but are important topics for further study.

3.3 Gas Dynamics Equations

Section (1.4.4) introduced the one-dimensional gas dynamics equations of inviscid, compressible flow. In conservative vector form, the equations are:

$$\frac{\partial U}{\partial t} + [\nabla \cdot F(U)]^T = 0 \quad (3.1)$$

where U is the matrix of conserved properties, which in two-dimensional Cartesian coordinates is:

$$U = (\rho, \rho u, \rho v, \rho E)^T \quad (3.2)$$

and $F(U)$ is the flux tensor,

$$F(U) = \begin{pmatrix} \rho u, p + \rho u^2, \rho uv, \rho uE + up \\ \rho v, \rho uv, p + \rho v^2, \rho vE + vp \end{pmatrix} \quad (3.3)$$

with ρ , the density, u , x -velocity, v , y -velocity, and p , pressure. The total energy, E , is equal to the sum of internal and kinetic energies and is given by:

$$E = \left(e + \frac{u^2 + v^2}{2} \right) \quad (3.4)$$

where e is the internal energy. The gradient is taken with respect to the x and y directions, then by inspection, equation (3.1) can be expanded to:

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ \rho u E + up \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v \\ \rho uv \\ p + \rho v^2 \\ \rho v E + vp \end{pmatrix} = 0 \quad (3.5)$$

Equation (3.5) represents the conservative form of the two-dimensional gas dynamics equations which will be evaluated numerically [LeVeque, 1990].

3.4 The Second Order Godunov Finite Difference Method in One Dimension

By inspection, equation (3.5) represents a non-linear hyperbolic system of equations [LeVeque, 1991]. These equations can be solved numerically using a finite difference technique known as the Godunov [1961] method. The method is an explicit, upwind, conservative, finite difference scheme based on a second-order extension developed by Colella and Glaz [1985]. For non-linear gas dynamics the Godunov method by far the best choice among all different schemes [LeVeque, 1990]. Like most schemes, the basic goal of Godunov's method is to evaluate the values of conserved physical quantities at a new time step - i.e. mass, momentum, and energy. Ordinary methods compute the new time value by interpolation of the previous time values in nearby nodes. The Godunov method, however, computes the *flux* at the edge between every pair of cells and then calculates the new time value by summing all the fluxes into and out of each cell and adding the net flux to the previous value. Figure 3.1 illustrates the 1-D discretized system being examined here. The average values of the conserved quantities are known at some time step n . The goal of the calculation is to evaluate the

values of conserved quantities at the new time step $n+1$. The flux across the cell edge between any pair of cells at $i\Delta x$ and $(i+1)\Delta x$ is computed from the gas dynamic properties at the cell edge located at $(i+1/2)\Delta x$. The cell edge gas dynamic properties are in turn derived from a special solution to the general Riemann problem at the same location (i.e. general case of the shock tube problem, Chapter 1). The Riemann problem considered here is comprised of the left and right states corresponding to the cells to the left and to the right of the edge, respectively. In essence, the Godunov method treats the difference in values across a pair of cells as a discontinuity.

Godunov's first-order method assumes that the profiles for the conserved quantities are uniform within the cell and constant during the time step. The second-order Godunov method improves on the first by assuming the distributions within each cell are piece-wise linear functions in space and time. Colella's second-order extension in 1-D of Godunov's first-order method contains four main steps: 1) spatial interpolation, 2) constructing time-centered left and right states, 3) solving the Riemann problem at cells edges and 4) computing fluxes and performing conservative differencing. The text in the sub-sections below describe each step in more detail.

3.4.1. Step 1 - Spatial Interpolation

Step (1) involves spatial interpolation of the conserved quantities in each cell. As mentioned above, Godunov's first-order method assumes that the distribution in each cell is constant. Assuming linear distributions inside each cell is sufficient to make the scheme second order accurate in space [LeVeque, 1990]. Spatial interpolation assigns a simple linear distribution according to the relationship:

$$q(x) = q_i^n + \left(\frac{x - x_i}{\Delta x_i} \right) \Delta q_i^n, \quad x_{i-1/2} < x < x_{i+1/2} \quad (3.6)$$

where q is a gas dynamics quantity needed for the Riemann problem, namely, either

density, velocity, or pressure. By inspection, equation (3.6) is just the slope-intercept method for computing the equation of a line. The value of Δq_i^n has a particular significance. If the initial data are relatively smooth, it is desirable to perform spatial interpolation. However, where there are shock discontinuities, spatial interpolation will generate numerical diffusion. The problem of numerical diffusion was solved by van Leer [1979] who proposed a logical test. In relatively smooth regions, one performs spatial interpolation, but where there are shocks, then no interpolation is done. That is, in smooth regions, the scheme is second-order, but at the shock fronts the scheme reverts back to first-order [van Leer, 1979]. van Leer's expression for this condition is often referred to as the van Leer flux limiter or just the van Leer limiter, and is given by:

$$\Delta q = \min \left(\frac{1}{2} |q_{i+1}^n - q_{i-1}^n|, 2|q_{i+1}^n - q_i^n|, 2|q_i^n - q_{i-1}^n| \right) \quad \text{if } (q_{i+1}^n - q_i^n)(q_i^n - q_{i-1}^n) > 0;$$

$$\quad \times \text{sign}(q_{i+1}^n - q_{i-1}^n)$$

$$= 0 \quad \text{otherwise.} \quad (3.7)$$

3.4.2. Step 2 - Computing Time Centered Left and Right States

Step (2) involves extrapolating in time to the half time step, the values of the conserved quantities at each cell edge. These values then become the inputs to the Riemann problem at the cell edges. Recall that in the previous section the spatial interpolation provides second-order accuracy in space. However, the scheme is still first order accurate in time since the time step is resolved only to first-order. To improve the scheme to second order accuracy in time, a higher-order time stepping method must be used [LeVeque 1990].

Colella and Glaz [1985] achieve second-order accuracy in time by extrapolating the values needed as inputs to the Riemann problem (i.e. ρ , u , and p) along characteristics to the half time step (figure 3.2). For any pair of cells i and $i+1$, the method developed by Colella and Glaz [1985] is:

$$V_{i+1/2,L}^{n+1/2}, V_{i+1/2,R}^{n+1/2} \quad [V = (\rho, u, p)^T] \quad (3.8)$$

$$\rho_{i+1/2,L}^{n+1/2} = (\tilde{\rho}_L^{-1} - \beta_L^0 - \beta_L^-)^{-1} \quad (3.9)$$

$$u_{i+1/2,L}^{n+1/2} = \tilde{u}_L - \beta_L^- C_i \quad (3.10)$$

$$p_{i+1/2,L}^{n+1/2} = \tilde{p}_L - \beta_L^- C_i^2 \quad (3.11)$$

$$\rho_{i+1/2,R}^{n+1/2} = (\tilde{\rho}_R^{-1} - \beta_R^0 - \beta_R^+)^{-1} \quad (3.12)$$

$$u_{i+1/2,R}^{n+1/2} = \tilde{u}_R + \beta_R^+ C_{i+1} \quad (3.13)$$

$$p_{i+1/2,R}^{n+1/2} = \tilde{p}_R + \beta_R^+ C_{i+1}^2 \quad (3.14)$$

where the β 's are defined:

$$\begin{aligned} \beta_L^- &= - \left(\Delta u_i - \frac{\Delta p_i}{C_i} \right) \frac{\Delta t}{2 \rho_i^n \Delta x_i} && \text{if } \lambda_i^- > 0 \\ &= 0 && \text{otherwise} \end{aligned} \quad (3.15)$$

$$\begin{aligned} \beta_R^+ &= - \left(\Delta u_{i+1} - \frac{\Delta p_{i+1}}{C_{i+1}} \right) \frac{\Delta t}{2 \rho_{i+1}^n \Delta x_{i+1}} && \text{if } \lambda_{i+1}^+ < 0 \\ &= 0 && \text{otherwise} \end{aligned} \quad (3.16)$$

$$\begin{aligned} \beta_L^0 &= - \left(\frac{\Delta p_i}{C_i^2} - \frac{\Delta \rho_i}{\tilde{\rho}_L \rho_L^0} \right) c_i \frac{\Delta t}{2 \Delta x_i} && \text{if } \lambda_i^0 > 0 \\ &= 0 && \text{otherwise} \end{aligned} \quad (3.17)$$

$$\begin{aligned} \beta_R^0 &= - \left(\frac{\Delta p_{i+1}}{C_{i+1}^2} - \frac{\Delta \rho_{i+1}}{\tilde{\rho}_R \rho_R^0} \right) c_{i+1} \frac{\Delta t}{2 \Delta x_{i+1}} && \text{if } \lambda_{i+1}^0 < 0 \\ &= 0 && \text{otherwise.} \end{aligned} \quad (3.18)$$

The $\Delta\rho$, Δu and Δp are computed using equation (3.7). One defines the ρ, u , and p 's on the left, right, or zero state as:

$$\tilde{q}_L = q_i^n + \frac{1}{2} \left(1 - \frac{\Delta t}{\Delta x_i} \min(\lambda_i^+, 0) \right) \Delta q_i \quad (3.19)$$

$$\tilde{q}_R = q_{i+1}^n - \frac{1}{2} \left(1 + \frac{\Delta t}{\Delta x_i} \min(\lambda_{i+1}^-, 0) \right) \Delta q_{i+1} \quad (3.20)$$

$$q_L^0 = q_i^n + \frac{1}{2} \left(1 - \frac{\Delta t}{\Delta x_i} u_i \right) \Delta q_i \quad (3.21)$$

$$q_R^0 = q_{i+1}^n - \frac{1}{2} \left(1 + \frac{\Delta t}{\Delta x_{i+1}} u_{i+1} \right) \Delta q_{i+1} \quad (3.22)$$

where q is one of the primary physical quantities ρ, u , or p ., small c the sound speed, and uppercase C the Lagrangian sound speed defined as ρc . The term C , the Lagrangian sound speed is a term used in computational fluid dynamics and does not have units of velocity. The lambda's specify characteristic speeds and are defined $\lambda^0_i = u_i$, $\lambda^-_i = u_i - c_i$, and $\lambda^+_i = u_i + c_i$.

3.4.3. Step 3 - Finding the Riemann Solution

Step (3) is finding the solution to the Riemann problem for the extrapolated left and right states. This requires an algorithm known as a Riemann solver. The solver computes the solution of characteristics in $x-t$ space which emerge as a result of interaction between initial left and right states. For an Eulerian frame calculation with fixed mesh, one chooses the solution in $x-t$ space corresponding to $x/t = 0$, the vertical characteristic. This gives the solution in physical space for the location of the physical boundary between each cell, i.e.: the solution to the Riemann problem provides the cell edge values for ρ^* , u^* , and p^* at $(x, t) = (i+1/2, n+1/2)$.

Recall from the Riemann problem in Chapter 1 that any interaction between a left and right state will result in a unique solution which falls into one of 4 categories (figure 1.6). The general Riemann solution determines the density, velocity and pressure distributions in $x-t$ space resulting from two originally discontinuous states. The solutions are centered-waves, either compression (shocks) or expansions (rarefactions) which emanate along characteristics from the original point of discontinuity. Typically, the solution consists of 3 separate sets of characteristics corresponding to 3 waves. The first is the $u+c$ wave, which represents the right moving wave, the u wave which represents the "density wave" or contact surface between the fluid in each cell, and lastly, the $u-c$ wave the left moving wave (figure 3.3). (Note: the contact surface is distinct because diffusive properties of gases are neglected in the model). Here, u is the particle velocity in the lab frame of the gas, and c is the sound speed in the gas.

Figure 3.3 shows the solution of the Riemann problem for the shock tube initial condition. The left-moving wave (between states U_L^* and U_L) is a rarefaction, and the right moving wave is a shock. In the general Riemann problem, either may be shock or rarefaction depending on the initial left and right states. The regions U_L^* and U_R^* in figure 3.3 have equal and uniform pressure, p^* and velocity, u^* , but different densities. The p^* and u^* comprise the unique intersection point of the two wave curves through U_L and U_R in the $p-u$ plane (figure 3.4).

The solution to the Riemann problem cannot be obtained in closed form for an ideal gas, and a numerical iteration is required [Colella and Glaz, 1985]. The basic method of the Riemann solver algorithm is to iterate for p^* and u^* . Van Leer [1979] suggests as a first guess, a weighted average guess pressure of the form:

$$p^* = \frac{p_L[\rho c]_R + p_R[\rho c]_L + \rho_L c_L \rho_R c_R (u_L - u_R)}{\rho_L c_L + \rho_R c_R} \quad (3.23)$$

From the guess pressure one can compute left and right states of velocity. However, the relationship for velocity depends whether the resulting solution will be a shock or rarefaction. A shock exists when the pressure p^* is greater than the reference initial state pressure, and a rarefaction exists when p^* is less than the reference initial state pressure. The equations for the velocities based on pressure are given by [Colella, 1991]:

$$u_L^* = u_L - (p^* - p_L) / w_L \quad \text{if } p^* > p_L \quad (3.24)$$

$$= u_L + \frac{2(c_L - \sqrt{\gamma(p_L / \rho_L^\gamma)[p^* / (p_L / \rho_L^\gamma)]^{(\gamma-1)/\gamma}}}{\gamma - 1} \quad \text{if } p^* < p_L \quad (3.25)$$

$$u_R^* = u_R - (p^* - p_R) / w_R \quad \text{if } p^* > p_R \quad (3.26)$$

$$= u_R + \frac{2(c_R - \sqrt{\gamma(p_R / \rho_R^\gamma)[p^* / (p_R / \rho_R^\gamma)]^{(\gamma-1)/\gamma}}}{\gamma - 1} \quad \text{if } p^* < p_R \quad (3.27)$$

where w is the mass flux for a shock as is given by:

$$w(p) = \sqrt{\mathcal{M}_0 \rho_0 \frac{1 + (\gamma + 1)}{2\gamma(p - p_0) / p_0}} \quad (3.28)$$

The density also depends on whether the solution to p^* specifies a shock or rarefaction. Colella [1991] expresses the equations for density as specific volumes, i.e.:

$$\tau_L^* = (1 / \rho)_L = 1 / \rho_L - (p^* - p_L) / w_L^2 \quad \text{if } p^* > p_L \quad (3.29)$$

$$\tau_L^* = (1 / \rho)_L = \left[\frac{p^*}{p_L / \rho_L^\gamma} \right]^{-1/\gamma} \quad \text{if } p^* < p_L \quad (3.30)$$

$$\tau_R^* = (1 / \rho)_R = 1 / \rho_R - (p^* - p_R) / w_R^2 \quad \text{if } p^* > p_R \quad (3.31)$$

$$\tau_R^* = (1 / \rho)_R = \left[\frac{p^*}{p_R / \rho_R^\gamma} \right]^{-1/\gamma} \quad \text{if } p^* < p_R \quad (3.32)$$

Convergence of p^* and u^* employs the Newton iteration method by van Leer

[1979]. The Newton method estimates the first derivative of p^* with respect to u^* . Depending on whether the wave will be a shock or a rarefaction, van Leer [1979] specifies:

$$Z_L = \frac{(\rho_L c_L) + w_L^2}{2w_L^3} \quad \text{if } p^* > p_R \quad (3.33)$$

$$Z_L = \frac{\tau_L^*}{c_L^*} \quad \text{if } p^* < p_R \quad (3.34)$$

$$Z_R = \frac{(\rho_R c_R) + w_R^2}{2w_R^3} \quad \text{if } p^* > p_R \quad (3.35)$$

$$Z_R = \frac{\tau_R^*}{c_R^*} \quad \text{if } p^* < p_R \quad (3.36)$$

where Z_s is equal to $|dp^*/du^*|$ and c is the sound speed and is given by:

$$c_s = \sqrt{\gamma \frac{p_s}{\rho_s}} \quad \text{and} \quad c_s^* = \sqrt{\gamma p^* \tau_s^*}. \quad (3.37)$$

The subscript s represents either L or R . The new guess pressure is determined by:

$$p_{new}^* = p_{old}^* + \frac{(u_L^* - u_R^*)}{Z_L + Z_R} \quad (3.38)$$

When p_{new}^* is equal to p_{old}^* or u_L^* is equal to u_R^* within some small error $\epsilon = 10^{-6}$ in absolute units, the solution is said to have converged. The final velocity is chosen as the average of the two left and right velocities:

$$u^* = \frac{u_L^* + u_R^*}{2} \quad (3.39)$$

Typically, the characteristics from three waves solutions in $x-t$ space divide the solution space into six separate zones: denoted by L , $-$, $*L$, $*R$, $+$ and R as shown figure 3.5. The λ 's represent slopes dx/dt . The superscript "+" represents the right traveling

wave, the "-" represents the left wave, and the "0" represents the density wave. Each zone has a different state U . If the wave traveling to the right is a shock, then both the λ_R^+ and λ_L^+ characteristics are the same and there will be no "+" zone. Similarly if the left traveling wave is a shock, λ_L^- and λ_R^- will be the same and there will be no "-" zone. If either solution is a rarefaction, then each set of λ_L and λ_R characteristics represents the bounds of the rarefaction fan represented by the "-" or "+" zones. The equations for the left traveling wave characteristics are [Colella 1991]:

$$\lambda_L^- = u_L - c_L \quad \text{if } p^* < p_L \quad (3.40)$$

$$\lambda_L^- = u_L - w_L / \rho_L \quad \text{if } p^* > p_L \quad (3.41)$$

$$\lambda_L^- = u^* - c_L^* \quad \text{if } p^* < p_L \quad (3.42)$$

$$\lambda_L^- = u_L - w_L / \rho_L \quad \text{if } p^* > p_L \quad (3.43)$$

Similarly for the right traveling wave characteristics:

$$\lambda_L^+ = u^* + c_R^* \quad \text{if } p^* < p_R \quad (3.44)$$

$$\lambda_L^+ = u_R + w_R / \rho_R \quad \text{if } p^* > p_R \quad (3.45)$$

$$\lambda_R^+ = u_R + c_R \quad \text{if } p^* < p_R \quad (3.46)$$

$$\lambda_R^+ = u_R + w_R / \rho_R \quad \text{if } p^* > p_R \quad (3.47)$$

The values of density, velocity and pressure will vary depending on where in x - t space one chooses the solution. For the location in x - t space, it is sufficient to specify the slope (x/t) because all of the characteristics are straight rays emanating from $x = 0$. For a given (x/t) the following equations and conditions are used to obtain the physical space solution [Colella, 1991]:

$$\rho^* = \rho_L, u^* = u_L, p^* = p_L \quad \text{if } \lambda_L^- \geq \left(\frac{x}{t}\right) \quad (3.48)$$

$$\rho^* = \left[\frac{\left[\frac{(\gamma-1)}{(\gamma+1)} \left(u_L + \frac{2c_L}{(\gamma-1)} \right) \right]^2}{\gamma \frac{p_L}{\rho_L^\gamma}} \right]^{1/(\gamma-1)}, \quad u^* = \frac{(\gamma-1)}{(\gamma+1)} \left(u_L + \frac{2c_L}{(\gamma-1)} \right)$$

$$p^* = \frac{\rho^* \left[\frac{(\gamma-1)}{(\gamma+1)} \left(u_L + \frac{2c_L}{(\gamma-1)} \right) \right]^2}{\gamma} \quad \text{if } \lambda_R^- \geq \left(\frac{x}{t}\right) \text{ and } \lambda_L^- < \left(\frac{x}{t}\right) \quad (3.49)$$

$$\rho^* = \frac{1}{\tau_L^*}, u^* = u^*, p^* = p^* \quad \text{if } u^* \geq \left(\frac{x}{t}\right) \text{ and } \lambda_R^- < \left(\frac{x}{t}\right) \quad (3.50)$$

$$\rho^* = \frac{1}{\tau_R^*}, u^* = u^*, p^* = p^* \quad \text{if } \lambda_L^+ \geq \left(\frac{x}{t}\right) \text{ and } u^* < \left(\frac{x}{t}\right) \quad (3.51)$$

$$\rho^* = \left[\frac{\left[\frac{(\gamma-1)}{(\gamma+1)} \left(u_R - \frac{2c_R}{(\gamma-1)} \right) \right]^2}{\gamma \frac{p_R}{\rho_R^\gamma}} \right]^{1/(\gamma-1)}, \quad u^* = \frac{(\gamma-1)}{(\gamma+1)} \left(u_R + \frac{2c_R}{(\gamma-1)} \right)$$

$$p^* = \frac{\rho^* \left[\frac{(\gamma-1)}{(\gamma+1)} \left(u_R + \frac{2c_R}{(\gamma-1)} \right) \right]^2}{\gamma} \quad \text{if } \lambda_R^+ \geq \left(\frac{x}{t}\right) \text{ and } \lambda_L^+ < \left(\frac{x}{t}\right) \quad (3.52)$$

$$\rho^* = \rho_R, u^* = u_R, p^* = p_R \quad \text{if } \lambda_R^+ < \left(\frac{x}{t}\right). \quad (3.53)$$

For the Godunov method in an Eulerian grid, $x/t = 0$, which, by inspection chooses the solution at $x = 0$, the cell edge.

3.4.4. Step 4 - Computing Fluxes and Finite Difference

Step (4) involves the calculation of fluxes and conservative differencing to obtain

values for density, velocity and energy at the new time. Once the values of density, velocity and pressure along the $x/t=0$ characteristics are known, the flux across the cell edge $i+1/2$ according to equation (3.5) is given by:

$$F_{i+1/2}^{n+1/2} = \begin{pmatrix} \rho_{i+1/2}^{n+1/2} u_{i+1/2}^{n+1/2} \\ \rho_{i+1/2}^{n+1/2} (u_{i+1/2}^{n+1/2})^2 + p_{i+1/2}^{n+1/2} \\ \rho_{i+1/2}^{n+1/2} u_{i+1/2}^{n+1/2} \left(\frac{\mathcal{P}_{i+1/2}^{n+1/2}}{(\gamma-1)\rho_{i+1/2}^{n+1/2}} + \frac{(u_{i+1/2}^{n+1/2})^2}{2} \right) \end{pmatrix} \quad (3.54)$$

The superscript $n+1/2$ denotes a time-centered quantity and the subscript $i+1/2$ (or $i-1/2$) represents the right (or left) cell edge. A simple finite difference gives the conserved quantities at the new time step according to:

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x_i} (F_{i-1/2}^{n+1/2} - F_{i+1/2}^{n+1/2}) \quad (3.55)$$

By inspection, the method just outlined above is completely explicit, that is, all values at the new time-step are computed from information at the current time-step. In addition, the conservative differencing in equation (3.55) is strictly based on the difference in flux between adjacent cells. The stability criterion will therefore require that in any time-step, the physical quantities carried on the characteristics in any arbitrary cell be permitted to advect to no more than the next adjacent cell. The maximum speed at which the characteristics advect information will be at the sound speed in the local medium. In an Eulerian (i.e. fixed-laboratory) frame, this speed translates into particle velocity in the fixed laboratory frame plus the sound speed where the particle velocity may be either positive or negative. The stability condition can be expressed by the Courant-Friedrichs-Lewy (CFL) [1928] condition, which specifies that all nodes must satisfy the conditions:

$$|\mu - c| \frac{\Delta t}{\Delta x} \leq 1, \quad |\mu + c| \frac{\Delta t}{\Delta x} \leq 1 \quad (3.56)$$

The terms on the left of the inequalities in equation (3.56) are often referred to as Courant or CFL numbers. Because the grid taken as a whole will most likely have velocities varying from zero to some maximum magnitude $|\mu \pm c|$ the CFL number will vary spatially. For the scheme considered here, the choice of CFL number is not crucial in terms of accuracy as long as it is less than or equal to one [Harten, 1983]. Using CFL numbers much smaller than unity increases the number of time steps to complete a calculation and therefore requires more computational time. However, using a CFL number too close to unity may also result in CFL violations in the multi-dimensional calculations to be discussed in the next section. For these two reasons, the work here uses CFL = 0.85. The time step is therefore determined by:

$$\Delta t = 0.85 \left(\frac{\Delta x}{\max(u \pm c)} \right) \quad (3.57)$$

3.5 Operator Splitting for Two-dimensional Calculation

For extension to two dimensions, the method uses Strang's [1968] technique of operator splitting. Operator splitting relies on the approximation:

$$\tilde{U}_{i,j}^* = U_{i,j}^n + \frac{\Delta t}{\Delta x_i} (F_{i-1/2,j}^x - F_{i+1/2,j}^x) \quad (3.58)$$

$$U_{i,j}^{n+1} \approx \tilde{U}_{i,j}^* + \frac{\Delta t}{\Delta y_j} (F_{i,j-1/2}^y - F_{i,j+1/2}^y) \quad (3.59)$$

where $\tilde{U}_{i,j}^*$ represents the intermediate solution obtained after differencing in one grid direction. In other words, for a single time-step, a sweep of the entire grid is first done in one direction -- the fluxes computed and conservatively differenced -- then a sweep is repeated in the other direction. However, this intuitively does not properly treat the

coupled derivative terms, which creates an error that grows with each time step.

Fortunately, Strang [1968] showed that in continuous (i.e. smooth, not shock) regions, if the original one-dimensional scheme was at least second-order accurate, then sweeping first in the x-direction then y-direction for one time step, and y-direction then x-direction for the next time step and thus alternating this way, maintains second-order accuracy. Strang began by considering a generic 2-D hyperbolic system of equations (such as Euler's equations) with a general form:

$$U_t = AU_x + BU_y, \quad U(0) = U_0 \quad (3.60)$$

where the subscripts t , x , and y imply taking the partial derivative, and the matrices A and B are symmetric but do not necessarily commute (i.e. AB not necessarily equals BA). Strang proposed the analogous second-order expression to the same equation:

$$U^{n+1} = S_{\Delta t} U^n \quad (3.61)$$

where the $S_{\Delta t}$ is a combination operator consisting of linear operators:

$$S_{\Delta t} = L_{\Delta t/2}^x L_{\Delta t}^y L_{\Delta t/2}^x \quad (3.62)$$

$L_{\Delta t}^x$, known as the Lax-Wendroff operator [Strang 1968], is given by:

$$L_{\Delta t}^x = \left(I + \Delta t A \partial_x + \frac{(\Delta t)^2}{2} A^2 \partial_x^2 \right). \quad (3.63)$$

where I is the identity matrix, Δt is the differential time step and ∂_x implies the partial derivative with respect to x . By inspection, $L_{\Delta t}^x$ is the second-order accurate equivalent to the 1-D problem. That is, the 1-D system of equations $U_t = AU_x$ has a second-order accurate solution given by $U^{n+1} = L_{\Delta t}^x U^n$. Strang showed, using Taylor series expansions of this operator, that first sweeping in a half time step, in the x-direction then a full time

step in the y-direction then another half time step in the x-direction maintained second order accuracy for the 2-D case. That is, he showed that if permitted to operate on the scalar f :

$$S_{\Delta t} f = \left(I + \frac{\Delta t}{2} A \partial_x + \frac{(\Delta t)^2}{8} A^2 \partial_x^2 \right) \left(I + \Delta t B \partial_y + \frac{(\Delta t)^2}{2} B^2 \partial_y^2 \right) \left(I + \frac{\Delta t}{2} A \partial_x + \frac{(\Delta t)^2}{8} A^2 \partial_x^2 \right) f \quad (3.64)$$

then the result after some algebraic manipulation is:

$$\begin{aligned} &\approx f + \Delta t (A f_x + B f_y) + \frac{(\Delta t)^2}{2} (A^2 f_{xx} + (AB + BA) f_{xy} + B^2 f_{yy}) + O(\Delta t^3) \\ &= f(t + \Delta t) + O(\Delta t^3) \end{aligned} \quad (3.65)$$

which is just the Taylor series expansion to second-order in time for f evaluated at the new time $t + \Delta t$. Because each operator is a linear operator, L^y can be expanded to include two half time steps without a change in the order of accuracy. That is:

$$S_{\Delta t} = L_{\Delta t/2}^x L_{\Delta t/2}^y L_{\Delta t/2}^x L_{\Delta t/2}^y \quad (3.66)$$

Similarly, increasing the time step size by a scalar factor of 2 has no effect on the second order accuracy, and therefore, one can express the solution:

$$U^{n+2} = S_{2\Delta t} U^n \quad (3.67)$$

where

$$S_{2\Delta t} = L_{\Delta t}^x L_{\Delta t}^y L_{\Delta t}^x L_{\Delta t}^y. \quad (3.68)$$

Equation (3.68) basically confirms that by first sweeping horizontally then vertically for one time step then alternating for the second time step, the scheme remains second order accuracy if the one-dimensional scheme was originally at least second order accurate. The only new requirement is that the time step be set constant for two complete

steps or *four* sweeps total. However, as stated above, the result in equation (3.68) is proved only for continuous smooth regions.

Where the initial data includes a discontinuity (i.e. shock fronts) the solution cannot be shown to converge to any other than first order. However, work by Crandall and Majda [1980] proved theoretically for weak shocks, that if the exact solution to the discontinuity is used in the solution process (i.e. the Riemann solver) then the operator-split solution converges to the 2D weak wave solution which has only an error which is third order in space with the Rankine-Hugoniot relations for the shock solution. This theory provided hope that accurate numerical methods could be developed for strong shock problems in 2D. Work by Glaz, Colella, Glass and Deschaumbault [1985] showed that indeed, it was possible to compute highly accurate solutions to strong shock problems with operator splitting.

The operator splitting technique requires some small modifications to the 1-D second-order method. The first modification is in the computation of flux at the cell edges (equation 3.54). In the 1-D formulation, there are no transverse velocity flux terms. However, in 2-D these must be included as written in equation (3.3). That is, the flux should now be written as:

$$F_{i+1/2}^{x,n+1/2} = \begin{pmatrix} \rho_{i+1/2}^{n+1/2} u_{i+1/2}^{n+1/2} \\ \rho_{i+1/2}^{n+1/2} (u_{i+1/2}^{n+1/2})^2 + p_{i+1/2}^{n+1/2} \\ \rho_{i+1/2}^{n+1/2} u_{i+1/2}^{n+1/2} v_{i+1/2}^{n+1/2} \\ \rho_{i+1/2}^{n+1/2} u_{i+1/2}^{n+1/2} \left(\frac{\gamma p_{i+1/2}^{n+1/2}}{(\gamma-1)\rho_{i+1/2}^{n+1/2}} + \frac{(u_{i+1/2}^{n+1/2})^2 + (v_{i+1/2}^{n+1/2})^2}{2} \right) \end{pmatrix} \quad (3.69)$$

The transverse velocity, v , is assumed to be passively advected, i.e.: the gas dynamics in the current sweep direction does not affect velocity in the cross direction.

However, one still uses piece-wise linear interpolation and then extrapolation to the half time step to find the correct v at the cell edge. The choice of which v to choose will then depend on the Riemann solution to u^* at the characteristic $x/t = 0$. If u^* is negative, then v is being advected from the right. If u^* is positive, then v is being advected from the left. The method can be expressed by [Colella, 1991]:

$$\begin{aligned} v_{i+1/2}^{**+1/2} &= \bar{v}_L + \beta_L^i & \text{if } u^* \geq 0 \\ &= \bar{v}_R - \beta_R^i & \text{if } u^* < 0 \end{aligned} \quad (3.70)$$

where

$$\begin{aligned} \beta_L^i &= c_i \Delta v_i \frac{\Delta t}{2 \Delta x_i} & \text{if } u_i^* > 0 \\ &= 0 & \text{otherwise} \end{aligned} \quad (3.71)$$

and

$$\begin{aligned} \beta_R^i &= c_{i+1} \Delta v_{i+1} \frac{\Delta t}{2 \Delta x_{i+1}} & \text{if } u_{i+1}^* < 0 \\ &= 0 & \text{otherwise} \end{aligned} \quad (3.72)$$

By inspection, the second modification is just the addition of another conserved quantity in the final finite differencing. That is, the term ρv should be included in the vector U of equation (3.55). The last modification is to the CFL condition which should now become:

$$|u \pm c| \frac{\Delta t}{\Delta x} \leq 1 \quad \text{and} \quad |v \pm c| \frac{\Delta t}{\Delta x} \leq 1 \quad \text{for all cells.} \quad (3.73)$$

3.6 Boundary Condition Generation for a Uniform Cartesian Grid

The numerical algorithm here is applied to a uniform Cartesian grid. This has the advantage that the mathematical functions for complex boundaries are simple to approximate on the grid. One drawback however, is difficulties encountered if the

boundary surface is curved or at oblique angles to the x and y axes. Existing problems in many schemes have always been how to provide volume averaging within a cell while still considering issues of stability, accuracy, and if there are many boundary nodes, computational efficiency.

The text in this section presents methods for treating two types of boundaries. Chapter 6 will present a method for treating a third type. The first type is the open or free stream boundary, and the second is the impermeable boundary. The accuracy of these boundary conditions are benchmarked for accuracy against other computations as well as with experimental data. The results, given in Appendix B, show very good agreement.

3.6.1 The Open Boundary Condition

Open or free stream boundaries exist where fewer nodes are desired to reduce the computational effort. Inflow or outflow at an open boundary can be set by a forcing function at the boundary, or, to the free stream conditions in the boundary cell [van Leer, 1979]. For the free stream boundary condition, the flux at the boundary cell edge can be set equal to $F(U)$ for U inside the boundary cell. That is:

$$F_0^{n+1/2} = F(U_0^n) \quad (3.74)$$

where

$$U_0^n = U(\rho_0^n, u_0^n, v_0^n, p_0^n) \quad (3.75)$$

The subscript "0" represents the spatial index for the boundary cell.

3.6.2 The Impermeable Boundary Condition

An impermeable boundary, on the other hand, permits no flux to pass through normal to the surface. To satisfy this condition in Cartesian coordinates requires first, defining the nodes which lie adjacent to boundaries, second, defining a spatial angle for

each boundary node, and third, computing the Riemann solution such that the pressure and density correspond to a zero normal flux across the boundary.

The first step is defining boundaries. Cells which comprise the boundary must be labeled and assigned a reference angle θ , which is defined as the angle between the positive, x-axis and a normal vector into the boundary (figure 3.6). The method used here distinguishes between 3 classes of cells - normal interior gas cells, boundary gas cells, and null cells. For stability, the selection of points must be consistent such that any nodes included in the computation in one direction, must also be included in the computation in the other direction, i.e. boundary cells and interior gas cells, must be either boundary or gas cells in both the x- and y-directions. Conversely, any null cells, that is, cells inside a liquid which are not computed, must be null cells in both x- and y-directions. Note, however, that a boundary cell in the x-direction may be an interior cell in the y-direction and vice-versa. Operator splitting requires that the gas dynamics computation be updated in both directions according to the Strang splitting scheme to maintain accuracy. If one only updates in one direction of the sweep, then errors in the physical quantities at that node will grow with time. Appendix A provides sample subroutines which set boundaries for cylindrical objects and round or elliptical curves.

Modeling the zero-normal flux condition at the impermeable boundary employs a technique of *mirror imaging*. This technique utilizes the Riemann solver to predict the correct density and pressure for a shock or rarefaction contacting an impermeable surface. Gaydon and Hurlle [1963] explain the physics of shock reflection. A shock which impacts a rigid surface will stagnate and form a reflected shock which propagates back into the oncoming medium. However, within the reflected zone, the pressure and density will be higher while the velocity will go to zero relative to the surface. The analogous Riemann problem to this scenario is just the situation of two identical shocks approaching each other. Therefore this is the physical basis with which one applies the mirror

imaging technique.

One begins by creating an imaginary node opposite but directly adjacent to the boundary node, possessing the *same* density, tangential velocity and pressure, but *opposite* normal velocity. As with ordinary interior nodes, left and right states must be computed using time-centered differencing. However, by inspection, one can see that equations (3.6) through (3.14) when applied to 'mirrored' boundary nodes results in all the 2nd-order correction terms becoming zero, and the result is simply:

$$\rho_{0,L}^{n+1/2} = \rho_0^n \quad (3.76)$$

$$u_{norm0,L}^{n+1/2} = u_0^n \cos \theta_0^n + v_0^n \sin \theta_0^n \quad (3.77)$$

$$p_{0,L}^{n+1/2} = p_0^n \quad (3.78)$$

$$\rho_{0,R}^{n+1/2} = \rho_0^n \quad (3.79)$$

$$u_{norm0,R}^{n+1/2} = -u_{norm0,L}^{n+1/2} \quad (3.80)$$

$$p_{0,R}^{n+1/2} = p_0^n \quad (3.81)$$

These equations provide the inputs into the Riemann problem. The Riemann solver will iterate for the solution at $x/t = 0$ which, for the initial conditions in equations (3.76) through (3.81) can only be the zero-flux, zero-velocity solution at the boundary. The solution provides the correct higher pressure and density associated with the shock reflection layer, however, because the normal velocity is zero, no flux of mass or energy across the boundary can take place. The non-trivial tangential velocity at the boundary node:

$$u_{tan,0}^{n+1/2} = v_0^n \cos \theta_0^n - u_0^n \sin \theta_0^n \quad (3.82)$$

is decomposed back into x-y coordinates according to:

$$u^{*n+1/2}_0 = -u^{n+1/2}_{tan,0} \sin \theta_0^n \quad (3.83)$$

$$v^{*n+1/2}_0 = u^{n+1/2}_{tan,0} \cos \theta_0^n \quad (3.84)$$

and then all the properties inserted into equation (3.69) for the flux calculation and then final finite differencing. Conservative differencing is performed using equation (3.56) and operator splitting performed according to the Strang splitting technique in section 3.5.

An important note is that boundary nodes do not necessarily remain boundary nodes when the sweeping direction changes (e.g. a vertical wall appears as a boundary when sweeping in the x-direction but not the y-direction.) Also, the apparent angle of a boundary in one direction changes by $\pi/2$ when sweeping in the other direction.

3.8 The Transient Shockwave Upwind Numerical Analysis Method for ICF (TSUNAMI)

The methods outlines in sections 3.1 through 3.7 were written in a Fortran computer code and named the Transient Shockwave Upwind Numerical Analysⁱs Method for ICF or TSUNAMI code. The code as well as user reference, documentation and related boundary condition generating subroutines are given in the TSUNAMI Code section (Appendix A). The source code is maintained and updated at the University of California at Berkeley, Department of Nuclear Engineering in the Thermal Hydraulics Group. It can be obtained through UNIX electronic mail by sending a request to:

`tsunami@fusion.Nuc.Berkeley.EDU (128.32.142.96)`

One can also obtain more information by contacting the address or phone numbers below:

Department of Nuclear Engineering
Thermal Hydraulics Research Group
4118 Etcheverry Hall
University of California at Berkeley
Berkeley, CA 94720 USA
(510) 642-0421
(510) 643-9685 Fax

Figure 3.1. One dimensional discretized system for the Godunov method

Figure 3.2. Schematic representation of computing time centered left and right states as inputs into the Riemann problem.

Figure 3.3. Characteristic lines of the solution to the Riemann problem for the shock tube initial condition.

Figure 3.4 Wave curves and solution of the Riemann problem in the pressure-velocity plane [Colella and Glaz, 1985].

Figure 3.5 Representation of the possible set of characteristics in x - t space for the general Riemann problem which shows the division of the solution space into 6 zones.

Figure 3.6. Schematic representation of grid definition and nodalization of impermeable boundary cells. Shaded cells are boundary cells. Cells on the liquid side are null cells and not subject to computation.

4. COMPARISON OF EXPERIMENTAL AND NUMERICAL RESULTS

4.1 Introduction

The experiment provides an excellent benchmark for evaluating the accuracy of the TSUNAMI code. The interaction of shocks with the 48 hexagonally-packed jets is a complex multi-dimensional problem which will test the code's ability to predict shocks in complex geometries. The calculation simulates the jets as rigid cylinders and the flow is assumed independent of height. Four comparisons are presented below. The first three comparisons examine shock speed attenuation, transmitted shock pressure and wall loading by the initial gas shock as functions of Mach number. For these comparisons, the experimental data will come from two sets of runs, shocks impacting a solid cylindrical array using air as the driver gas, and shocks impacting a liquid jet array using helium as the driver gas. The experimental data are compared to TSUNAMI code calculations for various Mach number shocks. The fourth comparison examines the calculation's ability to estimate liquid velocity due to impulse delivered by the shock propagation. Lastly, this chapter discusses the velocity dependence of peak wall pressure in the LJUST experiment generated by liquid impact on the wall.

4.2 LJUST Experimental Diagnostics

The LJUST experimental data presented here focuses on two periods of time. The first period is from the arrival of the shock at the entrance to the test section to its impact on the vessel wall. Typically, the shock requires 200 to 500 microseconds to traverse the test section. The second period of time is from the beginning of liquid impact to the end of liquid impact. Typically, the liquid impact occurs between 1 ms to 3 ms after the gas shock. For the runs using solid rods, there is no liquid impact.

4.2.1. Typical Gas Shock and Liquid Impact Pressure Traces

The LJUST experiment has 5 pressure transducers located on the side of the test section and 3 on the vessel wall. Figure 4.1 shows a diagram of their locations and the distances between them. The transducers have a response time of 2 microseconds which coincides with the data acquisition system which acquires data at a 500 kHz sampling rate. Figure 4.2 shows a sketch of the typical outputs of the pressure vs. time curves at six recording positions. The transducers are labeled sequentially from A to F (figure 4.1).

For an experimentally generated shock (referred to as the 'primary shock'), transducer A, the first transducer to detect the shock, typically shows a sudden rise in pressure to a relatively constant pressure. The constant pressure at A corresponds to the theoretically constant pressure and velocity region behind the shock front (region 2 in figure 1.7). Several tens of microseconds later, the primary shock arrives at transducer B. The pressure at B rises at first to the same level as A, but within one to several microseconds, it rises again to several times the pressure at A and then drops to about two-thirds its maximum. The several times higher peak pressure at B corresponds to the shock reflecting off of the jet array. Part of the shock is transmitted and it arrives at transducer C several tens of microseconds later. Curiously, transducer C records two pressure peaks. The first is about 50% of the second, which is about half the maximum pressure at B. The shock propagates to transducers D and then E after several more tens of microseconds. The pressures at D and E are usually less than 10% of the maximum at B and exhibit small, multiple pressure peaks. The impact of the shock on the vessel wall at F is usually a factor of 2 to 3 higher than the pressures at D or E.

Figure 4.3 shows a typical LJUST pressure trace for liquid impact on the vessel wall. The transducer records 3 or 4 peaks. The pressure begins to rise about 1 to 2 ms after the shock first arrives at A. At approximately 2 ms, three to four large pressure

spikes arrive spaced several hundred microseconds apart. The pressure then decreases after about 4 ms. The peak pressure on the wall due to liquid is one the order of several MPa (several hundred psi).

4.2.3. LJUST Experimental Diagnostics

This section defines the variables and describes the analysis methods applied to the experimental data. The arrival time of the shock at a transducer is defined as the time when the measured pressure rises to half its peak value (figure 4.2 and figure 4.3). The arrival time of the primary shock at transducer A is t_A , transducer B, t_B , and so on. The experimentally measured shock speed is an average speed derived from the distance between two transducers divided by the differences in arrival time. For example, the incoming shock speed (between transducers A and B) has speed:

$$u_{AB} = \frac{x_B - x_A}{t_B - t_A} \quad (4.1)$$

The average Mach number of the primary shock between any two transducers is defined as the speed of the shock divided by the sound speed in the undisturbed gas. For example, the Mach number of the shock between A and B is given by:

$$M_{AB} = \frac{u_{AB}}{c_i} \quad (4.2)$$

where c_i is the sound speed, a constant which depends on the type of test gas used. Since the runs used either air or helium at room temperature (295 K), the sound speeds for both are computed simply from equation (1.14). For air, c_i is 344 m/s and for helium it is 1011 m/s.

One of the quantities used in the comparison between the experiment and calculation is the overall shock retardation coefficient which is defined as the difference between the entering Mach number of the shock and the exiting Mach number divided by

the entering Mach number, i.e.:

$$r = \frac{M_{AB} - M_{EF}}{M_{AB}}. \quad (4.3)$$

When the primary shock first reflects off of the cylinders, the pressure rises in the region between the jets and the reflected shock. For normal reflection off of a plane surface, Gaydon and Hurle [1963] give the analytical expression for reflected shock pressure ratio in an ideal gas as:

$$\frac{p_R}{p_2} = \frac{(3\gamma - 1)M_i^2 - 2(\gamma - 1)}{(\gamma - 1)M_i^2 + 2} \quad (4.4)$$

where p_R is the pressure in the reflected shock, p_2 , the pressure in the approaching shock, also equal to p_A , and M_i , the Mach number of the approaching shock, also equal to M_{AB} . Section 4.5.3 below examines the ratio of p_B/p_R (i.e. measured peak pressure at transducer B divided by predicted 1-D reflected shock pressure) and its dependence on approaching Mach number.

The impact pressure of shock driven liquids against a rigid surface raises concerns of waterhammer in ICF vessels. Therefore, another goal of the experiment is to find the relationship between impact velocity and the pressure exerted on the wall. The LJUST pressure transducers cannot directly measure the horizontal velocity of the liquid jets when they impact the vessel wall. However, the steps below provide an estimate.

Because transducer D's position coincides with the rear edge of the last jet (figure 4.1), the distance from the last row of jets to the vessel is equivalent to the distance from transducer D to transducer F or x_{DF} . The time for the jets to traverse x_{DF} is the absolute difference between the time when form drag sets the last row of jets into motion and the time the jets first impact the wall. Intuitively, the form drag begins to set the last row of jets into motion when the primary shock arrives at transducer D, i.e. t_D . Similarly, the

time the jets first impact the wall (t_w) coincides with the first pressure spike from liquid impact (figure 4.3). As with the other arrival times, t_w is taken at the mid-point of the pressure rise from the background pressure to its peak. Because the jet undergoes acceleration, the velocity is not constant. Here, the analysis requires an assumption about the physics of the jet acceleration. The TSUNAMI calculation provides a time-dependent net drag on the jets which is based on the assumption of rigid cylinders. The results in section 4.6 indicate that the drag on the cylinders results in roughly linear increase in velocity. Hence, for simplicity the jets are assumed to undergo constant acceleration a . Therefore, from simple physics:

$$x_{DF} = \frac{1}{2} a (t_w - t_D)^2. \quad (4.5)$$

For constant acceleration, the impact velocity, v_w , is equal to $a(t_w - t_D)$. Combining this with equation (4.5) and solving for v_w yields:

$$v_w = 2 \frac{x_{DF}}{t_w - t_D}. \quad (4.6)$$

4.3 LJUST Experimental Results

This section presents the primary LJUST experimental data used to compare with the TSUNAMI calculations in sections that follow. The first tables are test matrices which present the initial pressures for the air and the helium shock runs. The tables which follow provide arrival times, peak pressure and the liquid impact pressure data.

4.3.1. Test Matrix

Tables 4.1 through 4.2 tabulate the initial conditions used for two sets of runs. The first set of runs is for shocks in an air test gas impacting solid cylinders. For most of

these cases, the driver gas is also air. In several cases, marked with asterisks, the driver gas is helium, which generates a higher Mach number primary shock for the same diaphragm ratio [Gaydon and Hurle, 1963]. The second set of runs are for shocks in a helium test gas impacting liquid jets. The driver gas in these cases was all helium. The tables are listed by a reference run number which corresponds to an ascending order of Mach number.

Table 4.1. Text matrix for shocks in air impacting solid rod array.

Run Number	Theoretical Mach No.	p_4/p_1	p_1 [Pa]	p_4 [Pa]
1	1.033	1.16	1.01×10^5	1.17×10^5
2	1.068	1.36	1.01×10^5	1.38×10^5
3	1.049	1.25	8.27×10^4	1.03×10^5
4	1.068	1.36	2.27×10^4	3.10×10^4
5	1.150	1.92	8.61×10^4	1.65×10^5
6	1.160	2.00	2.76×10^4	5.51×10^4
7	1.165	2.04	1.01×10^5	2.07×10^5
8	1.173	2.11	1.01×10^5	2.14×10^5
9	1.181	2.18	3.79×10^4	8.27×10^4
10	1.209	2.44	3.10×10^4	7.58×10^4
11	1.218	2.52	1.01×10^5	2.55×10^5
12	1.244	2.80	5.65×10^4	1.58×10^5
13	1.267	3.04	3.86×10^4	1.17×10^5
14	1.278	3.18	4.55×10^4	1.45×10^5
15	1.295	3.39	1.93×10^4	6.55×10^4
16	1.323	3.75	1.10×10^4	4.13×10^4
17	1.392	4.81	3.58×10^4	1.72×10^5
18	1.417	5.26	1.93×10^4	1.01×10^5
19	1.416	5.24	2.89×10^4	1.52×10^5
20	1.455	6.00	3.45×10^3	2.07×10^4
21	1.464	6.20	1.44×10^4	8.96×10^4
22	1.583	9.19	1.10×10^4	1.01×10^5
23	1.803	18.57	9.65×10^3	1.79×10^5

24	1.964	30.00	8.96×10^3	2.69×10^5
25	2.389	105.00	1.38×10^3	1.45×10^5
26	2.410	111.43	2.41×10^3	2.69×10^5
*27	2.597	25.00	6.89×10^3	1.72×10^5
*28	2.617	25.81	2.14×10^4	5.51×10^5
29	2.938	525.00	2.76×10^2	1.45×10^5
*30	2.911	39.39	2.27×10^4	8.96×10^5
31	3.169	1055.56	6.20×10^2	6.55×10^5
*32	3.176	56.67	2.07×10^4	1.17×10^6
*33	3.272	64.52	2.14×10^4	1.38×10^6

*Helium driver gas used to drive shocks into air test gas.

Table 4.2. Text matrix for shocks in He impacting liquid jet array.

Run Number	Theoretical Mach No.	p_4/p_1	p_1 [Pa]	p_4 [Pa]
1	1.153	2.05	7.58×10^3	1.55×10^4
2	1.185	2.35	3.51×10^4	8.27×10^4
3	1.272	3.39	3.10×10^4	1.05×10^5
4	1.369	5.00	1.24×10^4	6.20×10^4
5	1.414	5.94	1.10×10^4	6.55×10^4
6	1.420	6.08	3.51×10^4	2.14×10^5
7	1.422	6.15	8.96×10^3	5.51×10^4
8	1.595	11.72	1.10×10^4	1.29×10^5
9	1.603	12.09	2.96×10^4	3.58×10^5
10	1.634	13.51	5.10×10^4	6.89×10^5
11	1.640	13.80	3.45×10^4	4.75×10^5
12	1.676	15.75	6.89×10^3	1.09×10^5
13	1.753	20.77	8.96×10^3	1.86×10^5
14	2.464	274.29	2.41×10^4	6.62×10^6

4.3.2. Arrival Time Data

Tables 4.3 and 4.4 list the arrival time data for the shocks corresponding to the runs listed in tables 4.1 and 4.2. All times are given in microseconds. The arrival of the

shock at transducer A triggers the data acquisition system. All other arrival times are given relative to t_A . The determination criteria for the shock arrival time was described above in section 4.2.3.

Table 4.3. Arrival time data for shocks in air impacting a solid rod array.

Run Number	Arrival Times [microseconds]					
	t_A	t_B	t_C	t_D	t_E	t_F
1	0	220	350	450	540	690
2	0	212	348	498	634	820
3	0	212	382	524	646	830
4	0	208	356	510	640	873
5	0	204	352	504	610	768
6	0	190	306	456	566	753
7	0	188	312	444	556	728
8	0	186	304	446	558	744
9	0	186	312	442	552	711
10	0	180	310	438	550	705
11	0	178	294	432	540	694
12	0	176	286	424	534	713
13	0	172	278	414	522	701
14	0	170	280	418	*	*
15	0	168	272	408	514	690
16	0	166	342	490	578	784
17	0	156	256	370	494	666
18	0	154	248	380	480	658
19	0	154	252	384	488	663
20	0	150	250	380	480	630
21	0	148	244	374	472	650
22	0	120	198	298	412	568
23	0	110	180	290	386	533
24	0	92	152	194	296	469
25	0	90	144	224	292	462
26	0	84	138	208	296	410
27	0	84	140	250	296	446
28	0	74	122	182	254	372
29	0	74	128	216	342	424
30	0	68	108	224	310	458
31	0	68	112	166	234	340
32	0	66	106	160	228	336
33	0	40	88	102	116	144

*data point not available

Table 4.4. Arrival time data for shocks in He impacting a liquid jet array.

Run Number	Arrival Times [microseconds]					
	t_A	t_B	t_C	t_D	t_E	t_F
1	0	64	102	111	146	201
2	0	62	108	132	168	228
3	0	58	90	134	186	255
4	0	54	96	128	166	234
5	0	52	78	118	156	210
6	0	52	91	134	176	245
7	0	52	112	*	436	*
8	0	46	76	110	148	206
9	0	46	88	114	152	210
10	0	45	79	109	141	189
11	0	45	80	106	139	189
12	0	44	72	104	134	184
13	0	42	72	106	146	205
14	0	30	48	72	104	151

4.3.3. Peak Shock Pressure Data

Tables 4.5 and 4.6 list the peak shock pressure corresponding to the runs listed in tables 4.1 and 4.2. Pressures are given in Pa. The peak pressure corresponds to the maximum pressure reached by the monotonically increasing pressure generated by the arrival of the shock (figure 4.2).

Table 4.5. Peak pressure data for shocks in air impacting a solid rod array.

Run Number	peak shock pressures [Pa]					
	P_A	P_B	P_C	P_D	P_E	P_F
1	1.05×10^5	1.05×10^5	1.05×10^5	1.05×10^5	1.11×10^5	1.19×10^5
2	1.30×10^5	1.41×10^5	1.36×10^5	1.16×10^5	1.19×10^5	1.46×10^5
3	9.37×10^4	1.02×10^5	8.96×10^4	7.58×10^4	7.86×10^4	9.51×10^4
4	2.62×10^4	4.41×10^4	1.10×10^4	2.21×10^4	1.65×10^4	4.48×10^4
5	1.20×10^5	1.45×10^5	1.12×10^5	1.03×10^5	1.02×10^5	1.41×10^5
6	3.86×10^4	7.30×10^4	1.52×10^4	3.17×10^4	2.76×10^4	4.31×10^4
7	1.44×10^5	1.72×10^5	1.12×10^5	1.19×10^5	1.25×10^5	1.70×10^5
8	1.45×10^5	1.83×10^5	1.36×10^5	1.25×10^5	1.25×10^5	1.75×10^5
9	5.51×10^4	7.72×10^4	4.13×10^4	4.55×10^4	4.82×10^4	6.82×10^4
10	4.82×10^4	8.68×10^4	2.07×10^4	3.31×10^4	2.62×10^4	7.58×10^4

11	1.59×10^5	2.06×10^5	1.15×10^5	1.26×10^5	1.26×10^5	1.87×10^5
12	9.03×10^4	1.25×10^5	8.48×10^4	6.55×10^4	6.55×10^4	1.00×10^5
13	6.55×10^4	9.17×10^4	6.00×10^4	4.48×10^4	4.34×10^4	6.82×10^4
14	7.86×10^4	1.45×10^5	2.76×10^4	1.79×10^4	*	*
15	3.45×10^4	6.75×10^4	3.31×10^4	1.24×10^4	1.10×10^4	3.96×10^4
16	2.07×10^4	4.55×10^4	8.27×10^3	1.79×10^4	1.65×10^4	2.93×10^4
17	7.51×10^4	1.19×10^5	7.24×10^4	3.79×10^4	4.62×10^4	7.17×10^4
18	4.13×10^4	7.17×10^4	2.34×10^4	2.07×10^4	2.48×10^4	4.07×10^4
19	6.27×10^4	9.85×10^4	6.00×10^4	3.51×10^4	3.79×10^4	5.79×10^4
20	8.27×10^3	4.82×10^4	4.13×10^3	1.93×10^4	1.79×10^4	3.45×10^4
21	3.38×10^4	6.68×10^4	1.86×10^4	1.72×10^4	1.72×10^4	3.55×10^4
22	2.76×10^4	6.34×10^4	2.62×10^4	8.27×10^3	8.27×10^3	1.03×10^4
23	3.51×10^4	6.41×10^4	2.41×10^4	2.27×10^4	2.41×10^4	3.38×10^4
24	3.79×10^4	7.65×10^4	2.69×10^4	2.55×10^4	2.41×10^4	3.72×10^4
25	9.65×10^3	3.03×10^4	4.13×10^3	1.38×10^3	2.76×10^3	1.21×10^4
26	1.58×10^4	4.34×10^4	1.17×10^4	1.03×10^4	1.03×10^4	1.83×10^4
27	5.44×10^4	6.68×10^4	5.86×10^4	5.17×10^4	5.17×10^4	5.38×10^4
28	1.72×10^5	5.57×10^5	1.03×10^5	6.13×10^4	7.51×10^4	2.20×10^5
29	2.76×10^3	1.24×10^4	1.38×10^3	1.38×10^3	1.38×10^3	3.45×10^3
30	2.15×10^5	3.68×10^5	1.10×10^5	5.79×10^4	1.21×10^5	3.22×10^5
31	6.89×10^3	3.31×10^4	4.13×10^3	1.38×10^3	1.38×10^3	1.03×10^4
32	2.38×10^5	1.05×10^6	1.14×10^5	7.24×10^4	7.24×10^4	3.67×10^5
33	2.65×10^5	8.92×10^5	1.34×10^5	8.61×10^4	7.24×10^4	4.31×10^5

*data point not available

Table 4.6. Peak pressure data for shocks in He impacting a liquid jet array.

Run Number	peak shock pressures [Pa]					
	p_A	p_B	p_C	p_D	p_E	p_F
1	1.03×10^4	1.25×10^4	5.31×10^4	1.45×10^4	1.52×10^4	2.69×10^4
2	5.31×10^4	8.06×10^4	2.55×10^4	2.55×10^4	2.55×10^4	8.06×10^4
3	5.51×10^4	7.99×10^4	2.48×10^4	8.20×10^3	6.89×10^3	2.34×10^4
4	2.55×10^4	3.93×10^4	2.55×10^4	1.86×10^4	1.86×10^4	4.62×10^4
5	2.07×10^4	3.72×10^4	1.24×10^4	*	9.65×10^3	*
6	2.48×10^4	4.34×10^4	1.58×10^4	3.45×10^3	3.45×10^3	8.96×10^3
7	7.99×10^4	1.35×10^5	1.79×10^4	2.76×10^4	3.03×10^4	5.41×10^4
8	3.17×10^4	5.93×10^4	6.89×10^3	4.82×10^5	4.13×10^3	1.52×10^4

9	8.75×10^4	1.56×10^5	7.37×10^4	2.55×10^4	1.86×10^4	7.37×10^4
10	1.07×10^5	1.85×10^5	3.82×10^4	3.10×10^4	3.31×10^4	6.41×10^4
11	1.58×10^5	4.20×10^5	2.14×10^5	8.89×10^4	8.89×10^4	1.23×10^5
12	2.24×10^4	4.17×10^4	1.55×10^4	7.24×10^3	5.86×10^3	1.55×10^4
13	3.17×10^4	5.03×10^4	2.21×10^4	4.82×10^3	4.82×10^3	1.55×10^4
14	1.79×10^5	5.65×10^5	3.72×10^5	4.13×10^4	4.13×10^4	2.07×10^5

*data point not available

4.3.4. Liquid Impact Data

Table 4.7 lists the arrival time of the first large pressure spike due to liquid impact and the maximum magnitude of pressure detected on the vessel wall during the liquid impact duration (figure 4.3). The data correspond to the same runs used with the shocks in helium impacting liquid jets.

Table 4.7. Wall impact arrival times and peak pressure data.

Run no.	t_w [ms]	p_{wmax} [Pa]
1	1.93	5.51×10^6
2	2.32	6.62×10^6
3	1.70	4.41×10^6
4	2.49	4.24×10^6
5	*	*
6	2.90	2.03×10^6
7	3.13	1.58×10^6
8	2.60	2.17×10^6
9	2.88	4.24×10^6
10	3.16	3.24×10^6
11	3.46	2.10×10^6
12	3.08	2.83×10^6
13	2.00	5.38×10^6
14	1.40	4.20×10^6

*data point not available

4.4 Numerical Modeling of the LJUST Experiment

Section 4.4 presents the specific details of the initial conditions and mesh generation methods used to model the LJUST Experiment.

4.4.1. Grid Set-up and Initial Conditions for Numerical Calculation

The TSUNAMI simulation of LJUST uses a 600 x 100 uniform sized mesh to approximate the last 60 cm of the shock tube (figure 4.1). The calculation is Eulerian and two-dimensional, examining only the horizontal plane (x - y) and assuming no dependence on the vertical direction. The cell dimension, Δx , is 9.495×10^{-5} m. From here on, x is defined as the length dimension and y the width dimension. The left half of the computational grid (300 cells) models a 30 cm section of the shock tube and the remaining portion models the 30 cm test section (the shock is assumed to move from left to right). The code models all 48 cylinders, each 10 cells in diameter with 3 cells between cylinders to simulate the 1.3 pitch-to-diameter ratio necessary for a 50% packing fraction. The computational grid terminates on the right side against the vessel wall. The end of the physical LJUST test section is open and separated from the wall an average of 3 cm. Venting in this region is three dimensional since gas can escape both vertically and horizontally after stagnating against the vessel wall. The TSUNAMI simulation neglects the three-dimension effects and the vessel wall curvature and models this region as a flat wall with 3 cm openings on each side (figure 4.1). As in the LJUST experiment, simulated cylinders are placed hexagonally packed array near the middle of the test section.

4.4.2. Initial conditions

Modeling the entire shock interaction from the initial diaphragm burst requires simulating the first several hundred microseconds prior to the shock arriving at the test

section. Modeling the entire length of the shock tube requires over 2,400 cells in the x -direction. Both are computationally costly and unnecessary. One can reduce the required computational effort by, first, using the analytical solution to Riemann's shock tube problem (section 1.4.7) as the initial condition, and second, by using the open boundary condition (section 3.4.1).

Recall from section 1.4 that for the shock tube initial conditions, the solution comprises three waves which separate x - t space into four constant regions denoted as (1) the undisturbed low pressure medium ahead of the shock, (2) the region between the shock and the contact surface, (3) the region between the contact surface and the rarefaction fan, and (4) the undisturbed high pressure medium to the left of the rarefaction (figure 1.7). For any known initially discontinuous states (1) and (4), the solution to the Riemann shock tube problem provides the constant states in regions (2) and (3). By inspection using this solution for the initial condition can eliminate the need to simulate the duration prior to the shock's arrival at the test section.

For the calculations in this chapter, the initial conditions begin with the shock front of known Mach number M_1 at the first transducer location (transducer A) in the test section (figure 4.2). The interval of time which this shock has traveled is Δt_s , and is equal to the distance from the diaphragm to transducer A (1.10 m) divided by the shock speed, i.e.:

$$\Delta t_s = \frac{1.10 \text{ (m)}}{M_1 c_1 \text{ (m/s)}} \quad (4.7)$$

where c_1 is the sound speed in region 1. The gas to the right of the shock (region 1) is assumed to be a stationary, ideal gas (either air or helium) at 17500 Pa (2.54 psia) pressure and 295 K temperature. Behind the shock front (region 2), equations (1.44) and (1.45) provide density and pressure in according to:

$$\rho_2 = \rho_1 \frac{(\gamma + 1)M_1^2}{(\gamma - 1)M_1^2 + 2} \quad (1.44)$$

$$p_2 = p_1 \frac{2\gamma M_1^2 - (\gamma - 1)}{\gamma + 1} \quad (1.45)$$

Equation (1.42) provides the particle velocity u_2 as a function of pressure ratio p_2/p_1 . Combining with (1.44) yields:

$$u_2 = \frac{2}{\gamma + 1} c_1 \left(M_1 - \frac{1}{M_1} \right) \quad (4.8)$$

Region 3 is the constant state to the left of the contact surface. The pressure and velocity are constant across the contact surface so $u_3 = u_2$, and $p_3 = p_2$. The contact surface therefore moves at the same velocity as the particle velocity in region 2. This places the position of the contact surface at a distance $(M_1 c_1 - u_2) \Delta t$, to the left of the shock front. The density to the left of the contact surface, ρ_3 , follows the isentropic flow relationships for expansion of gas from region 4. Hence, calculating the region 3 density requires the region 4 properties. One obtains the region 4 properties from the diaphragm pressure ratio (p_4/p_1) relationship in equation (1.59). Here, the driver gas in region 4 is assumed to be the same type of gas as in region 1 and also at 295 K. Combining equations (1.10), (1.44) and (1.59) and solving for ρ_3 as a function Mach number yields:

$$\rho_3 = \rho_4 \frac{p_3^{1/\gamma}}{p_2 \left[1 - \frac{\gamma - 1}{\gamma + 1} \left(M_1 - \frac{1}{M_1} \right) \right]^{\frac{2}{\gamma - 1}}} \quad (4.9)$$

To limit the size of the computational grid, the left hand boundary is made an open or free stream boundary [van Leer, 1979] (section 3.4.1). The choice of 600 cells in the x -direction is sufficiently long to model regions 1, 2 and 3 for Mach numbers in air or helium from 1 to 5. By inspection, this exempts the driver gas region from the

computational domain and reduces the computational domain and effort by 75%.

4.4.3. Numerical Diagnostics

Like the actual experiment, the TSUNAMI simulation of LJUST places pressure transducers on the test section side wall and vessel wall to record the transient pressure traces (figure 4.1). In addition, the code can record the density map of the entire flow field, the form drag over each cylinder, the impulse delivered to the cylinder and the pressure distribution on the back wall. The density map of the flow field is used for flow visualization and animation. The form drag and impulse are used to predict the velocity the jets attain, and the pressure distribution on the vessel wall records the non-uniformity of the impacting shock. One computes the form drag in the x -direction by integrating the directed pressure over the surface of the cylinder, i.e.:

$$\text{form drag} = D_k = \int_{S_k} p \hat{r} \cdot \hat{n} dS_k = \sum_{i,j} p_{i,j} \Delta A_{i,j} \cos \theta_{i,j} \quad (4.10)$$

where p is the pressure, $\hat{r}$ the x -direction unit vector, $\hat{n}$ the unit normal vector into the surface, S_k is the total surface area for cylinder k , the vector $\Delta A_{i,j}$ the discretized area at cell i,j and θ the angle the normal into the surface makes with the positive x -axis. The form drag is given for a unit height cylinder. By inspection, for a uniform integer grid, $\Delta A_{i,j} \cos \theta_{i,j}$ is just Δx for $\cos \theta$ positive and $-\Delta x$ for $\cos \theta$ negative. Therefore, one needs only to sum the pressures on all nodes with the respective signs to obtain the net form drag in the x -direction. Note, however, the drag component in the x -direction is not necessarily the maximum since the y -direction form drag is not necessarily zero. However, the information of interest is the velocity of the liquid in the x -direction which is the component normal to the vessel wall.

With the x -direction drag force known for each jet, the impulse per unit height delivered to the jet comes from the time integration of the drag, i.e.:

$$I_k = \sum_{n=0}^N D_k^n \Delta t^n. \quad (4.11)$$

where n is the number of the time step. The velocity a jet obtains if all the impulse is converted to liquid momentum is given by:

$$v_k = \frac{I_k}{\rho \pi r_o^2}. \quad (4.12)$$

for a jet of radius r_o .

4.4.4. LJUST Simulation Parameters

The TSUNAMI code calculations here simulate the LJUST shock interaction for a duration of 2 ms. Time for execution of the program per run was approximately 4 days on a Sun Microsystems Sparcstation 2. The simulations use air and helium. The properties of the materials are given in table 4.8. The initial background pressure was 17.5 kPa for all runs, and the Mach number was varied between 1.1 and 4.0. Table 4.9 gives the test cases run for the numerical simulation as functions of gas and Mach number.

Table 4.8. Gas Properties used in LJUST code calculation.

Property	Air	He
Molecular Wt.	0.029 kg/mole	0.004 kg/mole
gamma (c_p/c_v)	1.40	1.667
Initial temperature	295 K	295 K
Sound speed	344 m/s	1011 m/s
Initial pressure	17500 Pa	17500 Pa

Table 4.9. LJUST simulation test matrix.

Mach Number	Air	He
1.1	x	x
1.25	x	x

1.5	x	x
1.677		x
1.75	x	x
2.0	x	x
2.5	x	x
3.0	x	x
3.2	x	
3.5	x	x
4.0	x	

4.5. Comparison between LJUST and TSUNAMI

This section presents the comparison of the LJUST experimental results and the TSUNAMI computations. The first comparison is a qualitative comparison between the computed pressure-time curves and the experimental data. The next three are quantitative comparisons of shock speed attenuation, shock reflection strength and wall impact pressure.

4.5.1 Comparing Transducer Output Traces

Figure 4.4 shows a comparison between pressure vs. time curves between the LJUST experiment and the TSUNAMI calculation. The case is for a Mach 3.2 shock approaching the array of 48 jets. The LJUST experiment used liquid jets in this case. Both the computed results and the experimental curves are typical of those sketched in figure 4.2. One notable point in the computed pressure trace is the pressure detected at transducer B which rises to the pressure level at A, then suddenly rises again when the shock reflection occurs off of the surface of the cylinders. This appears as a distinct kink near the based of the transducer B curve. The corresponding experimental curve also exhibits this phenomenon, but the kink is not as well defined. However, the experimental curve for transducer B still shows an initially steep rise to the same pressure as at

transducer A, and then an even steeper rise to the maximum pressure at B. The two microsecond rise time needed for the transducer to respond to sudden changes is the likely cause for the experimental pressure trace having less definition. The subsequent trend for the pressure drop at transducer B from 100 to 225 microseconds is qualitatively similar.

Another notable point is the prediction by the code of unexpected double peaks at transducer C. The code predicts a separate, smaller magnitude pressure spike will arrive first at transducer C followed by a larger spike several microseconds later. The experimental results also record the same phenomenon. The TSUNAMI code also predicts smaller pressure shocks which arrive at transducers D, and E. These qualitatively match the decreasing pressure magnitude behavior seen in the experiment. By inspection, the experimental and computed arrival times and the pressure magnitudes in figure 4.4 for this case of a Mach 3.2 shock agree well quantitatively as well as qualitatively. The next section compares quantitatively various aspects of the shock velocity and pressure for various Mach numbers.

4.5.2 Comparison of Shock Speed Attenuation

Figures 4.5 and 4.6 show the plots of shock retardation (r) versus initial Mach number. Figure 4.5 compares computed results against experimentally obtained data for the shocks into air impacting a solid rod array, and figure 4.6 compares the results for shocks into helium for a liquid jet array. The shock retardation coefficient is defined by equation (4.3). The reduced data for both the experimental and numerical data are provide in Appendix D. The experiments have a variety of values for p_1 and p_4 giving different Mach numbers. Kawamura and Kawada [1957] show that shock retardation and shock reflection can be both non-dimensionalized relative to shock pressure ratio and therefore Mach number. The experimental data here are therefore also assumed to

depend on Mach number only. Both figures 4.5 and 4.6 show the trend of greater shock retardation for greater Mach number. The computed results in figure 4.5 agree well with the solid rod experimental results while the experimental data and the computed results are less well correlated for the liquid jet runs.

One notable feature in figures 4.5 and 4.6 is the lack of linearity and monotonicity in the second derivative of the TSUNAMI computed retardation curves. This observation is especially true for the helium runs. The retardation coefficient is computed solely from the shock arrival time at fixed positions in the test sections. If a change in Mach number can generate a spatial variation in the pressure distribution of the shock front, then this may provide an explanation for the observation. Figure 4.7 shows a series of grey scale images of the TSUNAMI computed density distributions in the gas. The shock propagation generates a highly chaotic, multi-dimensional flow inside the jet array as well as behind the array. Figure 4.8 shows the computed plot of the pressure distribution along the rear wall 20 microseconds after the arrival of the shock at transducer F for Mach numbers 1.25 and 1.5 in air. The curves confirm that the pressure distribution is spatially non-uniform, and varies considerably for the two different Mach number cases.

4.5.3 Comparison of Shock Reflection Off of the First Row of Jets

The next comparison examines the Mach number dependence of shock reflection off of the first row of jets. The primary shock which first passes transducer A and then impacts the jets immediately after passing transducer B generates a reflected shock pressure, p_B . Analytically, the pressure behind a normal reflected shock, p_R , is given by one-dimensional gas dynamics in equation (4.4). The ratio p_B/p_R is shown in figures 4.9 and 4.10, for the air and helium runs, respectively. The reduced data for both the experimental and numerical data are provide in Appendix D. Both sets of experimental data in figures 4.9 and 4.10 show the trend of lower p_B/p_R ratio for Mach number

increasing from 1 to 2. The TSUNAMI computed values show the same trend. The runs using shocks in air impacting solid rods (figure 4.9) show a fair agreement in the range from Mach number 2 to 4. The TSUNAMI computed results for helium shocks impacting the cylinder array appears to over-predict the reflected pressure above Mach 1.5. The experimental data suggests that the reflected pressure ratio is lower for liquid jets than for solid rods as the Mach number increases. This leads one to speculate that with the liquid jets, the higher Mach number shocks have a great ability to deform the liquid and therefore clear a path for the flow, thus reducing the peak reflected pressure relative to ideal normal shock reflection.

In figure 4.9, the TSUNAMI calculation demonstrates its ability to predict another unexpected result. Intuitively, the one-dimensional normal shock reflection from a plane surface should yield the a higher shock reflected pressure than a surface which has multiple openings that permit part of the primary shock to be transmitted. Therefore in all cases, one expects that the ratio p_B/p_R will be less than 1. For the most of the experimental and computed results, this is the case. However, in some of the lower Mach number shock cases for the shocks in air, the experimental data indicates that p_B/p_R is actually greater than 1 (figure 4.9). The TSUNAMI calculations predict the same unexpected effect, although over estimating p_B/p_R by about 15% in the range from Mach 1.1 to 1.5.

4.5.4 Comparison of Gas Shock Wall Pressure

The final comparison examines the wall pressure due to gas shock impact and its dependence on Mach number. The data are normalized against the incoming shock pressure p_A . Figure 4.11 shows the comparison between experiment and TSUNAMI for the air shocks on solid rods, and figure 4.12 shows the comparisons for helium shocks on liquid jets. The reduced data are given in Appendix D. The experimental data for the air

shocks impacting solid rods (figure 4.11) indicate that p_{wall}/p_A is roughly 1.2 between Mach number 1.1 and 2.0. After Mach 2.0, p_{wall}/p_A slowly rises to 1.5 at Mach number of 3. The TSUNAMI calculations predict a non-linear variation for p_{wall}/p_A versus Mach number which is roughly within 20% of the experimental values in the range of Mach number from 1.1 to 2.0. Experimental data points lie above and below the computed result. However, beyond Mach number of 2.0, the code over-predicts the p_{wall}/p_A ratio by approximately 20% above the average data. A possible cause may be three-dimensional effects. In the experiment, the shock which impacts the wall can vent out from the top and bottom and not just the sides of the test section. The code, being only two-dimensional models only permits the shock to vent from the sides.

In the runs with helium shocks impacting liquid jets (figure 4.12), the TSUNAMI code appears to always over-predict the experimental data. The code predicts a p_{wall}/p_A ratio roughly 2 to 3 times higher than the experiment. This result indicates a significant difference between shocks on solid rods and shocks on liquid jets. One might speculate that the additional pressure attenuation is caused by liquid motion and surface stripping which may cause greater attenuation of the shock pressure as it traverses the jet array. Also, there is some transfer of momentum and kinetic energy to the liquid, thus changing the gas dynamics. For 1 cm diameter jets, the effect is approximately a factor of 2 to factor of 3 reduction in the TSUNAMI predicted gas shock pressure. The dependence on jet diameter size is unknown and may be an important effect. That effect was not explored here. however, it may be important and is worthy of future study.

4.6 Liquid Impact on the Vessel Wall

The impact of liquid on the vessel raises concerns about waterhammer damage. One of the goals of the LJUST experiment is therefore to examine the characteristic impact pressure and its relationship with liquid velocity.

4.6.1. Stagnation Pressure of Liquid on the Vessel Wall

There are two limiting cases. For the first case, flow in pipes, the instantaneous arrest of liquid will generate waterhammer pressures according to the Joukowsky relationship [Rust, 1979]:

$$\Delta p = \rho c \Delta u. \quad (4.13)$$

where Δp is the pressure rise, ρ the density of the liquid, c the sound speed in the liquid and Δu the change in velocity of the liquid. In the second case, the impact of cylindrical jets against a vessel may be like the stagnation of liquid according to Bernoulli's relationship:

$$p_2 - p_1 = \frac{\rho(u_1^2 - u_2^2)}{2}. \quad (4.14)$$

where the subscripts 1 and 2 indicate the initial and final state. By inspection, the Joukowsky relationship for waterhammer yields a much higher and less desirable impact stress than Bernoulli's relationship due to the influence of the liquid sound speed in the Joukowsky relationship.

Figure 4.13 plots the peak pressure measured on the vessel versus the predicted velocity of the liquid jets. Table 4.7 lists the data for the calculation. The liquid velocity is determined by equation (4.6). Appendix D contains the lists for all the data reduction. The liquid in these runs was mechanical vacuum pump oil with a specific gravity of 0.9 relative to water. Figure 4.13 also plots the curve for the Bernoulli pressure relationship. The graph confirms that the impact of the liquid jet array on the wall generates a pressure which follows the Bernoulli stagnation relationship and not the Joukowsky waterhammer relationship.

4.6.2. Liquid Impulse delivered to the Jets.

As discussed in section 4.4.3, the TSUNAMI code computes a velocity of the liquid based on the computed form drag (equation 4.12). The accuracy of this computed velocity will depend on the validity of the code's assumption of stationary geometry. This section compares the calculation with two specific experimental cases where liquid impacts the wall. In one case, a Mach 3.20 in air shock impacts water jets and in the second case, a Mach 1.677 shock in helium impacts oil jets. Table 4.10 provides the experimental data. The liquid impact velocity in table 4.10 is derived from equation (4.6). The TSUNAMI code initial conditions were arranged identically to the experiment and a 2 ms duration simulated. The code computes the velocity of each of the 48 jets using equation (4.12), then sums and averages the velocity for the whole array. This provides the computed average array velocity as a function of time. Figure 4.14 shows a plot of the predicted average velocity of the liquid jet array as a function of time for the Mach 3.2 case. The code predicts that the velocity is close to 100 m/s after 2 ms. The experimentally obtained value is 100.6 m/s after 2.31 ms. Using linear extrapolation, then the velocity at 2.31 ms is roughly 115 m/s, or about 15% faster than the experimental value. Figure 4.15 shows the same plot of average predicted velocity versus time, but for the Mach 1.677 case. The velocity after 2 ms is approximately 60 m/s. However, experimentally, the impact of the liquid on the wall does not occur until 3.08 ms. By inspection the plot in figure 4.15 is roughly linear over the entire period. Linear extrapolation predicts a velocity of 90 m/s at 3 ms. This is about 20% faster than the experimentally obtained velocity of 72 m/s.

Table 4.10. Two cases of liquid impact data.

Mach No.	p_l [Pa]	p_s [Pa]	t_D [ms]	t_{wall} [ms]
*3.2	1.75×10^4	1.02×10^6	0.18	2.31
1.677	6.85×10^3	1.08×10^5	0.10	3.08

In both cases, the TSUNAMI code over-predicts the velocity of the liquid. Intuitively, this result is expected since the TSUNAMI code assumes that the jets are stationary and therefore computes a higher differential velocity between the gas flow and the liquid which increases the form drag. However, the difference between the code calculation and the experimentally obtained value was shown in these two cases to be only 20%.

Figure 4.1. LJUST test section schematic.

Figure 4.2. Typical pressure transducer output for 6 transducer locations.

Figure 4.3. Typical pressure transducer output for liquid impact on the vessel wall.

Figure 4.4. Comparison of pressure transducer curves between experiment and calculation.

Figure 4.5. Plot of shock retardation (r) vs. Mach number for air shocks onto solid rods.

Figure 4.6. Plot of shock retardation (r) vs. Mach number for helium shock impacting a liquid jet array.

Fig. 4.7. Computed shock wave interaction with a jet array shown at 75 microsecond intervals. Grey-scale shows mass density with magnitude increasing from light to dark.

Figure 4.8. Plot of the TSUNAMI computed pressure distributions on the vessel wall at $t = 20$ microsec. after the shock contacts the wall for each case.

Figure 4.9. Plot of p_B/p_R ratio for air shocks impacting a solid rod array.

Figure 4.10. Plot of p_B/p_R ratio for helium shocks impacting a liquid jet array.

Figure 4.11. Plot of p_{wall}/p_A ratio for air shocks impacting a solid rod array.

Figure 4.12. Plot of p_{wall}/p_A ratio for helium shocks impacting a liquid jet array.

Figure 4.13. Plot of peak wall pressure vs. velocity of liquid impact.

Figure 4.14. Plot of computed average jet array velocity vs. time for a Mach 3.2 shock in air impacting the jet array.

Figure 4.15. Plot of computed average jet array velocity vs. for a Mach 1.677 shock in helium impacting the jet array.

5. APPLICATION OF THE NUMERICAL METHOD TO THE HYLIFE ICF REACTOR

5.1 Introduction

As mentioned in section 1.1, each deuterium-tritium (DT) fusion microexplosion releases either 1800 MJ or 350 MJ of energy depending on whether the concept is HYLIFE-I or -II, and the resulting radiation release may consist of about 68% neutrons, 16% xrays and 16% debris kinetic energies. Glenn [1982] as well as Chen et al. [1990] have studied the x-ray ablation phenomenon and made predictions of the inner cavity conditions prior to the blast contacting and venting through the blanket. The goal of this chapter is to present the TSUNAMI computational results for blast venting through blankets in the HYLIFE ICF reactor.

Figures 1.1, 1.2 and 1.4 in chapter 1 show the interiors of the HYLIFE reactor designs [Blink et. al 1980, Moir 1990]. The basic design concept includes an annular array of falling liquid jets or slabs surrounding a central cavity roughly 50 cm in radius. The liquid is either molten lithium (HYLIFE-I) or lithium fluoride-beryllium difluoride (Flibe, HYLIFE-II) salt.

The HYLIFE-I design uses a 50% packing fraction of 20 cm cylindrical jets. The jets are packed roughly in a hexagonal geometry, and the total blanket thickness, including the volume between jets is 1.6 meters. The required thickness is determined by the maximum neutron depositions per atom (dpa) that the vessel wall material can sustain during the 30 year reactor lifetime [Monsler and Meier, 1981]. The fall height from the orifice plate to the surface of the lithium pool at the bottom of the vessel is nominally 8 meters. This height is mostly determined by the repetition rate and jet injection velocity [Petzoldt 1991]. The objective is to replace the "older" liquid present at the prior shot with "fresher," colder liquid, for the current shot because the surfaces as well as interior

of the liquid will be heated. In general, a slower repetition rate allows a longer fall height and slower injection velocity. The vessel radius in HYLIFE-I is 5 meters.

The HYLIFE-II design considers two possible blanket geometries. The first is a 50% packing fraction, stationary, hexagonal array, as in HYLIFE-I, but using 5 cm diameter jets. The second is a 58% packing fraction of oscillating and stationary 7 cm thick slabs of Flibe spaced 5 cm apart. The total blanket thickness is approximately 1.0 meters. The actual liquid thickness is around 0.5 m, which is thinner than required in HYLIFE-I because Flibe has approximately twice the macroscopic neutron attenuation coefficient as lithium. The height from orifice plate to pool is only 2 meters to permit the higher repetition rate. The vessel radius is 3 meters.

5.2 Initial Conditions

Glenn [1980] was the first to study x-ray ablation and vapor generation in the HYLIFE reactor's inner cavity. Glenn's numerical analysis included a diffusion model for radiation transport, which incorporates opacity data for lithium. His study provided time-dependent profiles for density, velocity, pressure and temperature for the vapor mass up to the time just before expanding vapor re-contacts the blanket. For simplicity and comparison purposes, Glenn's calculated profiles were scaled, and used as the initial condition for gas dynamics analysis with TSUNAMI. Figure 5.1 shows the linearly approximated profiles of Glenn's inner cavity solution used as the initial conditions for HYLIFE-I and -II calculations. The scaling parameters were yield, mass evaporated, and ratio of specific heat (γ). Glenn calculated that in the central cavity, the distribution of ablated mass is concentrated in a dense band of material about 10 cm thick near the perimeter. The velocity, highest at the outer edge, decreases toward the center of the cavity. The pressure distribution is uniform up to the edge of the perimeter.

Glenn's analysis was one dimensional, that is, a cylindrical geometry with radial

symmetry and no axial dependence. Glenn placed approximately 63% of the total x-ray and debris energy into a 1 meter line source. The density in the outer band near the perimeter is 46 times the density in the interior. The outward velocity begins at zero in the center of the cavity and increases linearly with radius to about 18% of its maximum value at 15 cm radius. From 15 cm to 30 cm, the outward velocity increases linearly again, but with greater slope to its maximum value at 30 cm. Glenn divided the total energy up into approximately 92.3% in the gas internal energy and 5.7% in the kinetic energy. Appendix A provides the small computer program called "yield.f" used to scale Glenn's inner cavity profiles just prior to blanket contact. Chen [1992] later obtained distributions similar in shape for the mass and energy in his two-dimensional inner cavity calculations for HYLIFE-II. However, at the time these calculations were done, Chen's results were not yet available, and hence, all the calculations, including the HYLIFE-II, are based entirely on Glenn's initial data.

5.3 Geometries and Parameters Tested

The calculations use two basic geometries. The first geometry is a 1/4 section simulation of either a 3 or 5 meter radius vessel with a hexagonally packed array of 5 cm or 20 cm jets at 50% packing fraction (figure 5.2). The second geometry is a 1/2 section simulation of a 3 meter radius vessel with a slab array blanket (figure 5.3). To study the parametric effect of varying yield while holding initial vapor mass constant, four runs with the HYLIFE-I geometry were performed with yields varying from 600 MJ to 2700 MJ. In addition, to study the parametric effect of varying initial mass, four runs were performed with the HYLIFE-II slab geometry with initial density varying from 1.5 to 27 kg/m³ with yield and initial pressure held constant.

Table 5.1. Initial Conditions for Various Runs

HYLIFE-I Geometry

Yield	600, 1200, 1800, 2700 MJ
Max. Init. Density	23 kg/m ³
Vessel Radius	5 m
Blanket Geometry	Annular Jet Array
Packing Fraction	50%, 20 cm diam jets
Material	Lithium
Ratio of Specific Heats (γ)	1.67

HYLIFE-II

Yield	350 MJ
Max. Init. Density	1.5, 2.9, 14, 27 kg/m ³
Vessel Radius	3 m
Blanket Geometry	Annular Jet Array (1) Slab Array (2)
Packing Fraction	50% (1), 5cm diam. 58% (2), 7cm th. slabs
Material	Flibe
Ratio of Specific Heats (γ)	1.2

For HYLIFE-I, the duration simulated was 1000 microseconds which required about 4 days of computational effort on a Sun Microsystems Sparcstation 2™, workstation. For HYLIFE-II, the duration simulated was 250 microseconds for the cylindrical jet blanket geometry and 500 microseconds for the slab. These runs typically required 10 days for the cylindrical jet case, and 4 days for the slab case. Typically the grids used 600 x 600 nodes with the maximum at up to 1000 x 1000 nodes. The HYLIFE-I case modeled approximately 50 cylinders arranged in a hex-packed pattern in one-fourth of the reactor cavity. The HYLIFE-II cylinder case modeled over 350 cylinders. The slab case utilized only 38 objects in the flow field. Runs were performed using a workstation because the total active memory size for all arrays usually exceeded the maximum permitted on the local Cray supercomputer.

5.4 Effect of Blast Venting on Liquid Motion

One goal of the HYLIFE blast venting calculations is to predict the liquid velocity resulting from blast venting. The high speed vapor flow will exert both form drag and viscous drag on the liquid jets. Glenn [1980] showed that form drag is many orders of magnitude larger than viscous drag. Therefore, in these calculations, as in the LJUST calculation in chapter 4, only the form drag is considered. The drag on the jets is a force which will accelerate the liquid toward the first structural wall. The velocity of each jet outward in a radial direction results from the form drag integrated over each jet surface and summed over time. The sub-sections below discuss average liquid blanket velocity, wall loading due to liquid impact and the velocity obtained by different jets at different locations in the flow field.

5.4.1 Liquid Blanket Velocities

The calculation of the jet velocity for the HYLIFE jets uses the same method as in chapter 4 for the LJUST simulation. Namely, one sums the pressure distribution around the surface of the jets and derives a net outward radial force and acceleration. Integrating the net outward acceleration on the jet over time yields the velocity. Table 5.2 presents the peak and averaged velocities for the jets. The maximum liquid velocity in HYLIFE-I on the inner most jets is 830 m/s. In this case, the assumption of fixed grid is not appropriate. For the HYLIFE-II conditions, the maximum liquid velocity is more than an order of magnitude lower (80 m/s for the inner most cylinders). At this velocity, the assumption of fixed grid is still questionable because the jets will move 1.6 diameters and alter the blanket geometry significantly in 1 millisecond, which is the characteristic time required for more than half of the vapor to escape from the inner cavity. The velocity of the gas will depend on factors such as yield and mass ablated. Section 5.7 discusses this in more detail. The averaged velocity for the entire blanket is 280 m/s and 20 m/s

respectively for HYLIFE-I and -II cylinder cases, but only 1.0 m/s for the HYLIFE-II slab case. In the slab case, the assumption of fixed grid appears reasonable. The large difference lies in the different form drags between different shapes. The cylindrical jet geometry offers greater flow resistance providing more opportunity for the vapor to perform $p dv$ work on the liquid.

5.4.2 Liquid Impact Wall Loading

Two factors in FSW design are the peak wall pressure and the total impulse due to liquid impact. From the LJUST experimental data in chapter 4, for a given average liquid density ρ and velocity u , the peak, liquid-impact wall pressure is approximately the Bernoulli stagnation pressure, $\rho u^2/2$. The impulse delivered to the wall is just the momentum change in the liquid. In the HYLIFE-I case, liquid impacts the wall at 280 m/s imposing a peak pressure of 19 MPa (2750 psi) which repeats every 0.67 seconds due to the 1.5 Hz repetition rate. This presents a problem for the HYLIFE-I case because of a high damage potential. On the other hand, for the HYLIFE-II cylinder case, the expected pressure will only be 0.4 MPa from the impact of 20 m/s liquid. The slower outward velocity has another benefit. If the radial component of velocity is sufficiently slow, the liquid, which has some initial injection velocity, may fall into the pool below before impacting the FSW. This may imply that the design of the liquid recovery structure at the base of the vessel will need to consider the geometry of the blanket and where the blast venting will direct the liquid.

In the HYLIFE-II cylindrical jet geometry case the liquid will not reach the wall until 75 ms after the fusion micro-explosion. The repetition rate being 8 Hz requires that the old liquid clear the vessel every 125 ms. For a two meter fall height, this gives a minimum downward injection velocity of 16 m/s. This implies the liquid may fall more than half way to the pool before impacting the FSW. In the HYLIFE-II slab jet geometry

case, the average velocity is only 1 m/s. The liquid impacts the pool before it reaches the wall. The analysis here neglects any initial upward velocity. In the actual ICF system, the blast venting may impart an upward vertical velocity to some of the liquid.

Table 5.2. Momentum Transfer Results

HYLIFE-I (50% p.f. Lithium Jets)

Max Liq. Velocity	830 m/s
Avg. Liq. Velocity	280 m/s
Impulse of the liquid (per unit height)	8.5×10^5 N-s/m
Max. Wall Press. from Liq.	19 MPa

HYLIFE-II (50% p.f. Flibe Jets)

Max Liq. Velocity	80 m/s
Avg. Liq. Velocity	20 m/s
Impulse of the liquid (per unit height)	1.3×10^5 N-s/m
Max. Wall Press. from Liq.	0.4 MPa

HYLIFE-II (58% p.f. Flibe slabs)

Max Liq. Velocity	11 m/s
Avg. Liq. Velocity	1.0 m/s
Impulse of the liquid (per unit height)	6.4×10^3 N-s/m
Max. Wall Press. from Liq.	2 kPa

5.4.3 Comparison with Previous HYLIFE-I Estimate

The HYLIFE-I average liquid velocity results computed by TSUNAMI are over an order of magnitude larger than that first computed by Glenn who predicted a 14 m/s average velocity imparted to the liquid. The reason for such a large difference in results lies in a combination of two factors. Glenn [1980] included heat transfer in his one-dimensional model which he cited as providing the means to remove a considerable amount of energy from the gas. Glenn used Hilpert's [1933] correlation for heat transfer coefficient based on experiments using cylinders with air crossflow. He adapted Hilpert's

equation by using a different Prandtl number. Section 5.7 will discuss the parametric effects of yield which are quite strong, and indicate that if the liquid removes a considerable amount of energy from the gas, then the momentum transfer would also be reduced. However, chapter 6 will show condensation on jet surfaces to be a small effect which supports the use of the adiabatic approximation. However, condensation on liquid droplets will be much greater due to the larger surface area availability. Second, Glenn's use of drag coefficients based on steady-state flow may grossly underestimate the form drag subsequent to a shock reflection. Glenn himself cited the importance of Mach effects such as shock reflection and flow separation, which he did not include.

5.4.4. Phenomenon of Last Row Cylinders Receiving More Impulse

Supersonic flow separation, an inviscid phenomenon is unlike boundary layer flow separation, a viscous phenomenon. Supersonic flow over a cylinder generates a high frontal pressure where the gas initially stagnates. However, as the gas flows around the sides of the cylinder, it experiences a decreasing pressure gradient which accelerates the gas flow. The gas undergoes further expansion as it flows around the back side of the cylinder. The gas velocity is directed rearward and its inertia causes the majority of mass to separate away from the cylinder forming a small wake region behind the cylinder which has low velocity (figure 5.4). This region was referred to as the region of cavitation by Courant and Friedrichs [1948, pp 277]. The pressure in the expanded stream flowing behind the cylinder is much lower than in the front. This entrains mass from the wake region and generates a low density region behind the cylinder. Figure 5.5 shows the pressure distribution over an outer cylinder calculated in the HYLIFE.

One consequence of supersonic flow separation is that the last row of cylinders in the array will experience more drag than the cylinders just immediately inside. This phenomenon occurs because the inner cylinders have other cylinders positioned farther

out in radius which re-direct the flow of gas sufficiently so that flow separation lasts for only a brief time and then the pressure behind the jet builds and flow separation stops. The outer jets, however, do not benefit from this and will endure longer periods where flow separation occurs. For example, figure 5.6 compares pressure distribution curves for different cylinders at different times. The cylinders in front (3 through 5) experience form drag until about 400 microseconds. However, the outermost jet (cylinder 6) continues to experience higher differential in pressure between its front and back. Figure 5.7 shows the impulse of cylinders 1 through 6. Cylinder 1 receives all its impulse in the first 400 microseconds. The acceleration of cylinder 6 (as determined by the slope of the curve in figure 5.7) is greater than either cylinder 4 or 5 indicating that it will possess more impulse as a consequence of blast venting.

5.5. Blast Venting Flow Visualization

Figures 5.8, 5.9 and 5.10 show the grey-scale images for the blast venting simulations for HYLIFE-I, HYLIFE-II cylinder, and HYLIFE-II slab cases respectively. The images are those of logarithmic density, with white being the highest and black being the lowest. A numerical grey-scale ruler is provided at the base of each figure.

5.5.1. HYLIFE-I Simulation

One-quarter of the reactor vessel is modeled for the cylinder cases and one-half for the slab case. In the HYLIFE-I simulation, 54 cylinders approximately 20 cm in diameter are placed in a hex-packed pattern from an inner radius of 0.5 meters to 2.1 meters. The initial conditions are taken directly from Glenn [1980]. Glenn assumed that all the vapor implodes into the central cavity, which is a conservative assumption. From figure 5.8, the first frame at 0 microseconds shows a high density and high pressure mass just prior to contact with the inner jets. At 50 microseconds, the venting has proceeded 1 meter or approximately 3 to 4 rows into the array. The faces pointed toward the central

cavity of the first row of jets show bright white but the jets are trailed by dark zones, indicating high density and pressure on the front of these cylinders but low density and pressure behind. The result is high form drag. By 100 microseconds, the front of the blast has exited beyond the edge of the blanket. Because the initial internal energy of the ablated vapor is so high, the leading edge of the blast front, once clear of the blanket, travels at close to 45,000 m/s as it expands out toward the vessel wall. The blast front reaches the wall at 150 microseconds and begins to exert pressure. Section 5.7 examines the pressures on the wall for various cases. The picture at 150 microseconds shows venting is preferential in the direct lines of sight. These lines of sight, for the hex-packed geometry lie directly down and at 60 degrees azimuthal angle relative to the 0 degree axis in the graph (figure 5.2). Vapor expands out in these two directions and impacts the FSW first in these directions, thus creating another concern, asymmetric wall loading. This non-uniform loading will also be examined in the following sections. By 250 microseconds, relatively steady venting from the inner cavity has established and there are signs of sustained flow separation on many of the outer jets. The inner jets no longer show regions of high density in front and low density behind.

5.5.2. HYLIFE-II (Cylinder) Simulation

Figure 5.9 shows the density flow visualization for the HYLIFE-II cylinder case. Approximately 350 - 5 cm diameter jets are inside the one-quarter reactor. The initial conditions follow the same profiles as shown in figure 5.1, but use the code `yield.f` in Appendix A to scale the profiles proportional to the yield. The reactor cavity is 3 meters in radius. The blanket of hex-packed jets extends from 0.5 m radius to 1.5 meter radius. Initially, the venting is similar to the HYLIFE-I case. The yield in HYLIFE-II is only one fifth of that in HYLIFE-I, but mass evaporated will also be less because the x-ray attenuation of Flibe is greater and therefore the energy is concentrated in less mass. The mass shown is based on a conservative assumption by Moir [1990] of 8.8 kg evaporated.

Because Chen [1992] estimates only about 0.5 kg evaporated, calculations were also performed for 0.5, 1.0, and 5.0 kg of mass evaporated. These results are described further below in the parametric study. At 100 microseconds, the blast has emerged from the blanket. Once clear of the blanket, the blast front expands at close to 25,000 m/s. At 150 microseconds, the blast front has already contacted the wall and formed a small shock reflection. The blast is transported preferentially in the downward direction and not in at the 60 degrees degree azimuthal angle (figure 5.2). This is unreasonable in light of the result in HYLIFE-I where venting was preferential in both the downward and 60 degree directions.

The problem was traced back to the use of the too coarse of a grid. In order to accommodate over 300 cylinders in a grid of only 1000 x 1000 nodes, the cylinders were approximated by a pitch of 21 cells and diameter of 16 cells, leaving only 5 cells between cylinders. For the HYLIFE-I case, the ratio was 40 to 31 cells for pitch to diameter. Because the cylinders are centered on a uniform integer grid, the gap (i.e. number of cells) between cylinders can vary by as much as a single node or 20%. The error on the HYLIFE-I is smaller, but the flow is also observed to be preferred in the downward direction.

5.5.3. HYLIFE-II (Slab) Simulation

Figure 5.10 shows the density flow visualization for the HYLIFE-II slab case. The initial condition begins with the same initial condition as for the cylinder case. Thirty-seven slabs comprise the blanket. Thirty-one slabs make up the main blanket which form an inner cavity surrounded on three sides. On the left, two rows of relatively thick slabs shield the FSW but have gaps for the beam lines (figure 5.3). This design minimizes the solid angle through which fusion radiation can stream out. For simplicity, the calculation uses the same initial condition as in the HYLIFE-II cylinder condition.

From figure 5.10, it takes about 120 microseconds before the leading edge of the blast reaches the outer edge of the blanket. The velocities for the expanding blast for the slab case seem to be slower than the cylindrical jet case where the blast's leading edge exits in less than 100 microseconds. This result is at first counter to physical intuition because one might conclude that venting should occur more quickly in the slab geometry which exhibits less flow resistance. The leading edge of the blast however, moves faster through a smaller channel than a wider channel. This does not violate the gas dynamics relationships which state that subsonic flow accelerates and supersonic flow decelerates upon entering an area decrease [Liepmann and Roshko, 1957, p.52]. The original flow in the central cavity is supersonic prior to reaching the first row of jets. However, after stagnating on the jet surfaces, it now has become subsonic. The subsonic flow, upon entering a contraction, accelerates. Because of conservation of mass, the narrower the channel for the flow, the faster the velocity.

At 240 microseconds, the ablated vapor contacts the FSW. It has a velocity close to 13,000 m/s. At this time, the blast also reaches the inside of the beam port protection slabs to the left, and begins to vent through the beam slots in the slabs. In the central cavity, the high density layer of stagnated gas begins to form a complex density distribution as a result of the multiple shock reflections off of the individual slabs. By 300 microseconds, a relatively steady venting has been established. But now, venting through the beam slots in the slabs on the left is also underway and gives rise to concerns on how to protect the optics from these jets. The wall loading, described in more detail in the next section, is also very asymmetric.

5.6. Gas Shock Wall Loading

Table 5.3 provides the local, temporal maximum peak and the spatial peak average pressure on the FSW for the 3 difference HYLIFE cases. The local temporal

peak pressure is the absolute maximum pressure calculated during the duration simulated. The peak average pressure is the maximum pressure on the wall averaged over the surface. The HYLIFE-I case shows that the pressure reaches as high as 35 MPa (5100 psi) while the peak average pressure is only 5 MPa (730 psi). For the HYLIFE-II cylinder case, the time of calculation was insufficient to fully assess the peak wall pressures, but given the available results, the maximum and the average peak pressures were both approximately the same at 1 MPa (145 psi). For the HYLIFE-II slab case, the maximum peak and peak average pressures were 3 MPa (435 psi) and 1 MPa (145 psi) respectively. Both the HYLIFE-I and HYLIFE-II slab cases exhibited considerable asymmetry. These values represent cyclic stresses that occur at the fusion repetition rate.

Table 5.3. Gas Shock on FSW Results

HYLIFE-I (50% p.f. Lithium Jets, 1 ms duration)

Max. Wall Press. from Gas	35 MPa
Peak Avg. Wall Press. from Gas	5.0 MPa

HYLIFE-II (50% p.f. Flibe Jets - 250 μ sec.)

Max. Wall Press. from Gas	1.1 MPa
Peak Avg. Wall Press. from Gas	1.0 MPa

HYLIFE-II (58% p.f. Flibe slabs - 500 μ sec.)

Max. Wall Press. from Gas	3.1 MPa
Peak Avg. Wall Press. from Gas	1.0 MPa

5.6.1. Asymmetric Wall Loading

According to Glenn and Young [1979] and Orth [1989], designing the FSW will require knowledge of both the pressure-time history and the peak pressure for short impulses. However, to provide this information, one needs to consider the non-uniform wall loading caused by the asymmetric blast. Figures 5.11 and 5.12 show wall pressures at various azimuthal angles vs. time within the HYLIFE-I and HYLIFE-II (slab) vessel

respectively. One observes that in the HYLIFE-I case (figure 5.11), the peak pressure at the zero degree azimuthal angle (figure 5.2) is much higher than at other sampled locations. Similarly, the pressure curves for the HYLIFE-II slab case (figure 5.12) show that the pressure on the wall reaches much higher levels at zero, 90 and 180 degrees. (figure 5.3) than at the other angles. By inspection, the high pressures are imposed on the wall at positions where there is the most direct line-of-sight to the central cavity. In the HYLIFE-I case, this causes the difference between maximum local peak and peak average pressure to be a factor of 7. In the HYLIFE-II slab case, it is a factor of 3. This indicates that asymmetric wall loading on the FSW will be an important factor in determining the optimum blanket geometry. The geometry should minimize the imparted velocity to the liquid, but distribute the wall loading from gas shock relatively uniformly on the FSW.

5.7 Parametric Study of Effects of Yield and Density

Because the numerical simulations require a significant computational effort, it is not efficient to re-compute the gas dynamics every time one changes a design parameter such as yield or density. One cannot avoid performing a TSUNAMI calculation if the design changes significantly, such as switching from cylinder to slab geometry. However, for cases such as changes in yield and initial gas density, having a parametric scaling relationship can save a considerable amount of computing time. Hence, another goal is to develop a the rough scaling methodology which can be inserted into a design code such as the one used by Bieri [1991] for parametric studies leading to cost optimization.

The goal of this parametric study is to determine the variation of liquid impulse and gas shock wall loading as functions of yield and density. The study chooses yield and density because, 1) the yield determines the size and cost of the beam driver [Bieri

1991] and 2) the total vapor density may vary by factors of 2 to 3 or more depending on the x-ray spectrum emitted by the fusion target, which is speculative and classified information.

5.7.1 Parametric Effects of Yield

Figure 5.13 shows the spatial average wall gas shock loading for the various yields with initial density profiles kept the same for all runs. Figure 5.14 shows the average wall pressure versus yield. The gas wall loading varies approximately linearly with yield between 600 to 2700 MJ. This is not surprising since the assumption of an ideal gas was used in the calculation and no heat transfer was permitted. The stagnation pressure of the gas therefore remains relatively constant during venting and varies directly with the yield.

Figure 5.15 shows normalized impulse delivered to the liquid during the venting process. Two sets of points are plotted. One for the average of the inner cylinders and one for the outer most cylinders. Two standard normalized curves, $y = x$ and $y = x^{1/2}$, are also plotted to show a possible relationship. From a rough scaling, impulse delivered to the blanket scales as the product of average form drag with the duration of venting, i.e.:

$$\begin{aligned} \text{Impulse} &\sim \text{Drag} \times \Delta t \sim C_D \rho \frac{u^2}{2} \Delta t \\ &\sim u^2 \left(\frac{l}{u} \right) \sim u \end{aligned}$$

where u is a characteristic spatial average gas particle velocity. For the conditions of constant density but varied yield, the form drag pressure roughly varies as the square of velocity while the time for venting might scale inversely with velocity. Hence, impulse, or momentum transfer scales roughly as velocity. Finally, velocity scales roughly as the square root of yield leading to the relationship that momentum transfer should also vary approximately as the square root of the yield, i.e.:

$$Yield \sim internal + kinetic \text{ energies}$$

$$\sim c_v T + \rho u^2 \sim u^2$$

$$\therefore Impulse \sim \sqrt{Yield}$$

The computed impulse delivered to the first row of cylinders shown in figure 5.15 supports this square root relationship. However, the computed impulse to the last row of jets follows a more linear profile. Other factors such as the initial local pressure, shock reflection and flow separation may affect the form drag. These effects were not quantified here and are left as interesting topics for future study. For conservatism, the impulse to the liquid can be assumed to vary as the square root of yield when the design changes call for a smaller yield and higher repetition rate.

5.7.2 Parametric Effects of Density

Figures 5.16 and 5.17 show similar charts for average wall pressure and normalized impulse delivered to the liquid for the four runs where the vapor mass was varied holding yield and initial pressure constant. The plot of average pressure on the wall in figure 5.16 shows that the peak spatial average wall pressure experienced during venting will be on the order of 1 MPa. Although the duration of time for which the calculation was performed is not long enough to include the final pressures for the higher density runs, the shapes of the curves suggest that the average wall pressure due to gas shock will be the same regardless of density. The only difference will be the duration. For higher densities, there is less specific kinetic energy in the gas, therefore velocities are lower. However, because of the assumption of ideal gas and fixed yield, the total internal energy and therefore stagnation pressure are constant regardless of initial evaporated mass.

Figure 5.17 again tries to compare normalized impulse delivered to the liquid versus initial mass evaporated. From a similar scaling argument as above, the impulse

imparted to the slabs will scale as the product of form drag and venting duration.

$$\begin{aligned} \text{Impulse} &\sim \text{Drag} \times \Delta t \\ &\sim C_D \rho \frac{u^2}{2} \Delta t \sim \rho u^2 \left(\frac{l}{u} \right) \\ &\sim \rho u \end{aligned}$$

For the case of fixed yield, the product of density and velocity squared which varies as the yield is roughly constant:

$$\begin{aligned} \rho u^2 &\sim \text{Yield} \sim \text{const.} \\ u &\sim \sqrt{\frac{\text{yield}}{\rho}} \end{aligned} \quad (5.4)$$

Substituting into the expression for impulse scaling results in:

$$\begin{aligned} \text{Impulse} &\sim \rho u \sim \rho \sqrt{\frac{\text{yield}}{\rho}} \\ &\sim \sqrt{\rho} \end{aligned} \quad (5.5)$$

which reduces to another square root relationship; that is, momentum transfer should scale approximately with the square root of the mass initially evaporated. Both normalized square root curves and a standard linear curve are plotted with the data in figure 5.17. The calculation indicates that the relationship has a dependence which is neither linear nor square root, but somewhere in between.

Figure 5.1. Simple linearly approximated profiles of Glenn's inner cavity solution used as the initial conditions for HYLIFE-I and -II calculations.

Figure 5.2. HYLIFE cylindrical geometry used in the TSUNAMI computation.

Figure 5.3. HYLIFE-II Half Reactor with Slab Blanket Geometry used in TSUNAMI calculation

Figure 5.4. Schematic representation of supersonic flow separation.

Figure 5.5. TSUNAMI computed pressure distribution over HYLIFE-I out cylinder at 900 microseconds, 2700 MJ yield.

Figure 5.6. Pressure distribution curves over various cylinders at different times.

Figure 5.7. Impulse imparted vs. time for a line of cylinders placed at increasing radii for the HYLIFE-I case. 2700 MJ yield.

Figure 5.8. HYLIFE-I flow simulation. Logarithmic density shown. White is maximum density (40 kg/m^3) and black is void (10^{-4} kg/m^3). One quarter of the reactor simulated.

Figure 5.9. HYLIFE-II flow simulation. Logarithmic density shown. White is maximum density (40 kg/m^3) and black is void (10^{-4} kg/m^3). One-quarter reactor and approximately 350 objects modeled.

Figure 5.10. HYLIFE-II slab geometry flow simulation. One-half reactor with 37 slabs modeled. Logarithmic density shown with white being the highest density (40 kg/m³) and black being void (10⁻⁴ kg/m³).

Figure 5.11. Pressure on FSW vs. time at various azimuthal positions for HYLIFE-I (2700 MJ Yield).

Figure 5.12 Pressure on FSW vs. time at various azimuthal positions for HYLIFE-II (350 MJ; slabs).

Figure 5.13. Integrated spatial average pressure on FSW for various initial yields with mass held constant.

Figure 5.14. Integrated spatial average pressure on the FSW versus yield at various times for mass held constant.

Figure 5.15. Normalized average liquid impulse delivered to liquid versus normalized yield for 1st and last row of cylinders in HYLIFE-I.

Figure 5.16. Integrated spatial average pressure on FSW for various initial density with yield (350 MJ) held constant.

Figure 5.17. Normalized average liquid impulse delivered to 2 Slabs vs. normalized initial mass with yield (350 MJ) held constant

6. EFFECTS OF CONDENSATION ON SHOCK REFLECTION

6.1 Introduction

The work in Chapter 5 assessed the gas dynamics consequences of blast venting in HYLIFE using the conservative assumption of adiabatic gas. This has the potential to grossly over estimate the shock on the FSW if the venting is not adiabatic. Because the blast material is vaporized liquid, it must condense out to a low enough pressure and density to permit the next shot. At early times, in the first tens of microseconds, the vapor is very hot and the liquid surfaces not exposed to the target very cold. The condensation is especially rapid and has the potential to draw mass and energy out of the vapor and thus greatly reduce both potential $p dv$ work done by the gas on the liquid during momentum transfer, and the final pressure on the wall.

In the limiting case for ICF, the transient, early-time condensation might be so strong as to absorb all the vapor mass and energy, thus completely attenuating any shocks on the FSW while only causing only a minimal momentum transfer to the liquid. This scenario would indeed greatly ease the task of the structural designers. On the other hand, condensation may not cause any significant change in the gas dynamics if condensation quickly heats up the liquid surfaces and prevents additional condensation. Therefore, the purpose of the work below is to obtain some preliminary assessment of early-time condensation in the HYLIFE-II system. The work consists of coupling transient conduction and convection in the liquid with the TSUNAMI gas dynamics code in a one-dimensional system. Necessary to this work is the development of a boundary condition based on kinetic theory which couples both sub- and supersonic gas dynamics with the condensation heat flux into the liquid.

Much of the ground work for transient condensation in ICF reactors comes from the studies by Bai and Schrock [1991] and Schrock et al. [1992]. The former paper discusses the condensation on droplets required to bring down the pressure to pre-shot conditions, while the latter paper focuses on the very early-time condensation of vapor on a cold surface. The latter serves as a beginning point for the work presented below. In that paper, Schrock et al. examined the problem of initially cold droplets suspended in a uniform gas medium initially at rest. Using Schrage's [1953] equation for condensation, Schrock et al. developed a method for computing the net condensation flux into the condensing surface and then numerically solving the time-dependent heat equation in the liquid. The study investigated the idealized problem of initially quiescent vapor in contact with a cold liquid surface using the assumption of isentropic flow in the vapor. Hence, the next step in improving the method is to replace the isentropic assumptions with a better method of estimating gas properties such as the second-order Godunov method used in the TSUNAMI code. The sections below will first outline Schrage's kinetic theory of condensation, then the modeling of the effect of condensation on the vapor, liquid and interface, and lastly, the numerical method used to solve the governing equations.

6.2 The Kinetic Theory of Condensation

If a cold liquid surface is suddenly placed in contact with hot vapor, the result will be a net condensation flux into the liquid. Schrage [1953] considered this net flux to be comprised of the difference between the impacting condensation flux and the evaporation flux (see figure 6.1). His analysis is based on the kinetic theory of phase change (reviewed by Collier 1972). On a microscopic level, the gas particles near the liquid interface impact with some frequency and distribution of molecular velocities. Schrage considered a Maxwellian velocity distribution given by:

$$\frac{dN_{u,v,w}}{N} = \left(\frac{m}{2\pi k_b T} \right)^{3/2} \exp \left[- \left(\frac{m}{2k_b T} \right) (u^2 + v^2 + w^2) \right] du dv dw \quad (6.1)$$

where the left hand side represents the fraction of the total number of molecules N with velocities between u and $u+du$, v and $v+dv$, and w and $w+dw$ in Cartesian space. On the right, m is the mass of a molecule, k_b the Boltzmann constant and T the temperature. This distribution assumes that the bulk gas is stationary. However, there must be some bulk motion of the vapor normal into the liquid interface if there is net condensation. Schrage [1953] was the first to consider effect. He derived the mass flux for flow through a plane normal to the direction of the bulk gas motion. The mass flux is the product of molecular mass and particle flux. Beginning with the skewed Maxwellian distribution:

$$\frac{dN_{u,v,w}}{N} = \left(\frac{m}{2\pi k_b T} \right)^{3/2} \exp \left[- \left(\frac{m}{2k_b T} \right) [(u-u_0)^2 + v^2 + w^2] \right] du dv dw, \quad (6.2)$$

where u_0 is the average bulk velocity of the gas toward the surface, Schrage integrated the distribution function over all velocities v and w , and velocity u either away or into (evaporation or condensation respectively) the interface, and then multiplied by the product of average particle density to obtain the particle flux, i.e. (for case of condensation - positive toward the interface):

$$\begin{aligned} \phi_N &= \int_0^\infty \int_0^\infty \int_0^\infty n_0 u \frac{dN_{u,v,w}}{N} \\ &= n_0 \int_0^\infty \int_0^\infty \int_0^\infty u \left(\frac{m}{2\pi k_b T} \right)^{3/2} \exp \left[- \left(\frac{m}{2k_b T} \right) [(u-u_0)^2 + v^2 + w^2] \right] du dv dw \end{aligned} \quad (6.3)$$

where ϕ_N is the particle flux and n_0 is the average particle density. For the case of condensation, the limits of integration for the u -velocity component are defined from 0 to ∞ . Using the identity:

$$\int_{-\infty}^{\infty} \exp(-a^2 x^2) dx = \frac{\sqrt{\pi}}{a}. \quad (6.4)$$

and integrating with respect to v and w gives:

$$\phi_N = n_0 \left(\frac{m}{2\pi k_b T} \right)^{1/2} \int_{-\infty}^0 u \exp \left[- \left(\frac{m}{2k_b T} \right) (u - u_0)^2 \right] du. \quad (6.5)$$

Schrage evaluated the integral on the right hand side of equation (6.5) and recast the equation as:

$$\phi_N = n_0 \left(\frac{k_b T}{2\pi m} \right)^{1/2} \left\{ \exp \left[-u_0^2 \left(\frac{m}{2k_b T} \right) \right] + u_0 \sqrt{\pi} \left(\frac{m}{2k_b T} \right)^{1/2} \left[1 + \operatorname{erf} \left(u_0 \left(\frac{m}{2k_b T} \right)^{1/2} \right) \right] \right\}. \quad (6.6)$$

Equation (6.6) is the expression for gas motion toward the interface (i.e. $u_0 > 0$). One obtains a similar equation:

$$\phi_N = n_0 \left(\frac{k_b T}{2\pi m} \right)^{1/2} \left\{ \exp \left[-u_0^2 \left(\frac{m}{2k_b T} \right) \right] + u_0 \sqrt{\pi} \left(\frac{m}{2k_b T} \right)^{1/2} \left[1 - \operatorname{erf} \left(-u_0 \left(\frac{m}{2k_b T} \right)^{1/2} \right) \right] \right\}. \quad (6.7)$$

if the bulk gas velocity is away from the interface ($u_0 < 0$). By substituting the expressions:

$$s = u_0 \left(\frac{\mu}{2R_0 T} \right)^{1/2} = \frac{u_0}{(\gamma R T)^{1/2}} \left(\frac{\gamma}{2} \right)^{1/2} = M \left(\frac{\gamma}{2} \right)^{1/2}, \quad (6.8)$$

and

$$\frac{k_b}{m} = \frac{R_0}{\mu} \quad (6.9)$$

into equation (6.6), multiplying by the molecular mass, m , and then using the ideal gas law, Schrage obtained as the impacting condensation mass flux:

$$G_{cond} = p \left(\frac{\mu}{2\pi R_0 T} \right)^{1/2} \left\{ e^{-s^2} + s \sqrt{\pi} [1 + \operatorname{erf}(s)] \right\} \quad \text{if } s > 0$$

$$= p \left(\frac{\mu}{2\pi R_o T} \right)^{1/2} \left\{ e^{-s^2} - s\sqrt{\pi} [1 - \text{erf}(-s)] \right\} \quad \text{if } s < 0 \quad (6.10)$$

where p is the local pressure of the vapor at the interface measured by a detector moving with the flow, R_o is the gas constant and μ the molecular weight. In equation (6.8), R is the material specific gas constant, γ the ratio of specific heats and M the Mach number. The quantity s represents the ratio of average bulk flow velocity to most probable molecular speed in the Maxwellian distribution at the state of the vapor at the interface.

One can rewrite the bracketed term on the right-hand-side of equation (6.10) as a correction factor, i.e.:

$$\begin{aligned} \Gamma(s) &= e^{-s^2} + s\sqrt{\pi} [1 + \text{erf}(s)] & \text{if } s > 0 \\ &= e^{-s^2} + s\sqrt{\pi} [1 - \text{erf}(-s)] & \text{if } s < 0 \end{aligned} \quad (6.11)$$

Therefore, the impacting condensation mass flux is then given as:

$$G_{cond} = p_w \Gamma \left(\frac{1}{2\pi R T_w} \right)^{1/2} \quad (6.12)$$

As mentioned above, the net mass flux is the difference between the impacting condensation and the evaporative mass fluxes. The evaporative flux is usually assumed to correspond to the particle flux emanating from a saturated vapor at the liquid surface temperature. The analysis to determine the evaporative mass flux is similar to the condensation flux, except bulk mass motion of the particles is neglected. This gives for the evaporative mass flux:

$$G_{evap} = p_u \left(\frac{1}{2\pi R T_u} \right)^{1/2} \quad (6.13)$$

For the impacting condensation flux, the liquid surface may not capture every particle which impacts. Similarly for the evaporative flux, not every molecule which

possesses sufficient energy to boil off will escape into the gas. The fractions of molecules which stick on impact or boil off into the gas are called accommodation coefficients or sticking and evaporation coefficients. These are assigned f_c and f_e , respectively. At equilibrium in a quiescent system, there is zero net flux so the impacting condensation flux must equal the evaporative flux. If less than the full kinetic theory mass flux sticks in condensation, then the same reduction must also take place for the evaporation. That is, at equilibrium the sticking coefficient must be the same as the evaporation coefficient. Usually, in non-equilibrium situations, one still assumes that these coefficients are equal. The values for accommodation coefficients vary widely in literature, but work by Mills [1965] indicates that it is less than 1 only when impurities are present at the interface. For this assessment, both coefficients are assumed to be unity. All factors combined together give for the net condensation mass flux (Schrage's equation):

$$G_k = f_c p_{vs} \Gamma \left(\frac{1}{2\pi RT_{vs}} \right)^{1/2} - f_e p_{ls} \left(\frac{1}{2\pi RT_{ls}} \right)^{1/2} \quad (6.14)$$

6.3 Modeling

Schrage's equation provides a means for calculating the effect of condensation if the properties at the liquid-vapor interface are known. These interface properties are derived from both the liquid as well as vapor and will depend on the model used to predict vapor and liquid behavior. However, limitations posed by gas dynamics must also be considered. The system is modeled as three parts - vapor, liquid and interface (see figure 6.1). Modeling for the liquid side and interface as well gas dynamics considerations are presented below. The vapor is assumed to be an inviscid, gamma-law gas whose dynamics are governed by the equations of inviscid, compressible flow. This

assumption permits the vapor to be analyzed using the same techniques found in the TSUNAMI code (chapter 3).

6.3.1 Liquid-Side Modeling

On the liquid side, transient conduction and convection into the layer are the effects considered. Using the same method as Schrock et al. [1992], the governing, time-dependent energy equation for the liquid is given as:

$$\frac{\partial T(x,t)}{\partial t} + u_l \frac{\partial T(x,t)}{\partial x} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2} \quad 0 \leq x \leq \infty \quad (6.15)$$

where α is the thermal diffusivity of the liquid and x is taken as positive into the surface. The origin is fixed at the interface which is actually moving into the vapor as the condensate layer accumulates. The effect of this interface velocity on the gas dynamics is assumed to be negligible because of characteristic velocities of the vapor are expected to be much greater than the absolute velocity of the interface. The validity of this assumption is based on the continuity of mass flux across the interface, discussed further below. The liquid geometry is a semi-infinite slab, and the initial condition assumes a known temperature distribution. The slab assumption can be justified if the characteristic diffusion length into the liquid, $\sqrt{\alpha \Delta t}$, is small compared to the radius of surface curvature. For the case of Flibe in the HYLIFE-II reactor, the diffusion length will only be on the order of several tens of microns during the first millisecond, much thinner than either jets or slabs which have thicknesses of many centimeters. The boundary conditions are given as:

$$q''_{surf} = -k_l \left. \frac{\partial T}{\partial x} \right|_{x=0} + Gh_{ls} \quad t \geq 0 \quad (6.16)$$

and

$$T(\infty, t) = T_{lm} \quad t \geq 0 \quad (6.17)$$

where k_l is the thermal conductivity and h_{ls} is the liquid stagnation enthalpy at the surface. Equation (6.16) states that the heat flux at the interface must equal the heat flux due to convection and conduction into the liquid at the interface. Equation (6.17) states the assumption that infinitely deep, the liquid is the original liquid temperature prior to contact with the vapor.

6.3.2. Interface Modeling

At the interface, two conditions must be satisfied. The mass flux out of the vapor must be the same as the mass flux into the liquid, and the energy flux out of the vapor must be the same as the energy flux into the liquid. The continuity of temperature across the interface is not enforced because, by inspection, kinetic theory permits unequal temperatures to exist on either side of the interface. The first condition is just a statement of mass continuity across the interface, which can be expressed:

$$G|_{x=0-} = \rho_v u_v = \rho_l u_l = G|_{x=0+}, \quad t \geq 0 \quad (6.18)$$

while the second can be expressed by modifying equation (6.16):

$$G h_v^0 = -k_l \left. \frac{\partial T}{\partial x} \right|_{x=0} + G h_{ls}, \quad t \geq 0 \quad (6.19)$$

where h_v^0 is the total vapor stagnation enthalpy. The continuity of mass flux across the interface states that the ratio of vapor velocity to interface velocity is proportional to the inverse ratio of the vapor density to the liquid density. For most cases considered below, the vapor density is roughly unity in metric (mks) units while the liquid density is 3 orders of magnitude greater. Hence neglecting the interface velocity in the gas dynamics is a reasonable assumption.

As written in equation (6.19), the model for heat flux across the interface considers only convection and conduction in the liquid. For simplicity, conduction in the vapor and more notably, radiation are neglected. The characteristic diffusion length for conduction in the vapor limits the effects, for a 1 millisecond time scale, to within only 1 micron of the interface. Conduction is assumed negligible by considering this diffusion layer to be a discontinuity and applying the kinetic theory to vapor slightly away from the interface and where it is not affected by conduction. As for radiation, it is beyond the scope of the work here. Chen [1992] examined radiation coupled with one-dimensional gas dynamics using the diffusion approximation which applies in the limit of an optically thick vapor. However, for this problem, radiation transport is possible from vapor close to as well as far away from the interface. For these mixed conditions, neither of the simple models for the limiting cases of an optically thick or thin media is applicable.

For closure, the functional relationships for liquid and vapor enthalpies must be specified. The specific heats, c_{pg} and c_{pl} , are assumed to be constants. The vapor enthalpy is assumed to consist of the sum of superheat, heat of vaporization and sensible heat. Since the vapor may be in motion, a kinetic energy contribution is also included. This contribution may be large because the condensation may cause the velocity to approach the sonic state. Hence the total vapor enthalpy is given as:

$$h_{vs}^0|_{x=0} = c_{pg} [T_{vs} - T_{sat}(p_{vs})] + h_{fg} [T_{sat}(p_{vs})] + c_{pl} [T_{sat}(p_{vs}) - T_{lm}] + \frac{u_{vs}^2}{2} \quad (6.20)$$

For consistency with the use of constant but different c_{pl} and c_{pg} , the heat of vaporization, h_{fg} must be specified as a linear function of $T_{sat}(p_v)$ given by:

$$h_{fg}(T_{sat}(p_v)) = h_{fg}(T_{ref}) + (c_{pg} - c_{pl}) [T_{sat}(p_v) - T_{ref}] \quad (6.21)$$

where T_{ref} is some reference temperature with a reference enthalpy. We use this form due to the limited thermodynamic information available for Flibe. For other materials, tabulated data should be used for h_{fg} , c_{pl} and c_{pv} if available. The temperature $T_{sat}(p_{vs})$ is the saturation temperature for the pressure of the vapor near the interface. The saturation temperature is obtained from the relationship for saturation pressure as a function of temperature (units in Kelvin) is given for Flibe by [Furakawa and Ohno 1980]:

$$p_{sat}(T) = \frac{101,300}{760} \times 10^{\left(9.407 - \frac{1.0054 \times 10^4}{T}\right)} \quad [Pa]. \quad (6.22)$$

Similar relationships exist for other materials. The liquid enthalpy at the interface is defined by:

$$h_u^o|_{x=0} = c_{pl}(T_u - T_{lm}). \quad (6.23)$$

In both the liquid and vapor, the reference datum temperature for the enthalpy, as used by Schrock et al. [1992] is the temperature T_{lm} infinitely deep into the liquid. It is important to note here that the enthalpy in the vapor at the interface as defined by equation (6.20) is not the same enthalpy used in the rest of the vapor. The reason for the different methods for computing enthalpy is that the vapor is assumed to be an ideal gas for the gas dynamics calculation and its enthalpy is defined by equation (1.25) in chapter 1, but for condensation heat transfer being considered here, the vapor has a different reference datum temperature.

6.3.3 Gas Dynamics Limitations - Choking

There exists the possibility that kinetic theory may predict a net condensation mass flux greater than the ability of gas dynamics to deliver the vapor toward the interface. If this should occur, then physically, the gas dynamics will set a limit on the maximum mass flux. This gas dynamics limiting phenomenon is calling *choking*, and

indeed, Schrock et al. [1992] predict choking in several cases where superheated Flibe vapor condenses on an initially cold Flibe surface.

The maximum gas dynamics flux depends on whether the vapor is initially sub- or supersonic relative to the interface. In the subsonic case, if kinetic theory and liquid conduction permit the surface to condense more than the simple convective (ρu) flux from the gas, then the interface will apply a *suction* on the gas until either the flux increases to satisfy kinetic theory or the flux reaches its gas dynamics maximum. However, any increase in mass flux can only come about if the suction is able to send a rarefaction upstream into the vapor, a possibility only if the vapor is originally subsonic.

One can derive the choking condition for a subsonic vapor with initial properties (ρ_1, u_1, p_1). From the isentropic relation (equation 1.12) and Riemann Invariant (equation 1.44), the mass flux for a flow which is expanded from some density ρ_1 and subsonic velocity u_1 to a new density ρ and velocity u , can be expressed as:

$$G_v = \rho u = \rho_1 \left(\frac{p}{p_1} \right)^{\frac{1}{\gamma}} \left[u_1 + \frac{2}{\gamma-1} (c_1 - c) \right]. \quad (6.24)$$

Expressing all terms in equation (6.24) as functions of ρ_1 , u_1 , p_1 , and p gives:

$$G_v = \rho_1 u_1 \left(\frac{p}{p_1} \right)^{\frac{1}{\gamma}} + \frac{2\rho_1 c_1}{\gamma-1} \left[\left(\frac{p}{p_1} \right)^{\frac{1}{\gamma}} - \left(\frac{p}{p_1} \right)^{\frac{\gamma+1}{2\gamma}} \right]. \quad (6.25)$$

Differentiating the mass flux in equation (6.25) with respect to p and setting it equal to zero yields the expression for pressure ratio at the maximum flux:

$$\left. \frac{p}{p_1} \right|_{G_v = G_{v,max}} = \left[\left(\frac{\gamma-1}{\gamma+1} \right) \left(\frac{u_1 + \frac{2}{\gamma-1} c_1}{c_1} \right) \right]^{\frac{2\gamma}{\gamma-1}}. \quad (6.26)$$

Substituting equation (6.26) into (1.44) and using some algebraic manipulation gives:

$$u|_{G_v=G_{v,max}} = \frac{(\gamma-1)u_l + 2c_l}{\gamma+1} = \frac{\gamma-1}{2}(u_l - u) + c_l = c|_{G_v=G_{v,max}}. \quad (6.27)$$

Equation (6.27) shows that the maximum mass flux of an originally subsonic flow occurs when the velocity is expanded to exactly the sound speed, that is, it is expanded to Mach 1.

For initially supersonic flow relative into the interface, the velocity of the vapor is greater than the local acoustic velocity. Under these conditions, there is no possibility for a rarefaction, which propagates at the acoustic velocity, to move upstream into the vapor. Hence, for the supersonic flow case, no further increase in flux is possible and the maximum flux is just the product of density and velocity (ρu) in the oncoming vapor.

6.4 Numerical Method

The purpose of this section is to present a numerical method for implementing the condensation model as a boundary condition for the TSUNAMI code. Specifically, the goal is to develop an explicit finite difference method for determining net condensation mass flux at any given time step and for arbitrary initial liquid and vapor conditions. It is assumed that the properties of both vapor and liquid are entirely known at the beginning of a time step. Appendix A lists the subroutine called "condbc.f" which provides one method of implementing in code described in detail below.

6.4.1 First Guess at the Condensation Flux

Four possible conditions can exist for condensation at the interface. The arriving vapor can be either subsonic or supersonic, and for each state, the flow may be either choked or not choked. One first evaluates whether the flow is subsonic or supersonic,

and then computes the maximum gas dynamics flux. The TSUNAMI code provides the vapor properties at the beginning of the time step. The maximum flux for subsonic flow into the interface is obtained from combining equations (6.25) and (6.26), which gives:

$$G_{v,max} = \rho c \left(M + \frac{2}{\gamma-1} \right) \left[\frac{\gamma-1}{\gamma+1} \left(M + \frac{2}{\gamma-1} \right) \right]^{\frac{2}{\gamma-1}} - \frac{2\rho c}{\gamma-1} \left[\frac{\gamma-1}{\gamma+1} \left(M + \frac{2}{\gamma-1} \right) \right]^{\frac{\gamma+1}{\gamma-1}} \quad \text{if } u < c. \quad (6.28)$$

For supersonic flow, the maximum flux is simply:

$$G_{v,max} = \rho u. \quad \text{if } u > c \quad (6.29)$$

Note that for an explicit method, only the properties at the beginning of the current time step are used to compute the new properties at the next time step with the implied assumption that the properties remain constant during the time step.

The next step is to compute the kinetic theory mass flux according to Schrage's equation (6.14). The vapor side temperature, pressure and velocity are obtained as, before, directly from the TSUNAMI code for the boundary vapor cell. On the liquid side, it is assumed that the liquid interface pressure corresponds to the saturation pressure, p_{sat} , for the liquid interface temperature, T_{ls} . Equation (6.22) gives the relationship for saturated Flibe vapor where the temperature is specified in Kelvin. However, it is important to note here that T_{ls} is not an explicitly known quantity. Instead, it is defined by the heat flux boundary condition, which is depends on the mass flux. The solution to T_{ls} is described in more detail below but for now, T_{ls} may be assumed to be the same temperature as in the adjacent node just slightly deeper into the liquid. Once both the maximum gas dynamics mass flux and the kinetic theory mass flux have been evaluated, the choice of flux must always be the smaller of the two, regardless if the kinetic theory indicates net condensation or net evaporation. That is, one chooses:

$$G = \min(G_k, G_{v,max}). \quad (6.30)$$

6.4.2 Iteration for Liquid Interface Temperature and Condensation Flux

The calculation of the first guess kinetic theory mass flux, G in the above step, required five interface variables - vapor pressure, temperature, and Mach number, and liquid pressure and liquid temperature. The assumption that the liquid interface pressure is equal to the saturation pressure at the liquid interface temperature as expressed in equation (6.22) reduced the dependence to four variables. For an explicit method, all the properties are known at the beginning of each time step. The exception is T_{li} , the liquid interface temperature, which is defined by a heat flux boundary condition (equation 6.19).

The boundary condition can be rewritten in finite difference form as:

$$Gh_{vs}^o = -k_l \frac{[T_i - T_{li}]}{\Delta x} + G[c_{pl}(T_{li} - T_{lm})] \quad (6.31)$$

where T_i is the temperature at the first interior liquid node, and Δx is the spatial mesh size. Equation (6.31) can be rearranged to show the dependence of T_{li} on net mass flux G ,

$$T_{li} = \frac{G(h_{vs}^o + c_{pl}T_{lm}) + \frac{k_l}{\Delta x}T_i}{Gc_{pl} + \frac{k_l}{\Delta x}}. \quad (6.32)$$

By inspection, equations (6.14) and (6.32) are coupled such that both must be simultaneously satisfied.

The simultaneous solution to G and T_{li} is obtained by iteration. The scheme used here is the Newton-Raphson method, an averaging technique that converges halfway to the solution with each iteration. To implement it requires some initial guess of the upper and lower temperature limits which define the initial domain of iteration. One can use

physical reasoning to deduce these limits. Considering first only the case of net condensation (i.e. $G > 0$), as the numerical solution is solved for each time step, the liquid surface temperature will advance. The largest increase in T_L that can possibly occur during the advancement of a single time step must correspond to the highest heat flux and therefore mass flux into the liquid. Conversely, the minimum T_L increase must correspond to zero flux or no temperature gradient at all. By inspection, the latter condition sets the lower temperature limit to the temperature in the adjacent liquid cell, or T_I from the notation used in equation (6.31). From the fact that T_L and G behave inversely to each other in equation (6.14), (i.e. the lower the guessed T_L , the higher the G) one deduces that the largest possible mass flux G is found by substituting T_I for T_L in equation (6.14). Finally, the upper limit of T_L is then found by inserting the upper limit mass flux into equation (6.32). In the case of evaporation where $G < 0$, the conditions are reversed, i.e. the upper limit corresponds to the zero-flux and the lower limit corresponds to the largest evaporative flux. The statements in the preceding paragraph can be stated mathematically as:

$$\begin{aligned} T_{ls-low} &= T_I \\ T_{ls-high} &= T_L(G(T_{ls-low})) \end{aligned} \quad \text{if } G_{1st\ guess} > 0 \quad (6.33)$$

and

$$\begin{aligned} T_{ls-high} &= T_I \\ T_{ls-low} &= T_L(G(T_{ls-high})) \end{aligned} \quad \text{if } G_{1st\ guess} < 0 \quad (6.34)$$

where T_{ls-low} is the lower limit of liquid surface temperature, and $T_{ls-high}$ is the upper limit of surface temperature, and $T_L(G)$ implies liquid surface temperature as a function of mass flux as defined in equation (6.32). Each iteration for $T_L(G)$ evaluates a new liquid surface temperature based on the most recent iteration of mass flux. Calling the most

current $T_L(G)$ as T_{L-new} , and the previous T_L , just T_L , the convergence criterion for this scheme is determined by some small ε such that:

$$\frac{|T_{L-new} - T_L|}{T_L} \leq \varepsilon. \quad (6.35)$$

If the scheme is not converged, then iteration must take place until the criterion in equation (6.35) is satisfied. This requires the computation of a new guess liquid surface temperature and the setting of new temperature limits. If T_L is too high, the mass flux will be too low. This causes the heat flux boundary condition in equation (6.32) to predict a lower surface temperature T_{L-new} . Hence the real surface temperature should be lower on next guess. If T_L is too low, then the predicted mass flux will be too high, and therefore the heat flux boundary condition predicts a higher T_{L-new} . Hence, one chooses a simple averaging technique such as:

$$\begin{aligned} T_{L-high} &= T_L \\ T_L &= \frac{(T_L + T_{L-low})}{2} \end{aligned} \quad \text{if } T_{L-new} < T_L \quad (6.36)$$

or else

$$\begin{aligned} T_{L-low} &= T_L \\ T_L &= \frac{(T_L + T_{L-high})}{2} \end{aligned} \quad \text{if } T_{L-new} > T_L \quad (6.37)$$

When the physics dictate that the previous guess surface temperature T_L is too high, the scheme resets the upper bound of the iteration domain and then uses the average of the lower limit and itself as the new guess. The converse situation is based on the same principle except in reverse. Note that T_{L-old} must be reset to the new guess T_L before the new computation of condensation mass flux. This scheme usually converges in 20 iterations to an ε less than 10^{-6} which should provide accuracy on the order of the numerical truncation error for a standard real number. By inspection, the scheme devised

above will still converge on the correct mass flux and liquid surface temperature in either choked or non-choked flow.

6.4.3 Liquid Conduction and Convection

After the correct mass flux and liquid interface temperature have been found, the next step is to advance the liquid temperature distribution one time step according to the energy equation (6.15). In explicit finite difference form, equation (6.15) can be rewritten:

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} [T_{i+1}^n - 2T_i^n + T_{i-1}^n] - \frac{G \Delta t}{\rho_i \Delta x} [T_i^n - T_{i-1}^n], \quad \text{if } G \geq 0 \quad (6.38)$$

where T_i^{n+1} is the liquid temperature at any node i at the new time step $n+1$ and Δt is the time step size. When the flux G is greater than or equal to zero (i.e. net condensation is occurring), the convective term on right hand side of equation (6.38) is evaluated using the upwind difference $T_i - T_{i-1}$. This makes physical sense because the vapor which condenses onto the interface (refer to figure 6.2) is convected into the liquid from left to right, that is from a node $i-1$ on the left to the node i . Hence the convection at node i is evaluated based on *upwind* data. For evaporation, the convective velocity reverses direction. Convection relative to the interface will instead be from right to left. Therefore the convection should be evaluated base on a finite difference from $i+1$ to i . Hence for evaporation, equation (6.38) should be modified to:

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} [T_{i+1}^n - 2T_i^n + T_{i-1}^n] - \frac{G \Delta t}{\rho_i \Delta x} [T_{i+1}^n - T_i^n], \quad \text{if } G < 0 \quad (6.39)$$

In either condensation or evaporation, the liquid interface temperature, T_{li} , computed by the method in the previous section becomes the T_0^n and by inspection, stability requires that the time step satisfy :

$$\Delta t < \left[\frac{2\alpha}{(\Delta x)^2} + \frac{G}{\rho_i \Delta x} \right]^{-1} \quad (6.40)$$

The boundary condition specified by equation (6.17), states that infinitely deep into the fluid, the temperature is a constant, T_{∞} . Implementing this in the context of finite differences implies that one simply fixes the last node in the liquid. However, care must be taken such that as time advances numerically, the temperature close to the last node not be allowed to rise significantly. If it does, then the lower fixed temperature of the last node would place an artificially gradient and heat flux at the end of the grid. For the calculations presented here, whenever the temperature at the second to last node increases by 0.001 degree, the cell size (Δx) is doubled, and new temperatures computed for each cell based on the average of temperatures in each previous pair of cells.

6.4.4 Godunov Flux at the Interface

Up to this point, the assumption has been made that all the gas dynamics behavior can be computed using the models in the TSUNAMI code. This is true everywhere except at the interface which is governed also by the kinetic theory. The Godunov method requires computation of mass, momentum and energy flux at the edge of the boundary cell (see figure 6.3). The mass flux out of the vapor comes directly from Schrage's equation with some gas dynamics limitations, but the momentum and energy fluxes need to be determined. The energy flux is straight forward to compute since the mass flux is already known. Physically, condensation removes some mass out of the gas at the last cell, and that mass carries with it some enthalpy. Intuitively, the energy lost at the interface is just the product of mass flux and vapor enthalpy just as stated in the heat flux boundary condition (equation 6.32). However, because the Rankine-Hugoniot equations used by the Godunov method used everywhere else in the vapor do not represent phase change, the enthalpy for the Godunov flux will not be the same as that

given by equation (6.20). Instead, the enthalpy will be specified by the last term in equation (3.57). That is:

$$h_w^0(\text{Godunov}) = \frac{p_{vs}}{(\gamma-1)\rho_w} + \frac{u_{vs}^2}{2} \quad (3.57)'$$

Hence, the energy flux is given by the product of mass flux and gas total enthalpy according to:

$$\text{energy flux} = G \left[\frac{p_{vs}}{(\gamma-1)\rho_w} + \frac{u_{vs}^2}{2} \right]. \quad (6.41)$$

The Godunov momentum flux requires finding the correct pressure and velocity at the interface for the problem of a semi-permeable boundary condition. The problem here is how to compute the momentum flux at the interface when not all of the available vapor condenses and therefore, some of it must pile up against the liquid. In the zero-condensation case, the liquid condenses nothing at all, and the vapor can only stagnate at the interface, and in the fully condensing case, the liquid absorbs all the oncoming vapor so there is complete outflow. These boundary conditions were discussed in chapter 3. One was the impermeable boundary and the other was the outflow boundary. In the impermeable case, a mirror image node was created on the other side of the interface and assigned equal pressure and density but opposite velocity. The Riemann solver, which takes the two states $U_L = (\rho_w, u_w, p_w)^T$ and $U_R = (\rho_w, -u_w, p_w)^T$, and computes the solution $U^* = (\rho^*, u^*, p^*)^T$ at the interface between them, was then used to predict the pressure rise and therefore the momentum flux. The reason the mirror imaging technique worked for the impermeable boundary condition was because the shock reflection problem is analogous to the head-on collision of two equal, but oppositely traveling shocks. In the outflow boundary, a similar node was created on the other side of the interface, but instead of opposite velocity, as in the impermeable boundary, the outflow boundary assigned identical density, pressure and velocity to the imaginary node. The Riemann

solution to two identical states gives just the same state at the interface between the two. This result eliminates any gradients at the boundary and permits the velocity to be continuous across the interface so anything which is convected to the boundary is convected out at the same velocity. In both boundary conditions, the density and pressure were kept the same and only the velocity varied.

From the two previous boundary conditions, the method one can pursue for the semi-permeable boundary condition, is to again create an imaginary node on the other side of the boundary and assign it the same density and pressure, but find a more general analogy for its velocity. The imaginary node should be able to mimic both the impermeable boundary and outflow boundary, and also evaporation. By inspection, if the boundary vapor node possesses the state $U_L = (\rho_v, u_v, p_v)^T$ and one assigns the imaginary node with state $U_R = (\rho_v, -u_v + u_s, p_v)^T$, where u_s is a pseudo-suction (or blowoff) velocity, this satisfies the previous boundary criteria. The condition u_s equals zero mimics the impermeable boundary, while the condition u_s equals $2u_v$ mimics the outflow boundary condition. For a semi-permeable boundary, u_s will then be some intermediate value between zero and the maximum suction (or blowoff) velocity as determined by gas dynamics.

The pseudo-suction velocity must also be consistent with the mass flux G imposed at the interface by kinetics and gas dynamics. This implies that the Riemann solution $U^* = (\rho^*, u^*, p^*)^T$ at the interface must satisfy the condition:

$$G = \rho^* u^*. \quad (6.42)$$

Without knowing specifically the pseudo-suction velocity in the right state which will yield the correct $\rho^* u^*$ at the interface, one needs to solve iteratively with the Riemann solver until the G and $\rho^* u^*$ converge. The difference between the two quantities can be

non-dimensionalized by the maximum vapor flux (equations 6.28 and 6.29) and expressed as:

$$\Delta G_{norm} = \frac{\rho^* u^* - G}{G_{vmax}}. \quad (6.43)$$

Equation (6.43) can serve as the basis for the convergence criterion. That is, if the absolute value of ΔG_{norm} does not match within some small permissible error ε , then the iteration proceeds with a new guess for the suction velocity. For a first guess, one can choose:

$$u_s = 2 \frac{G}{\rho_{vs}} \quad (6.44)$$

which exhibits the correct behavior in the limits that the interface is impermeable ($G = 0$) or outflow ($G = \rho_{vs} u_{vs}$). The Riemann solver converges on the correct u_s relatively quickly when one uses the following iteration scheme:

$$\begin{aligned} u_s[new] &= u_s[old] \times (1 - \Delta G_{norm}) & \text{if } G > 0 \\ u_s[new] &= u_s[old] \times (1 + \Delta G_{norm}) & \text{if } G < 0 \end{aligned} \quad (6.45)$$

When the suction velocity which gives the correct mass flux is finally determined, the momentum flux ($p + \rho u^2$) is computed using $U^* = (\rho^*, u^*, p^*)^T$.

6.5 Test Problem - Condensation in Initially Still Vapor

The methods for handling the condensation boundary condition are implemented in a FORTRAN subroutine called the "condbc.f" and is one of the subroutines provided in appendix A. The boundary condition was coupled to a one-dimensional version of the TSUNAMI code. The method is first benchmarked against three Flibe liquid-vapor cases

used by Schrock et al. [1992]. The three cases and properties of the Flibe are provided in the Tables 6.1 and 6.2 respectively.

Table 6.1. Conditions for Four Example Problems [Schrock et al. 1992]

Case	T_0 , K	p_0 , Pa	ρ_0 , kg/m ³	T_{∞} , K
1	5000	2.65×10^5	0.216	843
2	1645	2.65×10^5	0.656	843
3	1500	7.94×10^4	0.216	843

All the cases assume that cold uniform temperature liquid is suddenly brought into contact with hot vapor also initially uniform and at rest. The first case is that of superheated Flibe vapor at 5000 K and 265 kPa pressure contacting cold uniform liquid at 843 K. The second case is the of saturated vapor at 1645 K contacting liquid at 843 K, and the third case is that of saturated 1500 K vapor contacting cold 843 K liquid. The initial conditions were chosen because the kinetics mass flux will exceed the maximum available gas dynamics mass flux for early times, so the flow is choked. The objective was to study the choking duration and compare the predictions against an analytical solution.

Table 6.2. Flibe Properties (33% LiF, 67% BeF₂) [Schrock et al. 1992]

Property	Quantity
Liquid Thermal Diffusivity (α)	2.5×10^{-7} m ² /s
Liquid Thermal Conductivity (k)	1.20 W/m-K
Liquid Density (ρ)	2.02×10^3 kg/m ³
Liquid Const. Press. Spec. Heat (c_p)	2.38×10^3 J/kg-K
Heat of Vaporization (h_{fg})	5.56×10^6 J/kg

Vapor Pressure (p_{sat})	$\log_{10} p_{sat} \text{ (mm Hg)} = A - B/T_{ls} \text{ (K)}$ $A = 9.407, B = 1.0054 \times 10^4$
Average Molecular Weight (μ)	0.0339 kg/mole
Specific Heat Ratio (γ)	1.2*

*A constant ratio of specific heats is used. Schrock et al [1992] use a functional relationship for gamma which varies weakly with temperature and on average is approximately 1.2.

Schrock et al. [1992] give an analytical method for determining the liquid temperature which is based on the closed form solution by Carslaw and Jaeger [1959] for a constant heat flux on a semi-infinite slab. The solution assumes that convection is negligible and heat flux is constant on the surface. The temperature in the liquid is given by:

$$T_l(x, t) - T_{\infty} = \frac{2q_0''}{k} \sqrt{\alpha t} \operatorname{ierf}\left(\frac{x}{2\sqrt{\alpha t}}\right). \quad (6.46)$$

and the surface temperature is:

$$T_{ls}(t) = T_{\infty} + \frac{2q_0''}{k} \sqrt{\frac{\alpha t}{\pi}}. \quad (6.47)$$

Knowing the surface temperature and the analytical equations for isentropic expansion permits the calculation of the Schrage mass flux. This can be compared to the maximum gas dynamics flux and solved for the time when choking ends (i.e. when G becomes less than G_{vmax}). During the initial choked flow period, the gas dynamics flux is constant because the isentropic relations dictate that the choked condition must be itself a constant state if the gas possesses a constant stagnation state. Therefore, to better approximate the analytical solution, the numerical algorithm used for these runs neglected convection by truncating the convection terms in equations (6.31) and (6.38), the heat flux boundary condition and the energy equation respectively.

Figure 6.4 shows the computed condensation mass flux as a function of time for case 1. The initially flat, plateau region indicates the period of choking. Once the choking ends, the mass flux decreases as the surface continues to heat up. Table 6.3 gives the comparison between choking duration for both the analytical solution values and those computed by TSUNAMI in cases 1 through 3. The agreement with the analytical solution is within 1%. Each of the computed cases utilized a 300 node mesh for the vapor and 100 node mesh for the liquid. Figures 6.5 and 6.6 show graphs of the interface pressures and temperatures respectively, and figure 6.7 shows the temperature distribution in the liquid, all for case 1.

Table 6.3. Comparison of Choking Period and Peak Mass Flux

Case	Choking Duration (μ sec)	
	Analytical	TSUNAMI (cond. only)
1	0.709	0.700
2	0.984	0.980
3	7.40	7.44

One interesting phenomenon which the numerical calculation predicts is condensation induced shock reflection. Figure 6.8 shows a contour plot of the logarithmic density in $x-t$ space of the vapor for case 3. The horizontal axis represents the position in the vapor, and vertical axis time. The right edge of the plot is the condensing wall. The contours which emanate from the lower right corner are the characteristic lines of the rarefaction fan that result from the initial condensation. The flow is initially choked and so the surface condenses the maximum available mass flux. However, from figures 6.6 and 6.7, the liquid will heat up and reduce the condensation potential at the interface. Once the period of choking is over, the uncondensed vapor

which has been accelerated by the rarefaction will stagnate against the liquid generating a shock.

6.6 Test Problem - Effect of Condensation on the Shock Tube Problem

The second test problem is the *condensing* shock tube (see figure 6.9). The initial conditions are identical to case 1 above, except an imaginary diaphragm is assumed to hold the hot vapor at a 7mm standoff from the liquid surface. Both conduction and convection are considered. The vapor in the gap between the hot gas and the wall is assumed to possess the saturation pressure at the liquid surface temperature. This corresponds to a pressure less than 1 Pa. The liquid is also assumed originally uniform at 843 K. At time $t = 0$, the hot vapor begins to expand toward the liquid. Two boundary conditions are compared, an impermeable interface with no condensation versus a condensing surface. Figure 6.10 compares the density contour plots for the two cases. Because the shock propagates nearly into the vacuum, the pressure ratio is very high and gas dynamics predicts that the shock will be barely distinguishable from the contact surface. For a period close to 5 microseconds after contact, the condensing wall absorbs the entire gas flux. Then a reflected shock forms and moves to the left. Comparing the slopes of reflected shock shows that the condensation not only delays the shock reflection, but also reduces the wave velocity back into the oncoming gas.

Figure 6.11 shows the condensation mass flux at the interface as a function of time. The leading edge of the shock takes about 1 microsecond to reach the interface after which condensation begins. The condensation mass flux increases for the next 4 microseconds and then decreases because of liquid surface heat up. The peak flux is approximately 65 kg/m²s, which is lower than the 92 kg/m²s maximum flux for case 1 above (see figure 6.4). The peak mass fluxes between the two cases differ because of gas dynamics as well as kinetics. Gas dynamics predicts little or no distinction between the

contact surface and the shock for high pressure gas expanding into extremely low pressure. In the shock tube case, because the hot vapor is at a standoff distance and must expand nearly into vacuum to reach the liquid, the flow which first reaches the liquid is highly rarefied. The leading edge has very high velocity and high Mach number, but low pressure and density. Gas dynamics also predicts that the mass flux at the liquid surface will be time and space dependent according to the velocity characteristic lines discussed in chapter 1. The mass flux is constant and a maximum only for the zero-characteristic, which starts at the diaphragm position. All other positions in the shock tube such as at the liquid surface, have lower mass fluxes which increase with time toward the maximum mass flux. By inspection, in case 1 above, the vapor rests initially against the liquid and therefore the liquid interface is the diaphragm position, resulting in the constant maximum mass flux being condensed as long as the flow is choked. Hence, $92 \text{ kg/m}^2\text{s}$ is the maximum flux for both cases. Given an infinite amount of time, the mass flux at the liquid surface in the shock tube will eventually increase to the maximum. However, liquid surface heating reduces the kinetic theory condensation potential before the peak mass flux can rise to its maximum. Therefore the shock tube problem results in a lower mass and heat flux into the surface, resulting in a slower rise in liquid surface temperature. The lower mass flux extends the duration in which kinetic theory permits the complete condensation of all the vapor approaching the interface.

Once the surface temperature has risen beyond some level, complete condensation can no longer take place and a reflected shock will form, which propagates back into the gas. Figures 6.12, 6.13, and 6.14 respectively, show the density, velocity and pressure profiles in the gas at various times. The pressure and density behind the reflected shock increase quickly at first as excess mass which cannot be condensed piles up against the surface. But the rate of increase slows as the reflected shock moves away from the liquid surface. Gradually over a period greater than 20 microseconds, both pressure and density

increase to about 80% of their original stagnation values, while velocity decreases gradually during the same time period to about 10% of its maximum. The kinetic theory however, predicts that condensation, although diminished, continues to remove mass at over 10 kg/m²s during the entire computational period. In fact, at 24 microseconds, the velocity at the interface is still close to 100 m/s.

6.7 Effect on Initial Blast Venting in HYLIFE-II

To assess the impact of the early time condensation on the blast venting in HYLIFE-II, the vapor property profiles for the inner cavity calculations by Chen [1992] were used as the initial condition. The profiles, much like Glenn's [1980] profiles (figure 5.1) show a relatively uniform band of dense gas near the outer edge of the cavity and a velocity profile that decreases almost linearly from the maximum value at the edge to zero at the center. In this assessment, Chen's solution profiles were approximated by the linear profiles given in figure 6.15. The density in the outer band of vapor is assume uniform at 1.3 kg/m³. The velocity at the outer edge of the expanding vapor is 10,000 m/s and decreases linearly to zero at the center. Pressure in the entire cavity is assumed a uniform 30 MPa. The computation utilized a one-dimensional grid with 100 nodes in the liquid, and 5000 nodes in the vapor to account for the larger gas domain. Two cases are presented below, one with condensation and one without. Figure 6.16 compares the resulting contour plots for the densities showing almost no change in behavior. This is surprising considering the previous shock tube case, which showed that condensation could forestall shock reflection for a period of 4 microseconds. Both the liquid surface mass flux curve (figure 6.17) and the temperature distribution curves in the liquid (figure 6.18) indicate that the liquid does absorb a considerable amount of energy, but little effect is observed in the gas dynamics. Evaporation never occurs on the surface because the shock reflection is predicted to always maintain a high pressure on the surface.

The reason why the gas dynamics shows no varying with and without condensation is because the surface quickly heats up and shuts down the rapid condensation. The mass flux curve shows that the mass flux comes down to less than 1 kg/m²s after just 10 microseconds. The heat flux from the vapor at this condensation rate is large because the vapor is extremely energetic. However, the removed energy is small compared to the total energy in the gas. If the blast venting occurs over a period of 1 ms, and for the average of that time the mass flux is roughly constant at 1 kg/m²s, then the approximate amount of heat removed is just the product of mass flux and heat of vaporization. From the properties in table 6.2, this amounts to about 10 kJ/m² removed in 1 ms time. Typically, the slabs will have about 2 meters height and 1 meter length and 7 cm width, which translates into roughly 4 m² per slab. For 37 slabs in the cavity, this translates to roughly 150 m² of surface area. Hence, if only the surface area of the jets or slabs are considered, the total condensation removes only 1.5 MJ in 1 ms, which is negligible compared to the total vapor energy of 105 MJ. However, if a continuous spray can approximately 100 times more surface area, then this may greatly reduce FSW loading by the gas shock. The amount of surface area per unit volume of liquid varies roughly as the inverse of the characteristic dimension. The task for the designers then becomes choosing the quantity of spray and droplet size droplets which simultaneously maximizes the economics of pumping but minimizes the wall loading. For spray flow which is 1/10th the volumetric flow rate of the blanket, this translates into roughly 1/1000th the characteristic dimension of the slabs (i.e. millimeter sized droplets) to achieve the extra 100 times surface area.

With the current HYLIFE design, since the spray is on the outside of the blanket, this will not mitigate impulse the blanket receives, which is fortunately modest in the slab geometry case. However, the asymmetry in the gas shock loading on the FSW may be

significantly corrected by judicious placement of fine sprays near locations which will receive the highest loads.

Figure 6.1. Schematic representation of Shrage's kinetic theory of condensation.

Figure 6.2. Finite difference grid representation of the liquid. The Bulk liquid temperature is governed by conduction and convection (equation 6.38 or 6.39). The liquid interface temperature, T_{ls} , is defined by the heat flux boundary condition (equation 6.32).

Figure 6.3. Godunov flux for vapor mass, momentum and energy at the interface. The mass flux is determined by kinetic theory. The energy flux is computed from known enthalpy and kinetics mass flux. The momentum requires the Riemann solution to compute the pressure.

Figure 6.4. Net condensation mass flux versus time curve for case 1 of initially quiescent Flibe vapor in contact with cold liquid Flibe.

Figure 6.5. Interface pressure for liquid and vapor versus time curves for case 1.

Figure 6.6. Interface temperature for liquid and vapor versus time for case 1

Figure 6.7. Temperature distribution in the liquid at various times for case 1

Fig. 6.8 Logarithmic density contour plot for x-t space, case 1

Figure 6.9. Geometry used for condensation shock tube problem.

Figure 6.10. Comparison of density contour plots for identical shocks on an impermeable surface (left) and a condensing surface (right).

Figure 6.11. Net condensation mass flux versus time curve for superheated Flibe vapor at 5000 K and 2.65×10^5 Pa, at 6.7mm standoff distance from the surface.

Figure 6.12. Density profiles in the vapor at various times for the shock tube condensation problem

Figure 6.13. Velocity profiles in the vapor at various times for the shock tube condensation problem

Figure 6.14. Pressure profiles in the vapor at various times for the shock tube condensation problem

Figure 6.15. Simplified profiles of the inner cavity gas properties for the HYLIFE-II case from Chen [1992].

Figure 6.16. Comparison of density contour plots of the shock reflection with (top) and without (bottom) condensation for the HYLIFE-II case.

Figure 6.17. Mass flux at liquid surface for HYLIFE-II inner cavity vapor condensing on uniform, 843 K liquid Flibe.

Figure 6.18. Temperature distribution in the liquid at various times for HYLIFE-II inner cavity vapor condensing on uniform, 843 K liquid Flibe.

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Appendix A. TSUNAMI USER MANUAL AND SOURCE CODE

A-1.1 TSUNAMI User Manual - Introduction

TSUNAMI is written in FORTRAN, and can be compiled using all standard f77 compilers. This section describes the code implementation and outlines the architecture of TSUNAMI. A full source listing follows in the next section. TSUNAMI consists of a main program, several subroutines, a custom input deck generation program for custom geometry set-up, a custom output file subroutine, and 3 include files. The program and subroutine names are listed in Table A.1, with a brief description of the purpose of each.

The TSUNAMI code is extensively commented to aid review, revision, and updating. Because the code will be ultimately used for a variety of problems where additional routines will be required, such as the subroutine `custom_init.f`, the main sources are written as separate modules to allow ease of interchangeability and enhancement.

The complete source code is available via electronic mail or on magnetic media from:

Nuclear Thermal Hydraulics Group
Department of Nuclear Engineering
University of California at Berkeley
Berkeley, CA 94720
(510) 642-0421
(510) 643-9685 FAX
Email: tsunami@fusion.Nuc.Berkeley.EDU

Table A.1 - TSUNAMI program and subroutines.

Name	Purpose
tsunami.f	main program - accepts data input, initializes variables, and iterates through time steps, controls operator splitting sweep, controls output, and includes the subroutines listed below.
tsunami_in	subroutine called by main program to read in input deck.
tsunami_out	subroutine called by main program to direct output data handling.
checku	subroutine called by main to compute maximum velocity on the grid which is necessary for Courant number calculation and tracking.
shock1d	subroutine called by main to compute 1-D gas dynamics using a 2nd order Godunov integrator; code also performs conservative differencing for a single time step.
riemann	subroutine called by shock1d.f to compute the exact solution to the general Riemann shock problem.
convert	subroutine called by main which converts a vector of conserved quantities into physical quantities.
cmvgt	logical function $fn(x,y,z)$ which choses the real value 'x' if z is true, otherwise, choses real value 'y.'
ws	real function $fn(p,p0,\tau0,\gamma)$ which computes the mass flux across a shock for the given parameters.
condbc	subroutine called by shock1d which specifically handles condensation at the liquid gas interface using kinetic theory
custom_init.f	program which generates input decks to be read by tsunami_in.f.
custom_out.f	subroutine called by tsunami_out.f which handles customized output information.
tsn_geo.i	include file called by main and all subroutines which need the array dimensions and geometric constants for the grid being used.
tsn_inp.i	include file called by main and tsunami_in.f for miscellaneous run-time and error handling parameters.
tsn_out.i	include file called by tsunami_out.f and custom_out.f which require specific information on the items to be sent to the output file(s).
custom_init.i	include file used in the custom_init.f program to create input decks for the tsunami.f kernel.
custom_out.i	include file used in the custom_out.f subroutine for customized outputs.

TSUNAMI FLOW CHART TOP LEVEL SCHEMATIC

Fig. A.1 Flow diagram for TSUNAMI

GAS DYNAMICS SWEEP - 2nd ORDER GODUNOV INTEGRATOR FOR 1-D ARRAY

Fig. A.2 Specific flow diagram for Godunov Integrator

A-1.2 TSUNAMI User Manual - Input/Output Specifications

TSUNAMI is a three part program consisting of input data file generator (custom_init.f), the actual computation fluid dynamics kernel (tsunami.f) and the output data post processor (custom_out.f). The TSUNAMI code itself consists only of the computational kernel. However, sample input and output programs are included along with algorithms for placing standard objects in the flow field. The input file generator sets up the initial geometry, density, velocity, and pressure fields and then outputs them to an input deck file to be read by tsunami.f. The computational kernel computes the gas dynamics and outputs data to an output file which varies depending on the customization of the output program. For most purposes, the user must write the custom input and output programs. This section describes the specifications for the input and output programs.

Input Deck

The TSUNAMI gas dynamics kernel requires all the information to be defined for the initial condition. This consists of 8 variable arrays: rho, u, v, p, thetax, thetay, typex, and typey. These are all dimensionally the same size arrays, consisting of ncellx by ncelly number of nodes. Rho is the variable for density, u the x-velocity (positive to the right, negative to the left), v the y-velocity (positive up and negative down), p the pressure, thetax the x-angle of the node, thetay the y-angle of the node, and typex and typey, the type of node it is in the reference direction. The angles and the types are used for boundary condition calculations. Each set consists of the type flag, which first tells the code whether the node is a boundary, interior, or free node, and second, the angle which is made with the normal into the boundary node. Two sets are necessary because the operator splitting method changes reference axes when the direction of computation changes from horizontal to vertical. In actuality, only one angle needs to be stored for each node, however, because this would cost computational effort in recalculation of the

transverse reference angle every time step for every node, the decision was made to expend more memory storage for the sake of speed.

Rho, u, v, and p

Specifying rho, u, v, p should be a straight forward process except at object interiors, and boundaries. In the most free nodes, the rho, u, v, and p are just what their physically space averaged quantities should be. In object or wall interiors, the usual practice is to uniformly set the density of the material to a higher initial value, the velocities to zero, and the pressure to a uniform value equal to the minimum ambient. Also, both typex and typey are set to zero. A node which is flagged as having type zero is excepted from the gas dynamics calculation. At boundaries, rho,u,v, and p are specified the same as if they were free nodes.

Figure A.3. Example of type and angle specification for some arbitrary nodes.

Thetax, thetay, typex, and typey.

Thetax and thetay are the geometric variables which store the angle information for complex boundary gas dynamics calculation. Each element in the two arrays is complemented by another element in the typex or typey variable arrays. (See figure A.3) In a normal free and open node where gas can move in any direction, the thetax and thetay are both set equal to a real value of 1.0. When gas is only free to move into cells on either side in one direction (i.e. cell is sandwiched by other gas cells), but the cell is butted up against a type zero cell in the transverse direction (i.e. the cell is a boundary cell in the other direction), then one of the angles, either thetax or thetay will be determined and the typex or typey flagged, while the other variable is just type 1 and angle is zero. The angle is taken as the normal into the boundary. However, this value changes with the sweep direction. When sweeping horizontally, the angle into a boundary is taken with reference to the positive x-axis rotating counter-clockwise. When sweeping vertically, the angle is taken with reference to the positive y-axis rotating clockwise. (this is equivalent to a transformation from x-y coordinates to y-x coordinates in Cartesian space.)

INT FILE.DAT -- The input deck.

The form of the input deck is actually in unformatted binary real and integer in single precision. The first values are: the initial real number time t in seconds, the initial integer number of time steps n , the initial integer number of data frames $nframes$ to begin with, and the gamma constant for the gas. The reason why these are placed here are because a similar data file is output every certain number of user-specified time steps as a safety against system crashes. The calculation can be resumed from the point of interruption with most likely only a small loss in computational time. (See section labeled "Crash handling" in this chapter.)

Immediately following the first three values are the 8 arrays rho, u, v, p, typex, typey, thetax, and thetay. These are mixed sequentially and must be stored as columns. That is, the data must be organized written as in the example below:

```

write (11) t, n, nframes, gamma
do 10 i = 1, ncellx
  do 20 j = 1, ncelly
    write (11) rho (i,j)
    write (11) u (i,j)
    write (11) v (i,j)
    write (11) p (i,j)
    write (11) typex (i,j)
    write (11) typey (i,j)
    write (11) thetax (i,j)
    write (11) thetay (i,j)
  20 continue
10 continue

```

Example A.1 Sample algorithm for writing the input deck to TSUNAMI

Table A.2. Boundary condition variable definitions.

typex	real number flag which tells the TSUNAMI code what type of node is being computed when calculation is sweeping horizontally.
typey	real number flag which tells the TSUNAMI code what type of node is being computed when calculation is sweeping vertically.
Type	Purpose
0	used for nodes specifically inside objects to signal the code to skip gas dynamics computation.
1	normal open, free gas node.
2	left-handed boundary for objects in the flow field.
3	right-handed boundary for objects in the flow field.
4	open left-handed boundary node
5	open right-handed boundary node
6	closed left handed boundary node for walls (same as 2 but allows for differentiation between objects and walls).
7	close right-handed boundary node for walls (same as 3 but allows for differentiation between objects and walls)
8	left-handed condensing boundary node
9	right-handed condensing boundary node

The TSU_GEO.I File

The TSU_GEO.I file is a FORTRAN include file called by the compiler during FORTRAN compilation. The last 3 letters of in the file name are short hand for "geometry" -- and thus this file is used to configure the grid. The include file basically takes advantage of the FORTRAN "parameter" statement in specifying constants which

do not vary. Also, depending on the computer hardware, variables assigned using parameter statements may have faster access times in the memory storage. The standard parameters in this include file are:

Table A.3 The parameters for the tsu_geo.i include file

ncellx	the number of nodes in the horizontal direction (specified from 1 to ncellx)
ncelly	the number of nodes in the vertical direction (specified from 1 to ncelly)
nmax	the maximum dimension in number of nodes (equals the larger of ncellx and ncelly)
pi	the value of $\pi = 3.1415926954$
dx	the width of one node in the x-direction (meters)
dy	the width of one node in the y-direction (meters)

The TSU_INP.I File

The TSU_INP.I file is another include file which contains run time information. The file contains items which control the Courant condition and run time to quit. It also contains the input deck file name to be read by TSUNAMI. The parameters are:

Table A.4 The parameters for the tsu_inp.i include file.

courant	the CFL condition at which to run at (real no. must be less than 1.0)
tstop	the gas dynamics time to run up to before quitting. (Real no.)
initfile	character variable which stores name of input deck

The TSU_OUT.I File

The TSU_OUT.I file is another include file which contains output specific parameter information. The file contains items which control the time increment between outputs, flags which switch standard output on and off, transducer locations, and output file names. The parameters are:

Table A.5 The parameters for the tsu_out.i include file.

dt_frame	the physical gas dynamics time (real seconds) interval between frame dumps for animation purposes
nt_dump	the number of time steps executed before a dump is done to backup against system crashes which may terminate a run. This allows from restart of the code after the crash with only minor losses in computation time. (integer)

ifile#	flag which determines if output file is turned on or off. Currently there are 8 ifile flag variables. These represent rho, u, v, and p frame data, and rho, u, v, and p transducer data respectively. The # symbol is an integer from 1 to 8 which represents the referenced variable. The value of an ifile variable must be either 0 (zero) for off and 1 for on.
icustom	this is another flag like ifile, exit it controls the on/off for the custom_out.f subroutine. 1 for on, 0 for off.
ntx#	these are the variables for the grid location of the transducers. # is an integer from 1 to 6 representing 6 channels for transducer data. All 6 channels are dumped if the corresponding ifile flag is on. None are output is the ifile flag is off. The actual value for ntx# or nty# is an integer corresponding to the grid location where one wants the transducer put.
nty#	
dfile	character filename for the dump file.
file#	8 character variables which store the names of the rho, u, v and p frame output files, and the rho, u, v, and p transducer data files. # is an integer from 1 to 8.
cfile	character filename for the custom output file.

The CUSTOM_INIT.I File

The CUSTOM_INIT.I file is another include file which contains run time information. Except, this only is good for the custom_init.f program which is used to create the input deck. This file appears in the program header along with the tsu_geo.i and the tsu_inp.i files in the custom_init.f program. The file is recommended as a parameter specification location for things such as the initial Mach number of a shock, gas properties (e.g. gas constant R or gamma, or molecular weight). This file is also used to store custom grid specific coordinates such as position of objects, or boundaries.

The CUSTOM_OUT File

The CUSTOM_OUT.I file is another include file which contains run time information but now for the custom output. This is compiled in conjunction with the custom_out.f subroutine. The file is recommended as a for specifying array sizes for objects and the like if a custom output is desired, for example for drag on each individual object in the flow field, it may be desirable to track the total momentum transfer due to drag on an object. this would require information on object coordinates, density, relative

position in the reactor vessel, etc. Some of the information can be stored in the custom_init.i file and then it becomes redundant to specify it again in another include file. It is recommended that any compilation of the code include both custom_init.i and custom_out.i files in the header.

Running TSUNAMI on a UNIX System

To run the code there are 2 basic steps. The assumption here is that you are operating in a UNIX workstation or Cray UNICOS environment. The first step is to create the input data deck file. To this copy all the necessary include files and the program custom_init.f to the working directory and type:

```
% f77 custom_init.f
```

There is no restriction on the name of the custom_init.f file. One may chose whatever name for the program as long as the output is in the format needed. On most UNIX systems, the compiling and linking are done all in one step. The resulting file is a.out. Execute this program by typing:

```
% a.out
```

On Cray UNICOS systems, compiling, linking and running is done using:

```
% cft77 custom_init.f
```

```
% ld custom_init.o
```

```
% a.out
```

The resulting file will be in machine binary format and have several megabytes size for a typical 200 x 200 grid. The filename will be whatever the name is given in the initfile variable in the tsu_inp.i file. The second step, once the initial

conditions file exists is to compile the TSUNAMI kernel and custom output routines together. This is done by using:

```
% f77 tsunami.f custom_out.f
```

or the Cray equivalent. To enhance computational speed, optimization should also be used. On Digital DECstations or Sun Sparcstations, computing speed can be increased up to 3 times by using compiling with the fast option:

```
% f77 -fast -O4 tsunami.f custom_out.f (Sun Sparcstation)
```

or

```
% f77 -fast tsunami.f custom_out.f (DECstation)
```

Compiling with the fast option usually requires that the code be "clean." This means that mathematical operations within the custom routines must be written with no inter-species numerical operations. That is, mathematical operation should be done in either all integer or all floating point in the correct precision. One needs to take care that real constants all include decimal points, any integers are converted to floating point when doing math on real numbers, and vice-versa. Division by zero, or numerical solutions which go to infinity must be avoided. Failure to produce "clean" code may result in a crash and core dump during execution. The actual TSUNAMI kernel has been repeatedly tested and executed under the highest optimizations with no crash and correct solution convergence. If a problem exists during a run, resulting in a crash, then more than likely, the initial conditions or the output subroutines may be fault.

A-2. tsunami.f Source Code

```
c-----
c      program tsunami
c-----
c Transient Shockwave Upwind Numerical Analysis Method for ICF
c-----
c      version 1.1  August 1992
c-----
c
c      James C. Liu, Xiang Ming Chen, Per F. Peterson, Phil Colella,
c      Virgil E. Schrock
c
c      Department of Nuclear Engineering and Mechanical Engineering
c      University of California at Berkeley
c      Berkeley, California 94720
c
c      (510) 642-0421
c      (510) 643-9685 FAX
c      tsunami@four-lab4.Berkeley.EDU (Internet)
c-----
c      Work performed under the auspices of the United States
c      Department of Energy for the Lawrence Livermore National
c      Laboratory under contract W-7405-ENG-48.
c-----
c
c This program uses 2nd order Godunov method and Riemann Solvers to
c compute gas dynamics in Inertial Confinement Fusion Reactors.
c
c Basic components required to run this code are:
c      -TSUNAMI.F -- this code
c      -TSU_GEO.I -- geometric information include file
c      -TSU_INP.I -- run-time initial information include file
c      -TSU_OUT.I -- output data format include file
c
c A front end package may be used to supply the necessary initial data
c The files are one fortran file and one include file:
c      CUSTOM_INIT.F
c      CUSTOM_INIT.I
c
c For more explicit instructions, see TSUNAMI Documentation
c-----
c
c NOMENCLATURE
c
c rho = density
c u = velocity in x-direction
c v = velocity in y-direction
c p = pressure
c thetax = normal angle (radians) into surface in x-y frame
c thetay = normal angle (radians) into surface in y-x frame
c typex = type of node (interior, exterior, boundary, etc) in x frame
c typey = type of node (interior, exterior, boundary, etc) in y frame
c gamma = ratio of specific heats, adiabatic constant
c dx = delta x (grid spacing)
c dy = delta y (grid spacing)
c dt = time step
c ncellx = number of cells on grid in x-direction
c ncelly = number of cells on grid in y-direction
c t = time (accumulated)
c
```

```

c-----
c
      include "tsu_geo.i"
      include "tsu_inp.i"
      include "tsu_out.i"
c
c ::::: FLOW PROPERTIES
      dimension rho(1:ncellx,1:ncelly)
      dimension u(1:ncellx,1:ncelly)
      dimension v(1:ncellx,1:ncelly)
      dimension p(1:ncellx,1:ncelly)
c
c ::::: GRID & GEOMETRIC INFO
      dimension typex(1:ncellx,1:ncelly)
      dimension typey(1:ncellx,1:ncelly)
      dimension thetax(1:ncellx,1:ncelly)
      dimension thetay(1:ncellx,1:ncelly)
c
c ::::: DUMMY ARGUMENTS & TEMPORARY VARIABLES
      dimension q(1:6,1:nmax)
      dimension utemp(1:5,1:nmax)
      dimension temprho(1:ncellx,1:ncelly)
      dimension tempu(1:ncellx,1:ncelly)
      dimension tempv(1:ncellx,1:ncelly)
      dimension tempp(1:ncellx,1:ncelly)
c
c ::::: OPEN SEQUENTIAL OUTPUT FILES
      if (ifile1 .eq. 1) open (unit=11, file=file1, form='unformatted')
      if (ifile2 .eq. 1) open (unit=12, file=file2, form='unformatted')
      if (ifile3 .eq. 1) open (unit=13, file=file3, form='unformatted')
      if (ifile4 .eq. 1) open (unit=14, file=file4, form='unformatted')
      if (ifile5 .eq. 1) open (unit=15, file=file5, form='formatted')
      if (ifile6 .eq. 1) open (unit=16, file=file6, form='formatted')
      if (ifile7 .eq. 1) open (unit=17, file=file7, form='formatted')
      if (ifile8 .eq. 1) open (unit=18, file=file8, form='formatted')
      if (icustom .eq. 1) open (unit=19, file=cfile, form='formatted')
c
c ::::: SET UP INITIAL CONDITIONS
      call tsunami_in(t,n,nframes,gamma,rho,u,v,p,
        & typex,typey,thetax,thetay)
c
c ::::: INITIALIZE THE TEMP ARRAY VARIABLES
      do 10 i = 1,ncellx
        do 20 j = 1,ncelly
          temprho(i,j) = rho(i,j)
          tempu(i,j) = u(i,j)
          tempv(i,j) = v(i,j)
          tempp(i,j) = p(i,j)
        20 continue
      10 continue
c
c ::::: DETERMINE FIRST TIME STEP SIZE
      call checku(rho,u,v,p,gamma,umax,ctempmax,ixcoord,iycoord)
      dt = courant*min(dx,dy)/umax
c
c ::::: OUTPUT INITIAL CONDITION
      call tsunami_out(t,dt,n,nframes,gamma,rho,u,v,p,
        & typex,typey,thetax,thetay)
c
c-----
c 2-D COMPUTATION REQUIRES THAT S(U)=LxLyLx(U) i.e., SWEEP X
c THEN Y AND THEN X AND THEN X FOR 2ND ORDER OP. SPLITTING (STRANG)
c TIME STEP SIZE MUST REMAIN CONSTANT FOR 2 TIME STEPS.
c THEREFORE AFTER EACH CALCULATION, THE CFL CONDITION IS CHECKED.

```

```

c IF VIOLATED, THE TIME STEP IS REDUCED AND COMPUATION IS STARTED
c FROM THE BEGINNING AGAIN.
c
c ..... sweep x-direction.....
c
200   continue
      iflag = 0
      nedge = ncellx
      do 100 k2 = 1,ncelly
        do 110 k1 = 1,ncellx
          q(1,k1) = rho(k1,k2)
          q(2,k1) = u(k1,k2)
          q(3,k1) = p(k1,k2)
          q(4,k1) = v(k1,k2)
          q(5,k1) = thetax(k1,k2)
          q(6,k1) = typex(k1,k2)
110   continue
        call shock1d(q,utemp,dt,gamma,nedge)
        call convert(temprho,tempu,tempv,tempp,gamma,utemp,k2,iflag,nedge)
100   continue
      call checku(temprho,tempu,tempv,tempp,gamma,umax,ctempmax,
&      ixcoord,iycoord)
      if((dt*umax/min(dx,dy)).ge.1.) then
        print*, 'CFL violation',umax,ctempmax,ixcoord,iycoord
        dt = 0.7*min(dx,dy)/umax
        goto 200
      endif
c
c ..... sweep y-direction.....
c
      iflag = 1
      nedge = ncelly
      do 120 k1 = 1,ncellx
        do 130 k2 = 1,ncelly
          q(1,k2) = temprho(k1,k2)
          q(2,k2) = tempv(k1,k2)
          q(3,k2) = tempp(k1,k2)
          q(4,k2) = tempu(k1,k2)
          q(5,k2) = thetay(k1,k2)
          q(6,k2) = typey(k1,k2)
130   continue
        call shock1d(q,utemp,dt,gamma,nedge)
        call convert(temprho,tempu,tempv,tempp,gamma,utemp,k1,iflag,nedge)
120   continue
      call checku(temprho,tempu,tempv,tempp,gamma,umax,ctempmax,
&      ixcoord,iycoord)
      if((dt*umax/min(dx,dy)).ge.1.) then
        print*, 'CFL violation',umax,ctempmax,ixcoord,iycoord
        dt = 0.7*min(dx,dy)/umax
        goto 200
      endif
c
c ..... sweep y-direction.....
c
      iflag = 1
      nedge = ncelly
      do 140 k1 = 1,ncellx
        do 150 k2 = 1,ncelly
          q(1,k2) = temprho(k1,k2)
          q(2,k2) = tempv(k1,k2)
          q(3,k2) = tempp(k1,k2)
          q(4,k2) = tempu(k1,k2)
          q(5,k2) = thetay(k1,k2)
          q(6,k2) = typey(k1,k2)

```

```

150      continue
        call shock1d(q,utemp,dt,gamma,nedge)
        call convert(temprho,tempu,tempv,tempp,gamma,utemp,k1,iflag,nedge)
140      continue
        call checku(temprho,tempu,tempv,tempp,gamma,umax,ctempmax,
&          ixcoord,iycoord)
        if((dt*umax/min(dx,dy)).ge.1.) then
            print*, 'CFL violation',umax,ctempmax,ixcoord,iycoord
            dt = .7*min(dx,dy)/umax
            goto 200
        endif
c
c ..... sweep x-direction.....
c
        iflag = 0
        nedge = ncellx
        do 160 k2 = 1,ncelly
            do 170 k1 = 1,ncellx
                q(1,k1) = temprho(k1,k2)
                q(2,k1) = tempu(k1,k2)
                q(3,k1) = tempp(k1,k2)
                q(4,k1) = tempv(k1,k2)
                q(5,k1) = thetax(k1,k2)
                q(6,k1) = typex(k1,k2)
170          continue
            call shock1d(q,utemp,dt,gamma,nedge)
            call convert(temprho,tempu,tempv,tempp,gamma,utemp,k2,iflag,nedge)
160          continue
            call checku(temprho,tempu,tempv,tempp,gamma,umax,ctempmax,
&              ixcoord,iycoord)
            if((dt*umax/min(dx,dy)).ge.1.) then
                print*, 'CFL violation',umax,ctempmax,ixcoord,iycoord
                dt = 0.7*min(dx,dy)/umax
                goto 200
            endif
c
c .....assign temp values to rho,u,v, and p.....
c
        do 180 i = 1, ncellx
            do 190 j = 1, ncelly
                rho(i,j) = temprho(i,j)
                u(i,j) = tempu(i,j)
                v(i,j) = tempv(i,j)
                p(i,j) = tempp(i,j)
190          continue
180        continue
c
c ::::: OUTPUTS & ACCUMULATED TIME UPDATE
        call tsunami_out(t,dt,n,nframes,gamma,rho,u,v,p,
&            typex,typey,thetax,thetay)
c
c ::::: OUTPUT RUN_TIME DIAGNOSTICS TO SCREEN
        print*,t,tstop,dt,umax,ctempmax,ixcoord,iycoord
c
c ::::: COMPUTE NEW TIME STEP
        call checku(rho,u,v,p,gamma,umax,ctempmax,ixcoord,iycoord)
        dt = courant*min(dx,dy)/umax
c
c ::::: RUN UNTIL tstop (PARAMETER FROM tsu_inp.i FILE)
        if(t.le.tstop) then
            goto 200
        endif
c
        print *, 'number of time steps was: ', n

```



```

        print *, 'number of frames was: ', nframes
c
c :::::: CLOSE FILE UNITS & QUIT
300    continue
        if(ifile1.eq.1) close (11)
        if(ifile2.eq.1) close (12)
        if(ifile3.eq.1) close (13)
        if(ifile4.eq.1) close (14)
        if(ifile5.eq.1) close (15)
        if(ifile6.eq.1) close (16)
        if(ifile7.eq.1) close (17)
        if(ifile8.eq.1) close (18)
        if(icustom.eq.1) close (19)
        end
c
c -----
      subroutine tsunami_in(t,n,nframes,gamma,rho,u,v,p,
&          typex,typey,thetax,thetay)
c -----
c :::::: READS IN INITIAL CONDITIONS FROM INPUT FILE "INITIAL.DAT"
c
      include "tsu_geo.i"
      include "tsu_inp.i"
c
      dimension rho(1:ncellx,1:ncelly)
      dimension u(1:ncellx,1:ncelly)
      dimension v(1:ncellx,1:ncelly)
      dimension p(1:ncellx,1:ncelly)
      dimension typex(1:ncellx,1:ncelly)
      dimension typey(1:ncellx,1:ncelly)
      dimension thetax(1:ncellx,1:ncelly)
      dimension thetay(1:ncellx,1:ncelly)
c
c :::::: READ IN DATA FILE
      open(29,file=initfile,form='unformatted')
      read(29) t,n,nframes,gamma
      do 10 i = 1, ncellx
        do 20 j = 1,ncelly
          read(29) rho(i,j)
          read(29) u(i,j)
          read(29) v(i,j)
          read(29) p(i,j)
          read(29) typex(i,j)
          read(29) typey(i,j)
          read(29) thetax(i,j)
          read(29) thetay(i,j)
20        continue
10      continue
      close(29)
      return
      end
c
c -----
      subroutine checku(rho,u,v,p,gamma,umax,ctempmax,
&          ixcoord,iycoord)
c -----
c :::::: RETURNS VALUE OF MAX SPEED OF EITHER u+c,u-c,v+c, OR v-c
c
      include "tsu_geo.i"
c
      dimension rho(1:ncellx,1:ncelly)
      dimension u(1:ncellx,1:ncelly)
      dimension v(1:ncellx,1:ncelly)
      dimension p(1:ncellx,1:ncelly)

```

```

c
c ::::: SET INITIAL DEFAULT RETURN VALUES
      umax = 1.
      ctempmax = 0.
      ixcoord = 1
      iycoord = 1

c
c ::::: DETERMINE MAX VELOCITY BY CHECKING ALL COMBINATIONS
      do 100 i=1,ncellx
        do 110 j=1,ncelly
          umax_old = umax
          ctemp = sqrt(gamma*p(i,j)/rho(i,j))
          umax = max(umax,abs(v(i,j)-ctemp),abs(v(i,j)+ctemp),
&                abs(u(i,j)-ctemp),abs(u(i,j)+ctemp))
          if(umax_old.ne.umax) then
            ctempmax = ctemp
            ixcoord = i
            iycoord = j
          endif
110      continue
100      continue
      return
      end

c
c-----
      subroutine tsunami_out(t,dt,n,nframes,gamma,rho,u,v,p,
&      typex,typey,thetax,thetay)
c-----
c ::::: OUTPUT RESULTS TO DATA FILES
c
      include "tsu_geo.i"
      include "tsu_out.i"

c
      dimension rho(1:ncellx,1:ncelly)
      dimension u(1:ncellx,1:ncelly)
      dimension v(1:ncellx,1:ncelly)
      dimension p(1:ncellx,1:ncelly)
      dimension typex(1:ncellx,1:ncelly)
      dimension typey(1:ncellx,1:ncelly)
      dimension thetax(1:ncellx,1:ncelly)
      dimension thetay(1:ncellx,1:ncelly)

c-----backup dump every nt_dump number of timesteps-----
      if(nt_dump .ne. 0) then
        check = mod(float(n),float(nt_dump))
        if(check .eq. 0.) then
          open (unit=30, file=dfile, form='unformatted')
          write(30) t,n,nframes,gamma
          do 10 i = 1, ncellx
            do 20 j = 1,ncelly
              write(30) rho(i,j)
              write(30) u(i,j)
              write(30) v(i,j)
              write(30) p(i,j)
              write(30) typex(i,j)
              write(30) typey(i,j)
              write(30) thetax(i,j)
              write(30) thetay(i,j)
20          continue
10          continue
          close(30)
        endif
      endif
c

```

```

c-----frame info output loop-----
c
c ::::: OUTPUT DENSITY, VELOCITY, & PRESSURE EVERY dt_frame SECONDS
      if (dt_frame .eq. 0.) goto 1111
      t_old = mod(t,dt_frame)
      t = t + 2.*dt
      n = n + 2
      if((mod(t,dt_frame).lt.t_old).or.(2.*dt.gt.dt_frame)
        & .or.(t.eq.2.*dt))then
c
c ::::: OUTPUT LOG(10) OF DENSITY IF ifile1 = 1
      if (ifile1 .eq. 1) then
        do 100 j = 1,ncelly
          do 110 i = 1,ncellx
            write(11) log(rho(i,j))/2.303
110          continue
100        continue
          write(11) t
        endif
c
c ::::: OUTPUT x-VELOCITY IF ifile2 = 1
      if (ifile2 .eq. 1) then
        do 200 j = 1,ncelly
          do 210 i = 1,ncellx
            write(12) u(i,j)
210          continue
200        continue
          write(12) t
        endif
c
c ::::: OUTPUT y-VELOCITY IF ifile3 = 1
      if (ifile3 .eq. 1) then
        do 300 j = 1,ncelly
          do 310 i = 1,ncellx
            write(13) v(i,j)
310          continue
300        continue
          write(13) t
        endif
c
c ::::: OUTPUT LOG(10) OF PRESSURE IF ifile4 = 1
      if (ifile4 .eq. 1) then
        do 400 j = 1,ncelly
          do 410 i = 1,ncellx
            write(14) log(p(i,j))/2.303
410          continue
400        continue
          write(14) t
        endif
        nframes = nframes + 1
      endif
c
c -----stuff to output every time step-----
1111 continue
c
c ::::: OUTPUT DENSITY TRANSDUCER TRACES
      if (ifile5 .eq. 1) then
        write(15,900) t,rho(ntx1,nty1),rho(ntx2,nty2),rho(ntx3,nty3),
        & rho(ntx4,nty4),rho(ntx5,nty5),rho(ntx6,nty6)
      endif
c
c ::::: OUTPUT X-VELOCITY TRANSDUCER TRACES
      if (ifile6 .eq. 1) then
        write(16,900) t,u(ntx1,nty1),u(ntx2,nty2),u(ntx3,nty3),

```

```

      &      u(ntx4,nty4),u(ntx5,nty5),u(ntx6,nty6)
      endif
c
c :::::: OUTPUT Y-VELOCITY TRANSDUCER TRACES
      if (ifile7 .eq. 1) then
        write(17,900) t,v(ntx1,nty1),v(ntx2,nty2),v(ntx3,nty3),
      &      v(ntx4,nty4),v(ntx5,nty5),v(ntx6,nty6)
      endif
c
c :::::: OUTPUT PRESSURE TRANSDUCER TRACES
      if (ifile8 .eq. 1) then
        write(18,900) t,p(ntx1,nty1),p(ntx2,nty2),p(ntx3,nty3),
      &      p(ntx4,nty4),p(ntx5,nty5),p(ntx6,nty6)
      endif
c
c-----CUSTOM OUTPUT-----
      if (icustom .eq. 1) then
        call custom_out(t,dt,n,nframes,gamma,rho,u,v,p,
      &      typex,typey,thetax,thetay)
      endif
c-----
      900      format(6(e11.4,1x),e11.4)
c-----
      return
      end
c
c-----
      subroutine shockld(q,utemp,dt,gamma,nedge)
c-----
c :::::: 2nd ORDER GODUNOV INTEGRATOR
c
      include "tsu_geo.i"
c
      dimension q(1:6,1:nmax)
      dimension utemp(1:5,1:nmax)
      dimension u(1:4,1:nmax)
      dimension dq(1:4,1:nmax)
      dimension charc(1:2,1:nmax)
      dimension c(1:nmax)
      dimension fhalf(1:4,1:nmax+1)
      dimension qstar(1:4)
      dimension qt1(1:4)
      dimension qtr(1:4)
      dimension ql0(1:4)
      dimension qr0(1:4)
      dimension ql(1:4)
      dimension qr(1:4)
c
c :::::: ALL INFO CARRIED BY 6 ELEMENTS OF THE q MATRIX
c :::::: rho,u,p,v,theta, AND type RESPECTIVELY
c
c :::::: SET FOR CONSTANT GAMMA EVALUATION; FUTURE MODIFICATION FOR
c :::::: VARIABLE GAMMA REAL GASES IN THE WORKS; ALSO, xbyt = 0
c :::::: FOR EULERIAN FRAME CALCULATION.
c
      ql(4) = gamma
      qr(4) = gamma
      xbyt = 0.
c
c :::::: CONVERT PRIMARY QUANTITIES OF DENSITY, VELOCITY, PRESSURE
c :::::: TO CONSERVED QUANTITIES (U VECTOR), & FIND SOUND SPEED
c :::::: AND CHARACTERISTICS.
      do 10 i = 1,nedge
        utemp(5,i) = q(6,i)

```

```

        if(q(6,i).gt.0.)then
            u(1,i) = q(1,i)
            u(2,i) = q(2,i)*q(1,i)
            u(3,i) = q(3,i)/(gamma-1.)+q(1,i)*(q(2,i)**2.+q(4,i)**2.)/2.
            u(4,i) = q(4,i)*q(1,i)
            c(i) = sqrt(gamma*q(3,i)/q(1,i))
            charc(1,i) = q(2,i) + c(i)
            charc(2,i) = q(2,i) - c(i)
        endif
10      continue
c
c ::::: COMPUTE 2ND ORDER SLOPES FOR (FCT) FLUX-CORRECTED TRANSPORT
c ::::: FROM VAN LEER'S SLOPES FOR THE MUSCL SCHEME
      do 200 i = 1,nedge
        if(q(6,i).eq.1.)then
          do 210 k=1,4
            if((q(k,i-1)-q(k,i))*(q(k,i)-q(k,i+1)).gt.0.)then
              dq(k,i) = min(abs(0.5*(q(k,i-1)-q(k,i+1))),abs(2.*
&              (q(k,i-1)-q(k,i))),abs(2.*(q(k,i)-q(k,i+1))))*
&              sign(1.,(q(k,i+1)-q(k,i-1)))
            else
              dq(k,i) = 0.
            endif
210      continue
          else
            do 220 k=1,4
              dq(k,i) = 0.
220      continue
            endif
200      continue
c
c ::::: COMPUTE FCT LEFT & RIGHT STATES TO SEND TO THE RIEMANN SOLVER
c -----
c ::::: VARIABLE NAME CONVENTION
c ::::: Variables are named the following way:
c ::::: first set of 4 to 6 characters:
c           same name which can be referenced in the code documentation
c ::::: trailing l:      Left state
c ::::: trailing r:      Right state
c ::::: trailing m:      - (minus)
c ::::: trailing p:      + (plus)
c ::::: trailing 0:      zero state
c ::::: trailing v:      transverse direction velocity (either u or v)
c ::::: EXAMPLE: betalm --> refers to BETA, left, minus state
c -----
      do 300 i = 1,nedge
        if((q(6,i).eq.1.).or.(q(6,i).eq.3.).or.(q(6,i).eq.5.)
&        .or.(q(6,i).eq.7.))then
          do 310 k = 1,4
            qtl(k) = q(k,i-1)+0.5*(1.-dt/dx*max(charc(1,i-1),0.))*dq(k,i-1)
            qtr(k) = q(k,i)-0.5*(1.+dt/dx*min(charc(2,i),0.))*dq(k,i)
            ql0(k) = q(k,i-1)+0.5*(1.-dt/dx*q(2,i-1))*dq(k,i-1)
            qr0(k) = q(k,i)-0.5*(1.+dt/dx*q(2,i))*dq(k,i)
310      continue
            betalm = -(dq(2,i-1)-dq(3,i-1)/q(1,i-1)/c(i-1))*dt/dx/2./q(1,i-1)
            betalo = -(dq(3,i-1)/(q(1,i-1)*c(i-1))**2.
&            -dq(1,i-1)/ql0(1)/qtl(1))*c(i-1)*dt/dx/2.
            betavl = c(i-1)*dq(4,i-1)*dt/dx/2.
            betarp = -(dq(2,i)+dq(3,i)/q(1,i)/c(i))*dt/dx/2./q(1,i)
            betaro = (dq(3,i)/(q(1,i)*c(i))**2.
&            -dq(1,i)/qr0(1)/qtr(1))*c(i)*dt/dx/2.
            betavr = -c(i)*dq(4,i)*dt/dx/2.
c
            betalm = cvmgt(betalm,0.,(charc(2,i-1).gt.0.))

```

```

        betal0 = cvmgt(betal0,0.,(q(2,i-1).gt.0.))
        betavl = cvmgt(betavl,0.,(q(2,i-1).gt.0.))
        betarp = cvmgt(betarp,0.,(charc(1,i).lt.0.))
        betar0 = cvmgt(betar0,0.,(q(2,i).lt.0.))
        betavr = cvmgt(betavr,0.,(q(2,i).lt.0.))
c
        ql(1) = 1./(1./qtl(1)-betal0-betalm)
        ql(2) = qtl(2)-betalm*c(i-1)*q(1,i-1)
        ql(3) = qtl(3)+betalm*(c(i-1)*q(1,i-1))**2.
        qr(1) = 1./(1./qtr(1)-betar0-betarp)
        qr(2) = qtr(2)+betarp*c(i)*q(1,i)
        qr(3) = qtr(3)+betarp*(c(i)*q(1,i))**2.
c
c ::::: SET PRESSURE AND DENSITY FLOORS TO FACILITATE CONVERGENCE
c ::::: FOR NEAR ZERO PRESSURE AND DENSITY CALCULATIONS
        ql(1) = max(1.e-03,ql(1))
        qr(1) = max(1.e-03,qr(1))
        psml = max(1.e-06,1.e-06*q(1,i-1)*q(2,i-1)**2./2.)
        psmr = max(1.e-06,1.e-06*q(1,i)*q(2,i)**2./2.)
        ql(3) = max(psml,ql(3))
        qr(3) = max(psmr,qr(3))
c
c ::::: SEND LEFT AND RIGHT STATES TO RIEMANN SOLVER
        call riemann(ql,qr,qstar,xbyt)
c
c ::::: COMPUTE AMOUNT OF PASSIVELY ADVECTED TRANSVERSE VELOCITY
        vleft = qtl(4)+betavl
        vright = qtr(4)+betavr
        vtemp = cvmgt(vright,vleft,(qstar(2).lt.0.))
c
c ::::: COMPUTE FLUX AT CELL EDGES
        fhalf(1,i) = qstar(1)*qstar(2)
        fhalf(2,i) = qstar(3)+qstar(1)*qstar(2)**2.
        fhalf(3,i) = qstar(1)*qstar(2)*(gamma*qstar(3)/(gamma-1.)/qstar(1)+
&          (qstar(2)**2.+vtemp**2.)/2.)
        fhalf(4,i) = fhalf(1,i)*vtemp
    endif
c-----
c ::::: if the point is a boundary point we use special treatment:
c
c ::::: For impermeable or symmetric BC's:
c ::::: we convert u and v to normal and tangential velocity components,
c ::::: send to the riemann solver, and convert back on return
c
c ::::: For outflow:
c ::::: we just compute the flux out normal to the node
c
c ::::: NODE TYPES:
c      type = 0      null node inside object (not tracked)
c      type = 1      gas node in open flow field
c      type = 2      impermeable to the left, object boundary
c      type = 3      impermeable to the right, object boundary
c      type = 4      outflow to the left, grid edge
c      type = 5      outflow to the right, grid edge
c      type = 6      impermeable to the left, grid boundary
c      type = 7      impermeable to the right, grid boundary
c-----
        if(q(6,i).ge.2.)then
            ql(1) = q(1,i)
            ql(2) = q(2,i)*cos(q(5,i))+q(4,i)*sin(q(5,i))
            ql(3) = q(3,i)
            qr(1) = q(1,i)
            qr(2) = -ql(2)

```

```

      qr(3) = q(3,i)
c
c ::::: SET PRESSURE AND DENSITY FLOORS TO FACILITATE CONVERGENCE
      ql(1) = max(1.e-03,ql(1))
      qr(1) = max(1.e-03,qr(1))
      psm = max(1.e-06,1.e-06*q(1,i)*q(2,i)**2./2.)
      ql(3) = max(psm,ql(3))
      qr(3) = max(psm,qr(3))
c
c ::::: TANGENTIAL COMPONENT OF VELOCITY
      vtan = q(4,i)*cos(q(5,i))-q(2,i)*sin(q(5,i))
c
c ::::: PROJECTION OF TANGENTIAL COMPONENT BACK ONTO AXES
c ::::: GIVES THE REMAINING u & v COMPONENTS
      q2temp = -vtan*sin(q(5,i))
      q4temp = vtan*cos(q(5,i))
c
c ::::: SEND LEFT AND RIGHT STATES TO RIEMANN SOLVER
      call riemann(ql,qr,qstar,xbyt)
c
c ::::: BOUNDARY IS IMPERMEABLE TO THE LEFT (type=q(6,i)=2 or 6)
      if((q(6,i).eq.2.).or.(q(6,i).eq.6.))then
        fhalf(1,i) = qstar(1)*q2temp
        fhalf(2,i) = qstar(3)+qstar(1)*q2temp**2.
        fhalf(3,i) = qstar(1)*q2temp*(gamma*qstar(3)
&          /(gamma-1.)/qstar(1)+(q2temp**2.+q4temp**2.)/2.)
        fhalf(4,i) = fhalf(1,i)*q4temp
c
c ::::: BOUNDARY IS IMPERMEABLE TO THE RIGHT (type=q(6,i)=3 or 7)
      else if((q(6,i).eq.3.).or.(q(6,i).eq.7.))then
        fhalf(1,i+1) = qstar(1)*q2temp
        fhalf(2,i+1) = qstar(3)+qstar(1)*q2temp**2.
        fhalf(3,i+1) = qstar(1)*q2temp*(gamma*qstar(3)
&          /(gamma-1.)/qstar(1)+(q2temp**2.+q4temp**2.)/2.)
        fhalf(4,i+1) = fhalf(1,i+1)*q4temp
c
c ::::: BOUNDARY IS OUTFLOW TO THE LEFT (type=q(6,i)=4)
      else if(q(6,i).eq.4.)then
        fhalf(1,i) = q(1,i)*q(2,i)
        fhalf(2,i) = q(3,i)+q(1,i)*q(2,i)**2.
        fhalf(3,i) = q(1,i)*q(2,i)*(gamma*q(3,i)
&          /(gamma-1.)/q(1,i)+q(2,i)**2.+q(4,i)**2.)/2.)
        fhalf(4,i) = fhalf(1,i)*q(4,i)
c
c ::::: BOUNDARY IS OUTFLOW TO THE RIGHT (type=q(6,i)=5)
      else if(q(6,i).eq.5.)then
        fhalf(1,i+1) = q(1,i)*q(2,i)
        fhalf(2,i+1) = q(3,i)+q(1,i)*q(2,i)**2.
        fhalf(3,i+1) = q(1,i)*q(2,i)*(gamma*q(3,i)
&          /(gamma-1.)/q(1,i)+q(2,i)**2.+q(4,i)**2.)/2.)
        fhalf(4,i+1) = fhalf(1,i+1)*q(4,i)
      endif
    endif
300    continue
c
c -----
c ::::: CENTRAL DIFFERENCING
      do 400 i = 1,nedge
        if(q(6,i).gt.0.)then
          do 410 k = 1,4
            utemp(k,i) = u(k,i) - dt/dx*(fhalf(k,i+1)-fhalf(k,i))
410          continue
          endif
400    continue

```

```

c-----
      return
      end
c
c-----
      subroutine convert(rho,u,v,p,gamma,utemp,k,iflag,nedge)
c-----
c ::::: subroutine to convert U=rho,rho*u,rho*E to rho,u,p.....
c
      include "tsu_geo.i"
c
      dimension rho(1:ncellx,1:ncelly)
      dimension u(1:ncellx,1:ncelly)
      dimension v(1:ncellx,1:ncelly)
      dimension p(1:ncellx,1:ncelly)
      dimension utemp(1:5,1:nmax)
c
c ::::: IF iflag = 0, WE ARE SWEEPING HORIZONTALLY
c ::::: REPLACE kth ROW OF PROPERTIES MATRIX
      if(iflag.eq.0) then
        do 100 n = 1,nedge
          if(utemp(5,n).gt.0.)then
            rho(n,k) = utemp(1,n)
            rho(n,k) = max(rho(n,k),1.e-03)
            u(n,k) = utemp(2,n)/utemp(1,n)
            v(n,k) = utemp(4,n)/utemp(1,n)
            p(n,k) = (utemp(3,n)/utemp(1,n) - (u(n,k)**2.+v(n,k)**2.)
            & /2.)*utemp(1,n)*(gamma-1.)
            p(n,k) = max(p(n,k),1.e-06)
          endif
100      continue
c
c ::::: ELSE IF iflag = 1, WE ARE SWEEPING VERTICALLY
c ::::: REPLACE kth COLUMN OF PROPERTIES MATRIX
      else
        do 200 n = 1,nedge
          if(utemp(5,n).gt.0.)then
            rho(k,n) = utemp(1,n)
            rho(k,n) = max(rho(k,n),1.e-03)
            v(k,n) = utemp(2,n)/utemp(1,n)
            u(k,n) = utemp(4,n)/utemp(1,n)
            p(k,n) = (utemp(3,n)/utemp(1,n) - (u(k,n)**2.+v(k,n)**2.)
            & /2.)*utemp(1,n)*(gamma-1.)
            p(k,n) = max(p(k,n),1.e-06)
          endif
200      continue
        endif
c
      return
      end
c
c-----
      subroutine riemann(ql,qr,q,xbyt)
c-----
c ::::: RIEMANN SOLVER SUBROUTINE FOR GIVEN LEFT AND RIGHT STATES
c ::::: FOR ARBITRARY xbyt AND GAMMA LAW GAS.
c ::::: EXACT SOLVER FOR SHOCKS AS WELL AS RAREFACTIONS
c-----
c ::::: This provides the phase space solution of Riemann problem.
c ::::: It requires Newton iteration to compute the pressure in the
c ::::: state between the two acoustic waves.
c-----
c
      dimension ql(1:4)

```



```

        dimension qr(1:4)
        dimension q(1:4)
c
c ::::: CHECK STATES TO SEE IF THEY'RE ALREADY HAVE SAME u & p
c ::::: IF THEY DO, RETURN
        if((ql(2).eq.qr(2)).and.(ql(3).eq.qr(3)))then
            q(2) = qr(2)
            q(3) = qr(3)
            q(1) = cvmgt(ql(1),qr(1),(xbyt.le.q(2)))
            q(4) = cvmgt(ql(4),qr(4),(xbyt.le.q(2)))
            return
        endif
c
c ::::: SET NUMBER OF ITERATIONS FOR CONVERGENCE & ACCURACY
c ::::: 5 ITERATIONS IS ADEQUATE FOR MOST APPLICATIONS; 10 ITERATIONS
c ::::: FOR VERY, VERY STRONG SHOCKS AND BETTER RAREFACTION RESOLUTION
        niter = 5
c
c ::::: COMPUTE SOME OFTEN NEEDED QUANTITIES
        psml = max(1.e-06,1.e-06*ql(1)*ql(2)**2./2.)
        psmr = max(1.e-06,1.e-06*qr(1)*qr(2)**2./2.)
        gamma = cvmgt(ql(4),qr(4),(ql(2).gt.qr(2)))
        gml = gamma - 1.
        gpl = gamma + 1.
        cl = sqrt(gamma*ql(3)/ql(1))
        cr = sqrt(gamma*qr(3)/qr(1))
        al = ql(3)/ql(1)**gamma
        ar = qr(3)/qr(1)**gamma
        p_old = (ql(3)+qr(3))/2.
c
c ::::: FIRST GUESS FOR p*
        p = (qr(1)*cr*ql(3) + ql(1)*cl*qr(3) + ql(1)*cl*qr(1)*cr*
&      (ql(2)-qr(2)))/((qr(1)*cr+ql(1)*cl))
        p = max(p,psml,psmr)
c
        ncounter = 0
        5
        continue
c
c ::::: COMPUTE ustar, GUESS DIFFERENTLY FOR EITHER SHOCK OR RAREFACTION
        ulss = ql(2) - (p-ql(3))/ws(p,ql(3),1./ql(1),gamma)
        ulsr = ql(2) + 2./gml*(cl-sqrt(gamma*al*(p/al)**
&      (gml/gamma)))
        urss = qr(2) + (p-qr(3))/ws(p,qr(3),1./qr(1),gamma)
        ursr = qr(2) - 2./gml*(cr-sqrt(gamma*ar*(p/ar)**
&      (gml/gamma)))
        ulstar = cvmgt(ulss,ulsr,(p.gt.ql(3)))
        urstar = cvmgt(urss,ursr,(p.gt.qr(3)))
c
c ::::: COMPUTE tau (INVERSE DENSITY)
        taulss = 1./ql(1) - (p-ql(3))/ws(p,ql(3),1./ql(1),gamma)**2.
        taulsr = (p/al)**(-1./gamma)
        taurss = 1./qr(1) - (p-qr(3))/ws(p,qr(3),1./qr(1),gamma)**2.
        taursr = (p/ar)**(-1./gamma)
        taulstar = cvmgt(taulss,taulsr,(p.gt.ql(3)))
        taurstar = cvmgt(taurss,taursr,(p.gt.qr(3)))
c
c ::::: COMPUTE cstar (SOUND SPEED TO LEFT AND RIGHT OF CONTACT SURF.)
        clstar = sqrt(gamma*p*taulstar)
        crstar = sqrt(gamma*p*taurstar)
c
c ::::: COMPUTE zl and zr (INV. VEL. DERIVATIVES FOR NEWTON ITERATION)
        zlr = taulstar/clstar
        zls = ((ql(1)*cl)**2. + ws(p,ql(3),1./ql(1),gamma)**2.)/
&      (2.*ws(p,ql(3),1./ql(1),gamma)**3.)

```

```

      zrr = taurstar/crstar
      zrs = ((qr(1)*cr)**2. + ws(p,qr(3),1./qr(1),gamma)**2.)/
&      (2.*ws(p,qr(3),1./qr(1),gamma)**3.)
      zl = cvmgt(zlr,zls,(p.lt.q1(3)))
      zr = cvmgt(zrr,zrs,(p.lt.qr(3)))
c
c ::::: CHECK FOR CONVERGENCE
      y = 1.e-06*max(cl,cr,abs(q1(2)),abs(qr(2)))
      z = abs(ulstar-urstar)
      if((z .lt. y) .or. (p.eq.p_old)) then
        goto 10
      endif
      ncounter = ncounter + 1
c
c ::::: COMPUTE NEW p
      p_old = p
      p = p + (ulstar-urstar)/(zl + zr)
      p = max(p,psml,psmr)
      if(ncounter.le.niter) goto 5
c
c ::::: SOLUTION EITHER HAS CONVERGED OR ITERATIONS RAN OUT
10  continue
      pstar = p
      ustar = 0.5*(urstar+ulstar)
c
c :::::      COMPUTE THE x-t SPACE CHARACTERISTICS THAT BOUND SOLUTION
c
      clambda0 = ustar
c
      clamlmr = q1(2) - cl
      clamlms = q1(2) - ws(pstar,q1(3),1./q1(1),gamma)/q1(1)
      clamrmr = ustar - clstar
      clamrms = clamlms
      clamlm = cvmgt(clamlmr,clamlms,(pstar .lt. q1(3)))
      clamrm = cvmgt(clamrmr,clamrms,(pstar .lt. q1(3)))
c
      clamlpr = ustar + crstar
      clamlps = qr(2) + ws(pstar,qr(3),1./qr(1),gamma)/qr(1)
      clamrpr = qr(2) + cr
      clamrps = clamlps
      clamlp = cvmgt(clamlpr,clamlps,(pstar .lt. qr(3)))
      clamrp = cvmgt(clamrpr,clamrps,(pstar .lt. qr(3)))
c
c ::::: DETERMINE THE PHYSICAL SPACE SOLUTION FOR AN xbyt
      if (xbyt .le. clamlm) then
        q(1) = q1(1)
        q(2) = q1(2)
        q(3) = q1(3)
      else if(xbyt .le. clamrm .and. xbyt .gt. clamlm) then
        c = (q1(2)+2.*cl/gml-xbyt)*gml/gp1
        q(2) = xbyt + c
        q(1) = (c**2./gamma/al)**(1./gml)
        q(3) = q(1)*c**2./gamma
      else if(xbyt .le. clambda0 .and. xbyt .gt. clamrm) then
        q(1) = 1./taulstar
        q(2) = ustar
        q(3) = pstar
      else if(xbyt .le. clamlp .and. xbyt .gt. clambda0) then
        q(1) = 1./taurstar
        q(2) = ustar
        q(3) = pstar
      else if(xbyt .le. clamrp .and. xbyt .gt. clamlp) then
        c = -1.*(qr(2)-2.*cr/gml-xbyt)*gml/gp1
        q(2) = xbyt - c

```

```

      q(1) = (c**2./gamma/ar)**(1./gml)
      q(3) = q(1)*c**2./gamma
    else if(xbyt .gt. clamrp) then
      q(1) = qr(1)
      q(2) = qr(2)
      q(3) = qr(3)
    endif
    q(4) = gamma
    return
  end

c
c-----
      function cvmgt(x,y,z)
c-----
c ::::: LOGICAL EXCHANGE FUNCTION CHOOSES x IF z is TRUE
c ::::: ELSE CHOOSES y.
c
      real x,y
      logical z
c
      if ( z .eqv. .true.) then
        cvmgt = x
      else
        cvmgt = y
      endif
      return
    end

c
c-----
      function ws(p,p0,tau0,gamma)
c-----
c ::::: FUNCTION WHICH COMPUTES MASS FLUX ACROSS SHOCK FRONT
c
      real p,p0,tau0,gamma
c
      ws = sqrt(gamma*p0/tau0*(1.+(gamma+1.)/2./gamma*(p-p0)/p0))
      return
    end
c-----

```

A-3.1 custom_init.f Source Listing - LJUST simulation

The source listing for custom_init.f given below is an example of the input deck generation subroutine used to generate the LJUST simulation. Segments of the subroutine use other subroutines such as roundbc.f to generate cylindrical boundaries. The subroutine roundbc is useful a variety of other TSUNAMI boundary generation needs. Also included at the end is the include file custom_init.i, which provides the parameters declared at the beginning of the custom_init.f.

```

c-----
c      program custom_init
c-----
c      This program generates input files for a specific
c      Gas Dynamics problem.
c-----
c      LJUST SIMULATION SHOCK ATTENUATION
c      April 1992
c-----
c      written by:
c
c      James C. Liu
c
c      Dept. of Nuclear Engineering
c      Thermal Hydraulics Laboratory
c      4118 Etcheverry Hall
c      University of California at Berkeley
c      Berkeley, CA 94720
c
c      (510) 642-0421
c      (510) 643-9685 FAX
c      tsunami@four-lab4.Berkeley.EDU (Internet)
c-----
c      Work performed under the auspices of the United States
c      Department of Energy for the Lawrence Livermore National
c      Laboratory under contract W-7405-ENG-48.
c-----
c
c      LJUST SIMULATION SHOCK ATTENUATION
c
c
c      |..... ) o o o o o o o o      open
c      |..... ) o o o o o o o o
c      |..... ) o o o o o o o o
c      3 .....2..... ) o o o o o o o o
c      |..... ) o o o o o o o o
c      |..... ) o o o o o o o o
c      |..... ) o o o o o o o o      open
c      |..... ) o o o o o o o o
c      C              S              jet array
c
c      zone 1 = ambient gas at rest
c      zone 2 = shocked zone 1 material that shock has traversed

```

```

c      zone 3 = expanding driver gas
c      C = contact surface
c      S = shock front
c-----
c      include "tsu_geo.i"
c      include "tsu_inp.i"
c      include "custom_init.i"
c
c      ::::: FLOW PROPERTIES
c      dimension rho(1:ncellx,1:ncelly)
c      dimension u(1:ncellx,1:ncelly)
c      dimension v(1:ncellx,1:ncelly)
c      dimension p(1:ncellx,1:ncelly)
c
c      ::::: GRID & GEOMETRIC INFO
c      dimension typex(1:ncellx,1:ncelly)
c      dimension typey(1:ncellx,1:ncelly)
c      dimension thetax(1:ncellx,1:ncelly)
c      dimension thetay(1:ncellx,1:ncelly)
c      dimension icyl(1:ncyl,1:4)
c
c      ::::: SET INITIAL CONDITIONS
c      t = 0.
c      n = 0
c      nframes = 0
c
c      ::::: ANALYTICAL GAS DYNAMICS RELATIONS USED TO GET SHOCK JUMP
c      gml = gamma - 1.0
c      gpl = gamma + 1.0
c      r1 = r0/wtmol
c
c      rho1 = p1/r1/temp1
c      u1 = 0.0
c      a1 = sqrt(gamma*p1/rho1)
c
c      p2 = p1*(2.*gamma*cmach**2.-(gml))/(gpl)
c      rho2 = rho1*(gpl*p2+gml*p1)/(gml*p2+gpl*p1)
c      u2 = 2.*a1/gpl*(cmach-1./cmach)
c
c      p4 = p2*(1-gml/gpl*(cmach-1./cmach))**(-2.*gamma/gml)
c      rho4 = p4/R1/temp1
c      u4 = 0.0
c
c      p3 = p2
c      u3 = u2
c      rho3 = rho4*(p3/p4)**(1./gamma)
c
c      nxs = nxc + int((cmach*a1-u2)*(tdist-dx*float(ncellx-nxc))/u2/dx)
c      nxs = min (nxs, ncstrt-5)
c
c      ::::: INITIAL CONDITIONS FOR LEFT OF CONTACT SURFACE
c      do 100 i = 1,nxc
c        do 110 j = 1,ncelly
c          rho(i,j) = rho3
c          u(i,j) = u3
c          v(i,j) = 0.
c          p(i,j) = p3
c          thetax(i,j) = 0.
c          thetay(i,j) = 0.
c          typex(i,j) = 1.
c          typey(i,j) = 1.
c        110 continue
c      100 continue
c

```

```

c ::::: INITIAL CONDITIONS FOR REGION BETWEEN C.SURF. & SHOCK
c      do 120 i = nxc+1,nxs
      do 120 i = 1,nxs
        do 130 j = 1,ncelly
          rho(i,j) = rho2
          u(i,j) = u2
          v(i,j) = 0.
          p(i,j) = p2
          thetax(i,j) = 0.
          thetay(i,j) = 0.
          typex(i,j) = 1.
          typey(i,j) = 1.
130      continue
120      continue
c
c ::::: INITIAL p1,rho1,u1 CONDITIONS TO RIGHT OF SHOCK
      do 140 i = nxs+1,ncellx
        do 150 j = 1,ncelly
          rho(i,j) = rho1
          u(i,j) = u1
          v(i,j) = 0.0
          p(i,j) = p1
          thetax(i,j) = 0.
          thetay(i,j) = 0.
          typex(i,j) = 1.
          typey(i,j) = 1.
150      continue
140      continue
c
c ::::: OPEN LEFT BOUNDARY & REFLECTING RIGHT WALL
      do 200 i = 1,ncelly
        typex(1,i) = 4.
        typex(ncellx,i) = 7.
        thetax(1,i) = pi
        thetax(ncellx,i) = 0.
200      continue
c
c ::::: SYMMETRIC BOUNDARIES ALONG TOP & BOTTOM w/ OPEN ENDS
      do 300 i = 1,nxstop
        do 310 j = 0,nystop-1
          typey(i,1+j) = 0.
          typey(i,ncelly-j) = 0.
          typex(i,1+j) = 0.
          typex(i,ncelly-j) = 0.
          rho(i,1+j) = rhow
          rho(i,ncelly-j) = rhow
310      continue
          typey(i,1+nystop) = 6.
          typey(i,ncelly-nystop) = 7.
          thetay(i,1+nystop) = pi
          thetay(i,ncelly-nystop) = 0.
300      continue
c
      do 320 i = nxstop+1,ncellx
        typey(i,1) = 4.
        typey(i,ncelly) = 5.
        thetay(i,1) = pi
        thetay(i,ncelly) = 0.
320      continue
c
      do 330 j = 0,nystop-1
        typex(nxstop+1,1+j) = 6.
        typex(nxstop+1,ncelly-j) = 6.
        thetax(nxstop+1,1+j) = pi

```

```

        thetax(nxstop+1,ncelly-j) = pi
330    continue
c
c ::::: COMPUTE CYLINDER BOUNDARIES
c ::::: icyl(n,1) = type (0 = half up, 1=half right, 2 = full)
c ::::: icyl(n,2) = x-coord of center of cylinder on grid
c ::::: icyl(n,3) = y-coord of center of cylinder on grid
c ::::: icyl(n,4) = radius in grid integer nodes
c ::::: CYLINDERS ARE HEX-PACKED WITH SPECIFIC P/D RATIO
c
c ::::: determine the spacial position and types for cylinders
      n = 1
      nd = 10
      id = int(float(nd)/2. +.5)
      npx = 12
      npy = 14
      ncstop = ncstrt + 7*npx + 1
c
      do 400 i = ncstrt,ncstop, (2*npx)
        do 410 j = npy+nystop+1,ncelly,npy
          icyl(n,1) = 2
          icyl(n,2) = i
          icyl(n,3) = j
          icyl(n,4) = id
          n = n + 1
          n = min( n , ncyl )
410      continue
400    continue
c
      do 420 i = ncstrt+npx,ncstop, (2*npx)
        do 430 j = npy/2+nystop+1,ncelly-npy/2,npy
          icyl(n,1) = 2
          icyl(n,2) = i
          icyl(n,3) = j
          icyl(n,4) = id
          n = n + 1
          n = min( n , ncyl )
430      continue
420    continue
c
      ncyla = n
c
      do 440 i = 1,ncyla
        itype = icyl(i,1)
        ixpos = icyl(i,2)
        iypos = icyl(i,3)
        id = icyl(i,4)
        call roundbc(itype,ixpos,iypos,id,rho,typex,typey,thetax,thetay)
440      continue
c
c ::::: WRITE INITFILE DATA FILE
      open(29,file=initfile,form='unformatted')
      write(29) t,n,nframes
      do 500 i = 1, ncellx
        do 510 j = 1,ncelly
          write(29) rho(i,j)
          write(29) u(i,j)
          write(29) v(i,j)
          write(29) p(i,j)
          write(29) typex(i,j)
          write(29) typey(i,j)
          write(29) thetax(i,j)
          write(29) thetay(i,j)
510      continue

```

```

500  continue
      close(29)
      end
c
c -----
      subroutine roundbc(itype,ixpos,iypos,id,rho,typex,typey,thetax,thetay)
c -----
c ::::: SETS UP REFLECTING BOUNDARIES AND COMPUTES THETAS ON GRID
c ::::: FOR CYLINDERS (EITHER 1/2 OR FULL)
c
c ::::: GRID & GEOMETRIC INFO
c
      include "tsu_geo.i"
      include "tsu_inp.i"
      include "custom_init.i"
c
      dimension rho(1:ncellx,1:ncelly)
      dimension typex(1:ncellx,1:ncelly)
      dimension typey(1:ncellx,1:ncelly)
      dimension thetax(1:ncellx,1:ncelly)
      dimension thetay(1:ncellx,1:ncelly)
c
      integer itype,id,ixpos,iypos,il,i,k
c
c ----- set x-sweep boundaries-----
      rd = float(id)
      do 100 i = 0, (id-1)
          xdim = sqrt(rd**2. - (float(i))**2.) +0.99
          il = int(xdim)
          xdim = float(il)
          phi = acos(xdim/sqrt(xdim**2.+(float(i))**2.))
c
c ::::: IF itype = 0, we have 1/2 a cylinder facing up from horiz. boundary
c ::::: IF itype = 1, we have 1/2 a cylinder facing out from vert. wall
c ::::: IF itype = 2, we have a full cylinder in the flow
c ::::: id = radius
c ::::: ixpos & iypos ARE THE POSITION OF THE CENTER OF THE CYL. ON GRID
c
      if(itype.eq.0)then
          typex(ixpos-il,iypos+i) = 3.
          typex(ixpos+il,iypos+i) = 2.
          thetax(ixpos-il,iypos+i) = -phi
          thetax(ixpos+il,iypos+i) = pi + phi
          do 110 k = (ixpos-il+1), (ixpos+il-1)
              typex(k,iypos+i) = 0.
              rho(k,iypos+i) = rhow
110      continue
      else if(itype.eq.1)then
          typex(ixpos+il,iypos-i) = 2.
          typex(ixpos+il,iypos+i) = 2.
          thetax(ixpos+il,iypos-i) = pi - phi
          thetax(ixpos+il,iypos+i) = pi + phi
          do 120 k = ixpos, (ixpos+il-1)
              typex(k,iypos-i) = 0.
              typex(k,iypos+i) = 0.
              rho(k,iypos-i) = rhow
              rho(k,iypos+i) = rhow
120      continue
      else if(itype.eq.2)then
          typex(ixpos-il,iypos-i) = 3.
          typex(ixpos+il,iypos-i) = 2.
          typex(ixpos-il,iypos+i) = 3.
          typex(ixpos+il,iypos+i) = 2.
          thetax(ixpos-il,iypos+i) = -phi

```



```

        thetax(ixpos+il,iypos+i) = pi + phi
        thetax(ixpos-il,iypos-i) = phi
        thetax(ixpos+il,iypos-i) = pi - phi
        do 130 k = (ixpos-il+1), (ixpos+il-1)
            typex(k,iypos-i) = 0.
            typex(k,iypos+i) = 0.
            rho(k,iypos-i) = rhow
            rho(k,iypos+i) = rhow
130      continue
        endif
100    continue
c
c ----- set y sweep boundaries -----
do 200 i = 0, (id-1)
    ydim = sqrt(rd**2. - (float(i))**2.) +0.99
    il = int(ydim)
    ydim = float(il)
    phi = acos(ydim/sqrt(ydim**2.+(float(i))**2.))
    if(itype.eq.0)then
        typey(ixpos-i,iypos+il) = 2.
        typey(ixpos+i,iypos+il) = 2.
        thetay(ixpos-i,iypos+il) = pi - phi
        thetay(ixpos+i,iypos+il) = pi + phi
        do 210 k = 0, (il-1)
            typey(ixpos-i,iypos+k) = 0.
            typey(ixpos+i,iypos+k) = 0.
            rho(ixpos-i,iypos+k) = rhow
            rho(ixpos+i,iypos+k) = rhow
210      continue
        else if(itype.eq.1)then
            typey(ixpos+i,iypos-il) = 3.
            typey(ixpos+i,iypos+il) = 2.
            thetay(ixpos+i,iypos-il) = -phi
            thetay(ixpos+i,iypos+il) = pi + phi
            do 220 k = 0, (il-1)
                typey(ixpos+i,iypos-k) = 0.
                typey(ixpos+i,iypos+k) = 0.
                rho(ixpos+i,iypos-k) = rhow
                rho(ixpos+i,iypos+k) = rhow
220      continue
            else if(itype.eq.2)then
                typey(ixpos-i,iypos-il) = 3.
                typey(ixpos+i,iypos-il) = 3.
                typey(ixpos-i,iypos+il) = 2.
                typey(ixpos+i,iypos+il) = 2.
                thetay(ixpos-i,iypos-il) = phi
                thetay(ixpos+i,iypos-il) = -phi
                thetay(ixpos-i,iypos+il) = pi - phi
                thetay(ixpos+i,iypos+il) = pi + phi
                do 230 k = 0, (il-1)
                    typey(ixpos-i,iypos-k) = 0.
                    typey(ixpos+i,iypos-k) = 0.
                    typey(ixpos-i,iypos+k) = 0.
                    typey(ixpos+i,iypos+k) = 0.
                    rho(ixpos-i,iypos-k) = rhow
                    rho(ixpos+i,iypos-k) = rhow
                    rho(ixpos-i,iypos+k) = rhow
                    rho(ixpos+i,iypos+k) = rhow
230      continue
            endif
200    continue
c
    return
end

```

```

c-----
c      CUSTOM_INIT.I
c-----
c      ::::: TSUNAMI geometric include file
c
c-----
c
c      SPECIFIC PROBLEM:
c          LJUST simulation shock attenuation
c          Grid resolution: 600 x 100
c
c-----
c
c          parameter (cmach = 3.0)
c          parameter (r0 = 8.3144)
c          parameter (wtmol = 0.029)
c          parameter (gamma = 1.4)
c          parameter (p1 = 17500.0)
c          parameter (templ = 295.0)
c          parameter (rhow = 25.0)
c          parameter (nxc = 5)
c          parameter (nxstop = 560)
c          parameter (nystop = 4)
c          parameter (ncyl = 48)
c          parameter (ncstrt = 386)
c          parameter (tdist = 1.1)
c-----

```

A-3.2 custom_init.f Source Listing - Elliptical Wall Chamber with X-ray Ablation

The source listing for custom_init.f given below is an example of the input deck generation subroutine used to generate the internal cavity with a rectangular plug in the middle of the cavity. The uniqueness of this subroutine is the ability to generate a curved, elliptical wall for the cavity. The subroutine places a curved structural wall into the grid and then nullifies all non-essential nodes outside of the vessel. The curvature follows an ellipse which satisfies the equation: $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$. By adjusting the major and minor radii, a and b respectively, one can generate a circular surface as well.

```

c-----
c      program custom_init
c-----
c      This program generates input files for a specific
c      Gas Dynamics problem.
c
c-----
c      INSIDE ELLIPTICAL CAVITY SHOCK WAVES
c-----
c      X
c      x-rays      |      | <----ablation shield
c      released    |      |

```

```

c |      here      |_____|
c |
c |
c |
c |
c |      back wall ----->
c |
c |
c |
c |      <-----elliptical wall
c |
c |
c |
c |
c |

```

```

c -----
c written by:

```

```

c      James C. Liu
c
c      Dept. of Nuclear Engineering
c      Thermal Hydraulics Laboratory
c      4118 Etcheverry Hall
c      University of California at Berkeley
c      Berkeley, CA 94720
c
c      (510) 642-0421
c      (510) 643-9685 FAX
c      tsunami@four-lab4.Berkeley.EDU (Internet)
c -----

```

```

c      Work performed under the auspices of the United States
c      Department of Energy for the Lawrence Livermore National
c      Laboratory under contract W-7405-ENG-48.
c -----

```

```

c
c      include "tsu_geo.i"
c      include "tsu_inp.i"
c      include "custom_init.i"
c

```

```

c :::::: FLOW PROPERTIES
c      dimension rho(1:ncellx,1:ncelly)
c      dimension u(1:ncellx,1:ncelly)
c      dimension v(1:ncellx,1:ncelly)
c      dimension p(1:ncellx,1:ncelly)
c

```

```

c :::::: GRID & GEOMETRIC INFO
c      dimension typex(1:ncellx,1:ncelly)
c      dimension typey(1:ncellx,1:ncelly)
c      dimension thetax(1:ncellx,1:ncelly)
c      dimension thetay(1:ncellx,1:ncelly)
c

```

```

c :::::: SET INITIAL CONDITIONS
c      t = 0.
c      n = 0
c      nframes = 0
c

```

```

c :::::: ANALYTICAL GAS DYNAMICS RELATIONS USED TO GET SHOCK JUMP
c      gml = gamma - 1.0
c      gpl = gamma + 1.0
c      r1 = r0/wtmol
c

```

```

c      rho1 = p1/r1/temp1
c      u1 = 0.0
c      a1 = sqrt(gamma*p1/rho1)
c

```

```

c ::::: INITIAL CONDITIONS
do 100 i = 1,ncellx
  do 101 j = 1,ncelly
    rho(i,j) = rho1
    u(i,j) = 0.0
    v(i,j) = 0.0
    p(i,j) = p1
    thetax(i,j) = 0.
    thetay(i,j) = 0.
    typex(i,j) = 1.
    typey(i,j) = 1.
  101 continue
100 continue
c
c ::::: REFLECTING BOUNDARY ALONG RIGHT
do 310 j = iyb1,iyb2
  typex(ixb2,j) = 7.
  thetax(ixb2,j) = 0.0
310 continue
c
  radx = float(iradx)
  rady = float(irady)
c
c ::::: ELLIPSE CURVE FOR LEFT BOUNDARY Y-NODES
do 375 i = 0, iradx-1
  xlen = float(i)
  ylen = rady*sqrt(1.0-(xlen**2.)/(radx**2.))
  iylen = int(ylen)-int(float(int(ylen))/ylen)
  typey(ixl-i,iyl-iylen) = 6.
  if(xlen.ne.0.) then
    thetay(ixl-i,iyl-iylen) = -pi/2.+atan(-float(iylen)/xlen*
&      (radx**2.)/(rady**2.))
    else
      thetay(ixl-i,iyl-iylen) = -pi
    endif
c
c ::::: FILL VOID BELOW BOUNDARY NODE
do 376 j = 1,(iyl-iylen-1)
  rho(ixl-i,j) = rhow
  typex(ixl-i,j) = 0.
  typey(ixl-i,j) = 0.
376 continue
375 continue
c
c ::::: ELLIPSE CURVE FOR LEFT BOUNDARY X-NODES
do 385 j = 0, irady-1
  ylen = float(j)
  xlen = radx*sqrt(1.0-(ylen**2.)/(rady**2.))
  ixlen = int(xlen)-int(float(int(xlen))/xlen)
  typex(ixl-ixlen,iyl-j) = 6.
  if(ylen.ne.0.) then
    thetax(ixl-ixlen,iyl-j) = -pi/2.+atan(-float(ixlen)/ylen*
&      (rady**2.)/(radx**2.))
    else
      thetax(ixl-ixlen,iyl-j) = -pi
    endif
c
c ::::: FILL VOID LEFT OF BOUNDARY NODE
do 386 i = 1,(ixl-ixlen-1)
  rho(i,iyl-j) = rhow
  typex(i,iyl-j) = 0.
  typey(i,iyl-j) = 0.
386 continue
385 continue

```

```

c
c ::::: FILL VOID BELOW AND TO LEFT AND RIGHT
do 400 i = 1, ncellx
  do 401 j = 1, iyb1-1
    rho(i,j) = rhow
    typex(i,j) = 0.
    typey(i,j) = 0.
401    continue
400  continue
  do 410 i = 1, ixb1-1
    do 411 j = 1, ncelly
      rho(i,j) = rhow
      typex(i,j) = 0.
      typey(i,j) = 0.
411    continue
410  continue
  do 420 i = ixb2+1, ncellx
    do 421 j = 1, ncelly
      rho(i,j) = rhow
      typex(i,j) = 0.
      typey(i,j) = 0.
421    continue
420  continue
c
c ::::: PUT OBSTRUCTION IN THE CAVITY AT IX2,IY2
c ::::: 9 nodes wide, ilen=9 nodes on left and 12 nodes on right
c ::::: and 22 deg. slope along bottom
do 500 i = ix2+1, ix3-1
  do 501 j = (iy2-ilen1+1), iy2
    typex(i,j) = 0.0
    typey(i,j) = 0.0
    rho(i,j) = rhow
501    continue
500  continue
c
  do 510 j = (iy2-ilen1+1), iy2
    typex(ix2,j) = 3.0
    thetax(ix2,j) = 0.0
    typex(ix3,j) = 2.0
    thetax(ix3,j) = pi
510  continue
c
  do 520 i = ix2+1, ix3-1
    typey(i, iy2-ilen1) = 3.0
    thetay(i, iy2-ilen1) = 0.0
520  continue
c
c ::::: X-RAY ENERGY DEPOSITION INTO EXPOSED BOUNDARY NODES.
c ::::: COMPUTE INTENSITY
flag = 0.
do 600 j = (iy2-ilen1+1), iy2
  d_x = float(ix2 - ix1)*dx
  d_y = float(j - iy1)*dx
  rad2 = d_x**2.+d_y**2.
  rad = sqrt(rad2)
  flux = yield*0.16/4./pi/rad2
  e_den = atten*flux/rho_liq
  project = abs((d_x*cos(thetax(ix2,j))+d_y*
    & sin(thetax(ix2,j)))/rad)
  depth = -log(evap/e_den)/atten*project
  if (depth.gt.0.) then
    flag = 1.0
    rho(ix2,j) = rho_liq*depth/dx
    e_denavg = flux*(1.-exp(-atten*depth/project))/

```

```

&          rho_liq/depth
      pfrac = (e_denavg - evap)/e_denavg
      p(ix2,j) = flux*(1.-exp(-atten*depth/project))*gml/dx*pfrac
    endif
600  continue
c
do 610 i = ix1,ncellx
  d_x = float(i - ix1)*dx
  d_y = float(iybl - iy1)*dx
  rad2 = d_x**2.+d_y**2.
  rad = sqrt(rad2)
  flux = yield*0.16/4./pi/rad2
  e_den = atten*flux/rho_liq
  project = abs(d_y/rad)
  depth = -log(evap/e_den)/atten*project
  if (depth.gt.0.) then
    flag1 = 1.
    rho(i,iybl) = rho_liq*depth/dx
    e_denavg = flux*(1.-exp(-atten*depth/project))/
&          rho_liq/depth
    pfrac = (e_denavg - evap)/e_denavg
    p(i,iybl) = flux*(1.-exp(-atten*depth/project))*gml/dx*pfrac
  endif
610  continue
c
do 620 i = ixbl,ixl
  do 621 j = iybl,iy1
    if ((typex(i,j).ge.2.).or.(typey(i,j).ge.2.)) then
      d_x = float(i - ix1)*dx
      d_y = float(j - iy1)*dy
      rad2 = d_x**2.+d_y**2.
      rad = sqrt(rad2)
      if (rad2.gt.0.) then
        flux = yield*0.16/4./pi/rad2
        e_den = atten*flux/rho_liq
        if (typex(i,j).ge.2.) then
          project = abs((d_x*cos(thetax(i,j))+d_y*
&          sin(thetax(i,j)))/rad)
        else if (typey(i,j).ge.2.) then
          project = abs((d_x*sin(thetay(i,j))+d_y*
&          cos(thetay(i,j)))/rad)
        endif
        depth = -log(evap/e_den)/atten*project
        if (depth.gt.0.) then
          rho(i,j) = rho_liq*depth/dx
          e_denavg = flux*(1.-exp(-atten*depth/project))/
&          rho_liq/depth
          pfrac = (e_denavg - evap)/e_denavg
          p(i,j) = flux*(1.-exp(-atten*depth/project))*gml/dx*pfrac
        endif
      endif
    endif
  continue
621  continue
620  continue
c
c ::::: SYMMETRIC BOUNDARY ALONG TOP AND BOTTOM
do 300 i = ixbl,ixb2
  typey(i,iyb2) = 7.
  thetay(i,iyb2) = 0.
300  continue
do 302 i = ixl,ixb2
  typey(i,iybl) = 6.
  thetay(i,iybl) = pi
302  continue

```

```

c
c ::::: WRITE INITFILE DATA FILE
      open(29,file=initfile,form='unformatted')
      write(29) t,n,nframes,gamma
      do 700 i = 1, ncellx
        do 710 j = 1,ncelly
          write(29) rho(i,j)
          write(29) u(i,j)
          write(29) v(i,j)
          write(29) p(i,j)
          write(29) typex(i,j)
          write(29) typey(i,j)
          write(29) thetax(i,j)
          write(29) thetay(i,j)
710      continue
700      continue
      close(29)
      end

c-----
c      CUSTOM_INIT.I
c-----
c ::::: TSUNAMI geometric include file
c
c-----
c
c      SPECIFIC PROBLEM:
c      Inner elliptical cavity shock computation
c      Grid resolution: 192 x 64
c
c-----
c
      parameter (r0 = 8.3144)          !gas constant
      parameter (wtmol = 0.005267)     !molecular wieght
      parameter (gamma = 1.58)         !ratio of spec. heats
      parameter (p1 = 1.333)           !initial cavity pressure [Pa]
      parameter (templ = 295.0)        !initial cavity temp [K]
      parameter (rhow = 1.0)           !wall density [kg/m3] for video
      parameter (pw = 1.0)             !wall pressure [Pa] for video
      parameter (ix1 = 40)             !ablation shield position on grid
      parameter (iy1 = 64)             !ablation shield position on grid
      parameter (ix2 = 64)             !ablation shield position on grid
      parameter (iy2 = 64)             !ablation shield position on grid
      parameter (ix3 = 72)             !ablation shield position on grid
      parameter (iy3 = 64)             !ablation shield position on grid
      parameter (ixb1 = 11)            !cavity position on grid
      parameter (iyb1 = 5)             !cavity position on grid
      parameter (ixb2 = 190)           !cavity position on grid
      parameter (iyb2 = 64)            !cavity position on grid
      parameter (iradx = 30)           !major radius
      parameter (irady = 60)           !minor radius
      parameter (ilen1 = 9)            !ablation shield x-dim
      parameter (ilen2 = 12)          !ablation shield y-dim
      parameter (e_theta = .3805064)   !ablation shield cone angle
      parameter (yield = 2.0e7)        !fusion pellet yield
      parameter (evap = 3.578e7)       !wall material dissoc. energy
      parameter (rho_liq = 689.)       !density of wall material
      parameter (atten = 1.385e4)      !x-ray atten. coeff [m-1]
c-----

```

A-4. Sample Custom Output Subroutine

The following subroutine integrates the pressure around each cylinder in the LJUST simulation to find the form drag. It also computes momentum transfer, expected velocity and cylinder position if the jets are allowed to move. It also finds the average velocity for all the jets and the average position.

```
-----
      subroutine custom_out(t,dt,n,nframes,rho,u,v,p,
&      typex,typey,thetax,thetay,cmom,icyl)
-----
c ::::: USER CUSTOMIZED OUTPUT SUBROUTINE
c
      include "tsu_geo.i"
      include "tsu_inp.i"
      include "custom_init.i"
      include "custom_out.i"
c
c ::::: FLOW PROPERTIES
      dimension rho(1:ncellx,1:ncelly)
      dimension u(1:ncellx,1:ncelly)
      dimension v(1:ncellx,1:ncelly)
      dimension p(1:ncellx,1:ncelly)
c
c ::::: GRID & GEOMETRIC INFO
      dimension typex(1:ncellx,1:ncelly)
      dimension typey(1:ncellx,1:ncelly)
      dimension thetax(1:ncellx,1:ncelly)
      dimension thetay(1:ncellx,1:ncelly)
c
c ::::: DRAG, MOMENTUM, SPEED, AND OTHER
      dimension icyl(1:ncyl,1:4)
      dimension drag(1:ncyl)
      dimension cmom(1:ncyl)
      dimension speed(1:ncyl)
      dimension rdist(1:ncyl)
c
      ncyla = ncyl
c
      avgspeed = 0.
      avgdist = 0.
c
c ::::: compute form drag on cylinders here
      do 440 i = 1,ncyla
        drag(i) = 0.
        id = icyl(i,4) + 1
        do 230 ix = (icyl(i,2)-id), (icyl(i,2)+id)
          do 231 iy = (icyl(i,3)-id), (icyl(i,3)+id)
            if(typex(ix,iy).eq.2.) drag(i)=drag(i)-p(ix,iy)*dx
            if(typex(ix,iy).eq.3.) drag(i)=drag(i)+p(ix,iy)*dx
          231 continue
        230 continue
        cmom(i) = cmom(i) + drag(i)*2.*dt
        speed(i) = cmom(i)/1000./(pi*(float(id)*dx)**2.)
        rdist(i) = rdist(i) + speed(i)*2.*dt
        avgspeed = avgspeed + speed(i)
      440

```



```

      avgdist = avgdist + rdist(i)
440  continue
c
      write(19,901) t, (drag(1),l=1,ncyla)
      write(20,901) t, (cmom(1),l=1,ncyla)
      write(21,901) t, (speed(1),l=1,ncyla)
      write(22,901) t, (rdist(1),l=1,ncyla)
      write(23,902) t, avgspeed/float(ncyla), avgdist
c
901  format(48(e11.4,1x),e11.4)
902  format(2(e11.4,1x),e11.4)
c
      return
      end
c-----

```

A-5 tsu_geo.i Source Listing

The tsu_geo.i subroutine is an abbreviation for TSUnami GEOMetry include file. This subroutine provides the geometric dimensions of the grid. It can be included in any subroutine which needs to know the parameters of the computational grid. The example below is for the LJUST simulation. The variables ncellx and ncelly determine the number of nodes in the x- and y-directions. The variable nmax, is the larger of either ncellx or ncelly. The variable pi is just the constant π which is the ratio of perimeter to diameter for a circle. Finally, dx and dy are the cell sizes.

```

c-----
c      TSU_GEO.I
c-----
c      TSUNAMI geometric include file
c
c-----
c
c      SPECIFIC PROBLEM:
c      LJUST simulation shock attenuation
c      Grid resolution: 600 x 100
c      dx = dy = 9.525e-04 m
c
c-----
c      parameter (ncellx = 600)
c      parameter (ncelly = 100)
c      parameter (nmax = 600)
c      parameter (pi = 3.1415926954)
c      parameter (dx = 9.525e-04)
c      parameter (dy = 9.525e-04)
c-----

```

A-6 tsu_inp.i Source Listing

The tsu_inp.i subroutine is an abbreviation for TSUnami INPut include file. This subroutine provides the parameters TSUNAMI requires during run time. The example below is for the LJUST simulation. The variables "courant" and "tstop" are the CFL number used for the stability criterion during run time (must always be less than one), and the duration of the simulation, respectively. The parameter "initfile" is a character string which stores the name of the input deck produced by the custom_init.f program.

```
c-----
c      TSU_INP.I
c-----
c ::::: TSUNAMI runtime include file
c
c-----
c
c      SPECIFIC PROBLEM:
c      LJUST simulation shock attenuation
c      Grid resolution: 600 x 100
c      dx = dy = 9.525e-04 m
c
c-----
c      parameter (courant = 0.85)
c      parameter (tstop = 0.0015)
c      character*13 initfile
c      parameter (initfile = 'init_dat.file')
c-----
```

A-7 tsu_out.i Source Listing

The tsu_out.i subroutine is an abbreviation for TSUnami OUTut include file. This subroutine provides the parameters TSUNAMI uses to configure the output file to reflect the desired output quantities. The first entries, dt_frame and nt_dump are the time increment between outputting a frame of visualization data (for animation) and the number of time steps between a full memory dump (for insurance against system crashes). The next set of 8 ifile parameters are meant as switches or flags which turn outputting on or off. If the value is 1, then output is turned on. If the value is 0, then output is shut off. Two types of output are available by default. The first type is the flow map of the entire grid. These are output for animation and visualization purposes. A flow map is output every dt_frame seconds of simulated time. The second type is transducer output. These diagnostics output some quantity on the grid at a fixed position every time step. Six locations on the grid are available (more can be added by modifying the actual tsunami.f source code).

The 8 ifile variables switch on or off, the density map output, the u-velocity map, the v-velocity map, the pressure map, density transducers, u-velocity transducers, v-velocity transducers, and finally pressure transducers. The icustom flag turns the custom output subroutine on and off in the same way as the ifile flags. The filename definitions at the end of the include file provide the default output file names for their respective outputs.

```
c-----  
c      TSU_OUT.I  
c-----  
c ::::: TSUNAMI geometric include file  
c  
c-----  
c  
c      SPECIFIC PROBLEM:  
c      LJUST simulation  
c  
c-----  
c
```

```

c ::::: RUNTIME PARAMETERS
c ::::: dt_frame = time increment in computed seconds to output a frame
c ::::: nt_dump = number of timesteps between memory dumps (0=no dump)
           parameter (dt_frame = 0.000075)
           parameter (nt_dump = 100)
c
c ::::: OUTPUT FLAGS
           parameter (ifile1 = 1)
           parameter (ifile2 = 0)
           parameter (ifile3 = 0)
           parameter (ifile4 = 0)
           parameter (ifile5 = 1)
           parameter (ifile6 = 1)
           parameter (ifile7 = 1)
           parameter (ifile8 = 1)
           parameter (icustom = 0)
c
c ::::: TRANSDUCER LOCATIONS
           parameter (ntx1 = 303)
           parameter (nty1 = 96)
c
           parameter (ntx2 = 382)
           parameter (nty2 = 96)
c
           parameter (ntx3 = 427)
           parameter (nty3 = 96)
c
           parameter (ntx4 = 473)
           parameter (nty4 = 96)
c
           parameter (ntx5 = 515)
           parameter (nty5 = 96)
c
           parameter (ntx6 = 600)
           parameter (nty6 = 50)
c
c ::::: DEFINE FILENAMES
           character*8 dfile, file1, file5, cfile
           character*6 file2, file3, file4, file6, file7, file8
           parameter (dfile = 'dump_out')
           parameter (file1 = 'rho_grid')
           parameter (file2 = 'u_grid')
           parameter (file3 = 'v_grid')
           parameter (file4 = 'p_grid')
           parameter (file5 = 'rho_tran')
           parameter (file6 = 'u_tran')
           parameter (file7 = 'v_tran')
           parameter (file8 = 'p_tran')
           parameter (cfile = 'outdata')
c-----

```

A-8 yield.f Source Listing

The yield.f subroutine computes the density, and pressure values for the initial conditions in the HYLIFE simulations. These are scaled according to Glenn's [1980] results. The variables which can be changed for this calculation are the yield and the evaporated mass (the first two parameters below). The resulting profile is assumed to correspond to the profiles in figure 5.1, and share the same shape.

```
c-----
      program yield
c-----
c::   to compute density, velocity and pressure for      ::
c::   a given yield, mass evaporated and molecular props  ::
c-----
      parameter (yield = 2.7e09)
      parameter (emass = 15.)
      parameter (height = 1.0)
      parameter (radout = 0.44)
      parameter (rad1 = 0.15)
      parameter (rad2 = 0.30)
      parameter (rad3 = 0.44)
      parameter (pi = 3.141592654)
      parameter (gamma = 1.67)

c
      yield2 = .32*.6258*yield
      rho1 = emass/(height*pi*(46.*rad3**2.-45.*rad2**2.))
      rho2 = 46.*rho1

c
      vol = pi*rad3**2.*height
      p = 0.92345*(gamma-1.)*yield2/vol

c
      e_ke = yield2 - p/(gamma - 1.)*vol
      denom = 2.*pi*rho1*height*(rad1**3./3.+4.5*((rad2**3.-rad1**3.)/3.
&      - rad1*rad2**2./2. + rad1**3./2.)/(rad2 - rad1) - rad2**2./2.
&      + rad1**2./2.) + 5.5*pi*rho2*height*(rad3**2. - rad2**2.)
      u1 = sqrt(e_ke/denom)
      u2 = u1*5.5

c
      print*, 'rho1 = ', rho1
      print*, 'rho2 = ', rho2
      print*, 'u1 = ', u1
      print*, 'u2 = ', u2
      print*, 'p = ', p
      end
c-----
```

A-9 Condensation Boundary Condition Subroutine

The subroutine condbc.f is given for a one-dimension implementation. This subroutine computes the qstar values at the interface corresponding to $q1 = \rho$, $q2 =$ normal velocity, and $q3 =$ pressure at the boundary node for an ideal gas provided that the liquid temperature distribution tliq is given. Because the scheme is iterative, the time, t , time step dt , the solution in phase space, xbyt, and liquid cell size $dxlg$ are required inputs. The condensation is assumed to follow kinetic theory according to [Shrage 1953]. Details on the methodology and the scheme are given in chapter 6.

```

c-----
      subroutine cond_bc(q1,q2,q3,qstar,gamma,tliq,t,
      & dt,xbyt,dxlg,tls)
c-----
c
      include "xxcond.i"
      dimension tliq(0:ncellx)
      dimension tliqnew(0:ncellx)
      dimension ql(1:4)
      dimension qr(1:4)
      dimension qstar(1:4)
      real g,wtmol,r0,q1,q2,q3,gamma,t,dt
c
      niter = 15
      niter2 = 15
      fe = 1.
      fc = 1.
      wtmol = 0.035
      r0 = 8.3144
      rl = r0/wtmol
      gml = gamma - 1.
      gpl = gamma + 1.
      gminv = 1./gamma
c
c ----- gas props -----
c
c ::::: compute local ideal gas props
      rho = q1
      u = q2
      p = q3
      c = sqrt(gamma*p/rho)
      cmach = u/c
      tlloc = p/rl/rho
c
c ::::: compute ideal gas stagnation state props
      rho0 = rho*(1. + gml/2.*abs(u)/c)**(2./gml)
      u0 = 0.
      p0 = p*(1. + gml/2.*abs(u)/c)**(2.*gamma/gml)
      c0 = sqrt(gamma*p0/rho0)
      t0 = tlloc*(1. + gml/2.*abs(u)/c)**2.
c
c -----first guess for solution to mass flux -----

```

```

c
c :::::: guess liquid surface props = sub-surface props at tliq(1)
c :::::: guess vapor surface props. corresponds to isen.max. gas flux.
c
      tls = tliq(0)
      psat = 101300.*(10.**((9.407-1.0054e4/tls))/760.
      rhovs = rho
      uvs = u
      pvs = p
      cvs = c
      tvs = tloc
      cvsmach = cmach

c
c :::::: maximum mass flux possible from gas dynamics
c :::::: if super sonic, the mass flux is just the supersonic mass flux
      if (cmach.ge.1) then
        gvmax = rho*u
      else if (cmach.lt.1.) then
        gvmax = rho*(u+2.*c/gml)*(gml/gpl*(cmach+2./gml))**(2./gml) -
&          2.*rho*c/gml*(gml/gpl*(cmach+2./gml))**(gpl/gml)
      endif

c
c -----iteration to converge on mass flux, tls, and tvs-----
c
      n = 0
10    continue
c
c :::::: mass flux from shrage's theory
      s = cvsmach*sqrt(gamma/2.)
      bgamma = exp(-s**2.) + s*sqrt(pi)*(1+erf(s))
      gcond = fc*pvs*sqrt(1./(2.*pi*rl*tvs))*bgamma
      gevap = fe*psat*sqrt(1./(2.*pi*rl*tls))
      gk = gcond - gevap

c
c :::::: smaller of two fluxes limits
      g = min(gk,gvmax)

c
c :::::: heat flux BC at first node to get new tls and psat
      hgasi = gamma*pvs/gml/rhovs+uvs**2./2.
      hgas = cpl*(tvs-tlinf) + hfg
      hliq = cpl*(tls-tlinf)
      qrad = fe*rsigma*(tvs**4.-tls**4.)
      if (g.gt.0.) then
c
        tlsnew = (thcond/dxlg*tliq(1)+g*hgas)/(g*cp+thcond/dxlg)
        tlsnew = tliq(1) + dxlg/thcond*g*(hgas-hliq)
      else if (g.lt.0.) then
        tlsnew = (tliq(1) + (g*hfg*dx/thcond))/(1-cpl*dxlg/thcond)
      endif

c
c :::::: check if tls = tlsnew - if yes, converged, if no, iterate
      if (n.eq.1) then
        if (tlsnew.lt.tls) then
          tslow = tlsnew
          tlshigh = tls
        else
          tlshigh = tlsnew
          tslow = tls
        endif
      endif
      tdiff = abs(tls-tlsnew)/tls
      if ((tdiff.gt.1.0e-05).and.(n.le.niter)) then
        if (tlsnew.gt.tls) then
          tslow = tls
          tls = (tls+tlshigh)/2.
        else
          tlshigh = tslow
          tls = (tslow+tlsnew)/2.
        endif
      endif

```

```

        tslow = tls
        tls = (tls+tlshigh)/2.
    else if(tlsnew.lt.tls) then
        tlshigh = tls
        tls = (tls+tslow)/2.
    endif
    psat = 101300.*(10.**((9.407-1.0054e4/tls))/760.
    n = n + 1
    goto 10
endif
tliq(0) = tls
c
20    continue
c
c ----- temperature distribution in liquid -----
c
c ::::: compute finite diff. coeffs for liq calc.
        r11 = alpha*dt/(dxlg*dxlg)
        r12 = q*dt/(rho1*dxlg)
c
c ::::: energy balance check
c ::::: energy per square meter of slab - old
        tsum_old = 0.
        tsum_new = 0.
        do 25 i = 1, ncellx-1
            tsum_old = tsum_old + tliq(i)
25    continue
        esum_old = cpl*rho1*dxlg*tsum_old
c
c ::::: conduction of energy into liquid
        do 30 i = 1, ncellx-1
            tliqnew(i) = tliq(i) + r11*(tliq(i-1)-2.*tliq(i)+tliq(i+1))
            & - r12*(tliq(i)-tliq(i-1))
30    continue
c
c ::::: energy per sq. meter of slab -new
        do 26 i = 1, ncellx-1
            tsum_new = tsum_new + tliqnew(i)
26    continue
        esum_new = cpl*rho1*dxlg*tsum_new
        ediff1 = esum_new - esum_old
c
c ::::: reassign new temperatures to old array, but
c ::::: adaptive mesh doubles cell size everytime last cell increases
c ::::: by .001 of the liquid internal temperature
c
        tdiff = abs(tliq(ncellx-1)-tlinf)/tlinf
        if(tdiff.gt.0.001) then
            dxlg = 2.*dxlg
            tliq(1) = 2.*tliq(1) - tliq(0)
            do 40 i = 2, ncellx/2
                ii = 2*i
                iim1 = 2*i - 1
                iip1 = 2*i + 1
                tliq(i) = (tliqnew(iim1) + 2.*tliqnew(ii) + tliqnew(iip1))/4.
40    continue
            do 42 i = ncellx/2, ncellx
                tliq(i) = tlinf
42    continue
        else
            do 44 i = 1, ncellx-1
                tliq(i) = tliqnew(i)
44    continue
        endif
endif

```



```

      write(13,400) t*1.0e06,g,gk,gvmax,tvs,tls,pvs,psat,cvsmach
400      format(8(e10.3,1x),e11.4)
c
      ediffg = g*hgas*dt
c      print*, 'rho,u,p,e1,eg', rho,g/rho,p,ediff1,ediffg
c      print*, 'hgas,hgasi',hgas,hgasi-cpl*tlinf
c
c :::::: boundary condition for gas dynamics
c :::::: use Riemann solver...seek solution that satisfies mass flux
c :::::: iterate until G matchs
c
c...first guess
      ql(1) = rho
      qr(1) = rho
      ql(3) = p
      qr(3) = p
      ql(4) = gamma
      qr(4) = gamma
      nn2 = 0
      xbyt = 0.
c
      u_suc = 2.*g/rho
c      print*, 'u_suc',u_suc
      ql(2) = uvs
      qr(2) = -uvs + u_suc
c
600      continue
      call riemann (ql,qr,qstar,xbyt)
      gr = qstar(1)*qstar(2)
      g_diff = (gr-g)/gvmax
c      print*, 'u_suc',u_suc
c      print*, 'g_diff,gr,g ',g_diff,gr,g
c      print*, 'ul,ur',ql(2),qr(2)
      if(abs(g_diff).gt.0.001 .and. nn2.le.niter2) then
          u_suc = u_suc*(1.-g_diff)
          qr(2) = -uvs+u_suc
          nn2 = nn2 + 1
          goto 600
      endif
c
c :::::: check enthalpy
c      h1 = g*(gamma*p/gm1/rho + u**2./2.)
c      h2 = g*(gamma*qstar(3)/gm1/qstar(1) + qstar(2)**2./2.)
c      print*, 'h_flux0, hflux_rie',h1,h2
c
      return
      end
c=====

```

Appendix B. BENCHMARKS

To test the applicability of the approximate boundary conditions, three comparisons are presented here. The first two are qualitative comparisons of shock diffraction around a corner and shock flow past a cylinder while the third is a quantitative comparison with experimentally obtained shock retardation data. For the first two problems, iso-density contours provide a convenient method of visualizing the gas dynamics and comparing qualitative features. Non-dimensional units are used.

B.1. Shock Diffraction Around a Corner

The first benchmark is a comparison of density contour plots for a Mach 3 shock diffracting around a sharp corner. The TSUNAMI code used a 50x50 uniform grid. Figure B.1 shows the initial condition. The shaded region represents the solid corner. Region (1) is the undisturbed test gas. Region (2) is the gas behind the shock front. The calculation begins with the shock front one node away from the corner.

Figure B.1. Schematic of the initial condition used in the shock diffraction computation. Dotted lines represent freestream boundaries, and solid lines, reflecting or symmetric boundaries.

The gas, ideal, and adiabatic air has a ratio of specific heats $\gamma = 1.4$, which is assumed constant. The boundary to the left, right and top of figure B.1, is an open, "free stream"

boundary [van Leer, 1979]. The boundary along the lower edge represents a plane of symmetry. The shock tube that originally generated the shock is assumed to be sufficiently long, such that the region (2) is a constant state region during the whole duration of the calculation.

Figure B.2 shows the comparison of density contour plots between the TSUNAMI calculation and a previous calculation [Carafano, 1984]. Some discrepancies exist such as a higher wall shock speed at 90 degrees which results in a flatter and smoother profile than in the other calculation. Also, some of the internal details to the right of the vortex swirl are different. These differences may be attributed to coarser mesh spacing and shorter physical time of calculation in our calculations. Overall, however, most of the major phenomena such as the vortex swirl, transmitted shock front and downward propagating acoustic wave are all represented.

Figure B.2. Iso-density contours of Mach 3 shock in air diffracting around a corner. Left figure computed using TSUNAMI code with 50x50 grid, and right side computed by Carafano [1984] as presented by Hillier and Graham [1985].

B.2. Shock Flow Around a Cylinder

The second benchmark is a comparison of density contour plots for a Mach 1.65 shock flowing over a cylinder. The TSUNAMI code uses an 80x80 uniform grid. Figure

B.3 shows the initial condition. The shaded region represents the solid cylinder. The calculation begins with the shock front one node away from the cylinder. As in the preceding shock diffraction problem above, the gas is ideal and adiabatic air.

Figure B.3. Schematic of the initial condition used in the shock flow over a cylinder computation.

The boundaries on all four sides of the grid are free stream boundaries. The cylinder uses the approximate boundary conditions described in chapter 3, and the `roundbc.f` subroutine listed in appendix A-3.1. The cylinder is approximated by a 16 cell diameter region. Again, the shock tube that originally generated the shock is assumed to be sufficiently long, such that the shock gas region is a constant state region during the whole duration of the calculation. Figure B.4 shows density contours for calculated shock flow over a cylinder compared with a photograph of the real process [Bowman and Niblett, 1956]. Remarkably good agreement exists in the qualitative features between calculation and experiment. A small difference does exist in the width and curvature of the Mach stems which trail behind the cylinder. A closer inspection reveals that the cylinder in the photograph is somewhat elliptical, which may be the cause of the discrepancy.

Figure B.4. Comparison of iso-density contours for Mach 1.65 shock in air over a cylinder computed using TSUNAMI. 80x80 grid to Mach 1.65 shock through a bank of cylinders. (Only one cylinder shown). From Bowman and Niblett [1956].

The second benchmark suggests that number of nodes needed to model a round object like a cylinder is less than 16. The number of cells needs is not exactly known because the minimum number of nodes needed to approximate a 2 dimensional curvature was not specifically investigated. However, from the LJAST simulations in chapter 4 which used 10 cells diameter cylinders and still predicted reasonably accurate results, an estimate of about 8 to 10 cells for the characteristic diameter of a curved object like a cylinder appears to be the minimum.

B.3. Shock Retardation Experiment

In the third benchmark test, we attempt to predict the shock retardation for the experimental set-up shown in Figure B.5 and then compare the computed results with the experimental data of Kawamura and Kawada [1957]. The experiment presents a suitable benchmark because of its complex geometry. Air is the gas in both cases. Table B.1 gives a comparison of the results.

The main parameter measured in the experiment was the retardation coefficient. The retardation is given as distance r divided by the distance L (figure B.5) where r is the distance between the unimpeded shock front and the attenuated shock. The total length, L , is the distance from the cylinder center to the unimpeded shock front. The experimental results were obtained from photographic data of the shocks. Multiple runs were averaged to provide the single reported value. The researchers report standard deviations in their data of as much as 50% [Kawamura and Kawada, 1957].

The TSUNAMI calculation used a 100x26 grid to represent the experiment. The case of the plane, unimpeded shock propagation was run first until the shock had traversed a distance of 45 cm from the cylinder. The transit time for the unimpeded shock to move 45 cm was then recorded. The value of shock velocity was compared with the analytical Riemann solution and verified to be within 0.01% of the value for Mc , the analytical shock speed. Next, the same run is repeated with the blockage in place. The simulated duration is set to terminate at the same time the unimpeded shock traverses the 45 cm distance. When the calculation stops, the code locates the position of the steepest horizontal pressure gradient on the grid. The x-direction cell index at this position is now taken as the position of the retarded shock.

By inspection, the TSUNAMI calculations are mostly within 5% to 10% of the reported values, well within the reported margins of experimental error. The calculations for 58% blockage tended to under estimate the retardation while the calculations at 78% blockage over estimate the retardation. This was traced back to the nodalization and use of integer spaced grids which resulted in slightly smaller percentage blockage (57.7% - 15 cells) for the 58% case and slightly higher percentage blockage (76.9% - 20 cells) for the 75% case. The higher blockage, similar to the cases run in chapter 5, causes the flow to become actually faster in velocity with less blockage. This agrees in principle with equation (2.9) which says that a reduction in area increases the Mach number.

Figure B.5. Experimental apparatus used in experiment to study shock retardation with obstructions in the flow path. From Kawamura and Kawada [1957].

Table B.1. Shock Retardation Results.

Mach No.	Blockage	retardation [r/L]	
		Experiment	TSUNAMI
1.25	58%	3.2%	3.1%
	75%	5.4%	6.1%
1.36	58%	3.7%	3.3%
	75%	7.5%	8.0%

Appendix C. CALIBRATION AND ERRORS

C-1. Pressure Transducer Calibration.

The LJUST experiment used Kistler 601B1 miniature piezo-electric pressure transducers (figure 2.15). These transducers output a given charge for a given pressure on their surface. The charge is then converted to a proportional voltage signal using Kistler transducer amplifiers. (figure C.1). The voltage signal then becomes the input into any standard oscilloscope. The transducers each come from the manufacturer, Kistler Instruments, Clarence, New York, with a calibration curve showing the linearity in the charge output to the pressure applied to the crystal. The piezo-electric crystals inherently output a charge proportional to the pressure applied. The transducers are each recalibrated in our laboratory before installment into the LJUST experiment. Each transducer is calibrated in conjunction with its own charge amplifier and the same amplifier-transducer combination is used as a pair. If a transducer is switched with an amplifier, the calibration is performed again

The manufacturer lists a charge to pressure ratio for each transducer. Typically, this is between 1.0 and 1.2 picoCoulombs per psi. The amplifiers can then be set using the main dial on the face of the amplifier (figure C.1.). Because of differences in the calibrations of the transducer amplifiers in converting the charge signal to a voltage signal, the calibration to determine the setting on the amplifier must be performed prior to use.

The calibration used a Crosby dead weight tester to provide a known pressure source. Each transducer is subject to a known pressure, and then the reading from the data acquisition system recorded as described in chapter 2. The calibration requires about 30 seconds for each pressure measurement. This requires that the amplifiers output a constant voltage over that period of time for a constant input charge. The charge amplifiers have 3 time settings - short response, medium response, and long response. In

short response mode, the amplifier responds within 1 microsecond to any sudden changes in charge input. However, the voltage decays exponentially with time back toward ground after only about 0.1 second. In the long response mode, the amplifiers require about 0.1 second to respond to changes in pressure, but can sustain the output for 100 seconds. The exponential decay constant is roughly 1000 seconds. The manufacturer assures that the voltage output for a given charge is the same regardless if the amplifier is on long or short response modes. Calibration used a basic number of steps. listed in Table C.1.

Table C.1. Calibration procedures (cf. figure C.2).

1.	Turn on the data acquisition system and transducer amplifier (chapter 2.)
2	Screw the main plunger all the way down on the Crosby dead weight tester.
3.	Open the oil reservoir and fill with hydraulic oil to within 5 mm of the top
4.	Open the oil release valve and unscrew the main piston handle to draw oil into the system. Add more oil as it is drawn into the plunger chamber.
5.	When the plunger is roughly 70% to 80% withdrawn, close the oil release valve.
6.	Turn the plunger handle to force oil up into the test column.
7.	Mount the transducer and fitting into the Crosby dead weight tester (figure 2.15)
8.	Set the data acquisition system to continuous reading and output for the single amplifier and set the amplifier to the factory installed charger/psi output on the main dial.
9.	Set the Crosby dead weight tester to zero pressure.
10.	Zero the pressure using software on the PC data acquisition system.
11.	Set a new pressure on the dead weight tester and quickly screw the dial to the correct pressure. Record the pressure off of the PC monitor.
12.	Repeat steps 9 through 11 for higher and higher pressures until 10 points or more are obtained for the current amplifier setting.
13.	Plot the measured pressure to the actual pressure and fit the best straight line through the data. If the slope of the line is not 1.0, then correct the dial setting for pCb/psi on the amplifier by a proportional amount of $s \cdot m$ where s is the old setting and m is the slope of the fitted line. By inspection, if the amplifier is outputting a higher voltage than it should, then increasing the pCb/psi on the sensitivity dial decreases the sensitivity of the amplifier and therefore reduces the voltage output.
14.	Repeat the calibration to verify that the output pressure from the dead weight tester is actually being output digitally on the PC with a slope of 1.0.

C-2. Experimental Error Assessment

The relative error in the experiment is assessed using standard error propagation methods [Tsoulfanidis, 1983]. The relative error for a chain of errors in the experiment is defined by:

$$\frac{\delta F}{F} = \left[\left(\frac{\delta a_1}{a_1} \right)^2 + \left(\frac{\delta a_2}{a_2} \right)^2 + \dots + \left(\frac{\delta a_n}{a_n} \right)^2 \right]^{\frac{1}{2}} \quad (C.1)$$

where $\delta F/F$ is the relative uncertainty and $\delta a/a$ is the fractional uncertainty for some independent step in the chain of data acquisition. For this experiment, possible errors exist in the transducer calibration, the measurement of arrival time and the transducer response time. The effect of test section vibration and vessel ringing was not assessed.

C-2.1 Arrival Time Error

The transducer response time and measurement of arrival time are the key factors in the relative error expected in the arrival time. The transducers require 2 microseconds to sudden changes in pressure. For a time differential between transducers of only 40 microseconds on average, this translates into a 2/40th or 5% fractional uncertainty. The dimension of the transducer face is itself, about 5 mm in diameter. The average distance between transducers may be as little as 3 cm. Therefore, the fractional uncertainty is roughly of order 5/30 or 17%. The sampling rate of the computer is 500 kHz or 2 microseconds. Hence, this adds another 2/40 or 5% uncertainty. The above values summed together using equation (C.1) yields:

$$\left. \frac{\delta F}{F} \right|_{\text{uncertainty}} = \left[(0.05)^2 + (0.17)^2 + (0.05)^2 \right]^{\frac{1}{2}} = 0.18.$$

Therefore the uncertainty in the time measurement is roughly plus or minus 18%.

C-2.2 Pressure Measurement Error

Pressure calibration and transducer response time generate the majority of the error in the pressure measurement. All the pressure measurements were taken relative to some background pressure. This was added to the final pressure listed in the tables in both chapter 4 and in appendix D. The background pressure is usually sub atmospheric. For pressures below 100 Pa, a Hastings thermocouple gauge can yield very accurate pressure readings within 1 Pa. However, in the range above 100 Pa to 1 atmosphere absolute pressure, the pressure is difficult to assess except with conventional spring loaded gauges. The experiment utilized a spring loaded vacuum gauge which was calibrated to read atmospheric pressure with no vacuum and -29.92 inches of Hg relative to atmosphere with the suction of a mechanical vacuum pump calibrated to pull 1 Pa pressure vacuum. The linearity of the gauge was assumed. The error in the background pressure measurement was therefore roughly 0.5 inch of Hg, which is roughly 1.7 kPa. The relative uncertainty for a pressure reading of 20 kPa is then approximately 8.5%.

The pressure calibration on the dead weight tester was accurate to approximately 3 kPa, which for readings of 20 kPa corresponds to approximately a 15% uncertainty in pressure. The data acquisition system discriminates to within 10 millivolts. For most of the runs, the amplifiers were set to output approximately 0.05 volts/psi. This implies that the data acquisition is accurate to roughly 0.2 psi or 1.4 kPa. This corresponds to an uncertainty of 7% for a 20 kPa pressure reading. Summing these three affects yields:

$$\left. \frac{\delta F}{F} \right|_{\text{pressure uncertainty}} = \left[(0.085)^2 + (0.15)^2 + (0.07)^2 \right]^{\frac{1}{2}} = 0.19.$$

Other error may exist in the experiment. For example, because the PC data acquisition system can only sample the pressure once every 2 microseconds, there may be occasions such that the a pressure peak may rise and fall in that period. However, this was not assessed.

Figure C.1. A Kistler transducer amplifier.

Appendix D. DATA TABLES

The following tables are list the reduced data from the experiment as well as the computations. One computes velocity and Mach number according to the equations given in chapter 4:

$$u_{AB} = \frac{x_B - x_A}{t_B - t_A} \quad (4.1)$$

$$M_{AB} = \frac{u_{AB}}{c_I} \quad (4.2)$$

The positions x_A , x_B , etc. are given in figure 4.1 relative to the entrance to the test section. The sound speed, c_I , is the sound speed in the undisturbed test gas. For shocks into air, c_I is 344 m/s, and for helium, 1011 m/s. The shock retardation is given by:

$$r = \frac{M_{AB} - M_{EF}}{M_{AB}} \quad (4.3)$$

The reflected shock pressure for plane shock reflection is given by:

$$\frac{p_R}{p_2} = \frac{(3\gamma - 1)M_I^2 - 2(\gamma - 1)}{(\gamma - 1)M_I^2 + 2} \quad (4.4)$$

where p_2 is the pressure behind the approaching shock, or p_A in this case. The Mach number M_I , in this case is M_{AB} .

For the liquid impact cases, the velocity of the liquid is estimated using the method described in section 4.2.3. Equation 4.6 was derived to estimate the values., i.e:

$$v_w = 2 \frac{x_{DF}}{t_w - t_D} \quad (4.6)$$

The input data for the velocities come from Tables 4.4 and 4.7. The Bernoulli stagnation pressure for liquid is just given by $\rho v_w^2/2$ where the density is for the liquid.

Table D.1. Shock velocity for LJUST shocks in air impacting a solid cylinder array.

Run #	u_{AB} [m/s]	u_{BC} [m/s]	u_{CD} [m/s]	u_{DE} [m/s]	u_{EF} [m/s]
1	351.95	252.13	313.03	325.31	373.75
2	351.95	315.17	296.33	291.82	369.73
3	358.71	289.61	288.64	305.29	295.15
4	365.75	289.61	292.43	374.41	435.26
5	392.70	369.50	296.33	360.80	367.76
6	396.88	345.67	336.74	354.35	399.83
7	401.14	340.18	341.92	360.80	432.52
8	401.14	363.24	313.03	354.35	369.73
9	409.96	375.99	313.03	354.35	384.19
10	414.51	329.71	347.27	354.35	443.68
11	419.17	369.50	322.10	367.48	446.56
12	423.93	389.66	322.10	360.80	384.19
13	433.79	404.36	326.84	367.48	384.19
14	438.90	389.66	322.10	*	*
15	444.12	412.14	326.84	374.41	390.74
16	449.47	243.54	300.34	450.99	333.84
17	478.29	428.63	389.91	320.06	399.83
18	484.50	437.37	336.74	381.61	392.97
19	484.50	455.98	336.74	396.88	386.35
20	497.42	428.63	341.92	396.88	458.47
21	504.14	446.48	341.92	404.97	386.35
22	518.14	487.07	404.09	389.09	386.35
23	621.77	549.52	444.50	348.14	440.84
24	678.30	612.32	404.09	413.41	467.83
25	811.01	714.38	1058.33	389.09	397.52
26	829.03	793.75	555.63	583.64	404.53
27	888.24	765.40	404.09	862.77	458.47
28	888.24	793.75	635.00	450.99	603.25
29	1008.28	793.75	505.11	314.98	838.66
30	1008.28	892.97	740.83	551.22	582.80
31	1097.24	974.15	823.15	583.64	648.78
32	1097.24	1071.56	383.19	461.48	464.67
33	1130.49	1071.56	823.15	583.64	636.76

Table D.2. Mach numbers for LJUST shocks in air impacting a solid cylinder array.

Run #	M_{AB}	M_{BC}	M_{CD}	M_{DE}	M_{EF}	r
1	1.023	0.733	0.910	0.945	1.086	-0.06
2	1.023	0.916	0.861	0.848	1.074	-0.05
3	1.042	0.842	0.839	0.887	0.858	0.18
4	1.063	0.842	0.850	1.088	1.265	-0.19
5	1.141	1.074	0.861	1.049	1.069	0.06
6	1.153	1.005	0.979	1.030	1.162	-0.01
7	1.166	0.989	0.994	1.049	1.257	-0.08
8	1.166	1.056	0.910	1.030	1.074	0.08
9	1.191	1.093	0.910	1.030	1.116	0.06
10	1.205	0.958	1.009	1.030	1.289	-0.07
11	1.218	1.074	0.936	1.068	1.298	-0.07
12	1.232	1.132	0.936	1.049	1.116	0.09
13	1.261	1.175	0.950	1.068	1.116	0.11
14	1.275	1.132	0.936	*	*	*
15	1.291	1.198	0.950	1.088	1.136	0.12
16	1.306	0.708	0.873	1.311	0.970	0.26
17	1.390	1.246	1.133	0.930	1.162	0.16
18	1.408	1.271	0.979	1.109	1.142	0.19
19	1.408	1.325	0.979	1.153	1.123	0.20
20	1.446	1.246	0.994	1.153	1.332	0.08
21	1.465	1.298	0.994	1.177	1.123	0.23
22	1.506	1.415	1.174	1.131	1.123	0.25
23	1.807	1.597	1.292	1.012	1.281	0.29
24	1.971	1.779	1.174	1.201	1.360	0.31
25	2.357	2.076	3.076	1.131	1.155	0.51
26	2.409	2.307	1.615	1.696	1.176	0.51
27	2.581	2.224	1.174	2.507	1.332	0.48
28	2.581	2.307	1.845	1.311	1.753	0.32
29	2.930	2.307	1.468	0.915	2.437	0.17
30	2.930	2.595	2.153	1.602	1.694	0.42
31	3.189	2.831	2.392	1.696	1.885	0.41
32	3.189	3.114	1.114	1.341	1.350	0.58
33	3.285	3.114	2.392	1.696	1.850	0.44

Table D.3. Ratio of p_B/p_R for LJUST shocks in air impacting a solid cylinder array.

Run #	M_{AB}	$p_R(M_{AB})/p_A$	p_B/p_A	p_B/p_R
1	1.023	1.05	0.99	0.94
2	1.023	1.05	1.08	1.03
3	1.042	1.10	1.09	0.99
4	1.063	1.15	1.68	1.47
5	1.141	1.34	1.21	0.90
6	1.153	1.37	1.89	1.39
7	1.166	1.40	1.19	0.85
8	1.166	1.40	1.26	0.90
9	1.191	1.46	1.40	0.96
10	1.205	1.49	1.80	1.21
11	1.218	1.52	1.29	0.85
12	1.232	1.56	1.38	0.89
13	1.261	1.63	1.40	0.86
14	1.275	1.66	1.84	1.11
15	1.291	1.70	1.96	1.15
16	1.306	1.74	2.20	1.27
17	1.390	1.94	1.59	0.82
18	1.408	1.98	1.57	0.79
19	1.408	1.98	1.73	0.87
20	1.446	2.08	5.83	2.81
21	1.465	2.12	1.98	0.93
22	1.506	2.22	2.30	1.04
23	1.807	2.92	1.82	0.62
24	1.971	3.27	2.02	0.62
25	2.357	4.02	3.14	0.78
26	2.409	4.11	2.74	0.67
27	2.581	4.40	1.23	0.28
28	2.581	4.40	3.25	0.74
29	2.930	4.91	1.71	0.35
30	2.930	4.91	4.50	0.92
31	3.189	5.23	4.42	0.85
32	3.189	5.23	4.80	0.92
33	3.285	5.34	3.36	0.63

Table D.4. Shock velocity for LJUST shocks in helium impacting a liquid jet array.

Run #	u_{AB} [m/s]	u_{BC} [m/s]	u_{CD} [m/s]	u_{DE} [m/s]	u_{EF} [m/s]
1	1165.82	1127.96	4938.89	1133.93	1250.37
2	1203.43	931.79	1852.08	1102.43	1146.18
3	1286.42	1339.45	1010.23	763.22	996.67
4	1381.71	1020.54	1389.06	1044.41	1011.33
5	1434.86	714.38	*	101.76	*
6	1434.86	1099.04	1033.72	944.94	996.67
7	1434.86	1648.56	1111.25	1044.41	1273.53
8	1622.01	1020.54	1709.62	1044.41	1185.70
9	1622.01	1428.75	1307.35	1044.41	1185.70
10	1658.06	1224.64	1709.62	1202.65	1375.41
11	1658.06	1260.66	1481.67	1240.23	1432.72
12	1695.74	1530.80	1389.06	1322.92	1375.41
13	1776.49	1428.75	1307.35	992.19	1165.60
14	2487.08	2381.25	1852.08	1240.23	1463.20

Table D.5. Mach numbers for LJUST shocks in helium impacting a liquid jet array.

Run #	M_{AB}	M_{BC}	M_{CD}	M_{DE}	M_{EF}	r
1	1.153	1.116	4.885	1.122	1.237	-0.07
2	1.190	0.922	1.832	1.090	1.134	0.05
3	1.272	1.325	0.999	0.755	0.986	0.23
4	1.367	1.009	1.374	1.033	1.000	0.27
5	1.419	0.707	*	0.101	*	*
6	1.419	1.087	1.022	0.935	0.986	0.31
7	1.419	1.631	1.099	1.033	1.260	0.11
8	1.604	1.009	1.691	1.033	1.173	0.27
9	1.604	1.413	1.293	1.033	1.173	0.27
10	1.640	1.211	1.691	1.190	1.360	0.17
11	1.640	1.247	1.466	1.227	1.417	0.14
12	1.677	1.514	1.374	1.308	1.360	0.19
13	1.757	1.413	1.293	0.981	1.153	0.34
14	2.460	2.355	1.832	1.227	1.447	0.41

Table D.6. Ratio of p_B/p_R for LJUST shocks in helium impacting a liquid jet array.

Run #	M_{AB}	$p_R(M_{AB})/p_A$	p_B/p_A	p_B/p_R
1	1.153	1.381	1.21	0.88
2	1.190	1.472	1.52	1.03
3	1.272	1.670	1.45	0.87
4	1.367	1.891	1.54	0.81
5	1.419	2.011	1.69	0.84
6	1.419	2.011	1.76	0.87
7	1.419	2.011	1.80	0.89
8	1.604	2.412	1.79	0.74
9	1.604	2.412	1.87	0.78
10	1.640	2.485	1.72	0.69
11	1.640	2.485	2.66	1.07
12	1.677	2.559	1.86	0.73
13	1.757	2.714	1.57	0.58
14	2.460	3.790	3.15	0.83

Table D.7. Estimated velocities and corresponding Bernoulli stagnation pressures for liquid impacting the vessel wall.

Run #	M_{AB}	v_w [m/s]	$\rho v_w^2/2$ [Pa]
1	1.153	117.85	907.00
2	1.190	97.98	626.87
3	1.272	136.89	1223.74
4	1.367	90.84	538.83
5	1.419	*	*
6	1.419	71.55	334.34
7	1.419	77.06	387.76
8	1.604	77.62	393.39
9	1.604	86.09	484.03
10	1.640	63.97	267.25
11	1.640	70.20	321.76
12	1.677	72.03	338.85
13	1.757	113.19	836.59
14	2.460	161.43	1701.67

Table D.8. Shock arrival times for TSUNAMI simulation for LJUST with air shocks.

Mach #	t_A [μ s]	t_B [μ s]	t_C [μ s]	t_D [μ s]	t_E [μ s]	t_F [μ s]
1.10	0	197.1	314.3	467.5	587.5	806.1
1.25	0	174.0	278.2	399.0	512.3	727.1
1.50	0	144.7	232.3	338.3	442.5	647.0
1.75	0	124.2	199.7	290.9	385.3	572.4
2.00	0	109.0	175.5	255.0	343.0	517.0
2.50	0	87.0	139.5	201.0	276.0	431.0
3.00	0	73.0	117.0	169.0	232.0	367.0
3.50	0	62.5	99.0	144.0	195.0	317.0
4.00	0	54.5	86.4	125.0	174.0	279.0

Table D.9. Shock peak pressures for TSUNAMI simulation of LJUST with air shocks.

Mach #	p_A [Pa]	p_B [Pa]	p_C [Pa]	p_D [Pa]	p_E [Pa]	p_F [Pa]
1.10	1.50×10^5	1.74×10^5	1.35×10^5	1.48×10^5	1.47×10^5	1.75×10^5
1.25	2.00×10^5	2.76×10^5	2.25×10^5	1.81×10^5	1.83×10^5	2.60×10^5
1.50	2.96×10^5	5.32×10^5	3.95×10^5	2.53×10^5	2.34×10^5	4.13×10^5
1.75	4.11×10^5	9.11×10^5	6.16×10^5	2.58×10^5	2.12×10^5	5.24×10^5
2.00	5.43×10^5	1.46×10^6	4.20×10^5	3.51×10^5	2.59×10^5	6.20×10^5
2.50	8.61×10^5	3.01×10^6	6.82×10^5	4.48×10^5	3.45×10^5	1.58×10^6
3.00	1.24×10^6	5.20×10^6	9.92×10^5	5.17×10^5	4.69×10^5	2.59×10^6
3.50	1.70×10^6	8.05×10^6	1.35×10^6	6.96×10^5	6.20×10^5	4.86×10^6
4.00	2.23×10^6	1.13×10^7	1.76×10^6	9.03×10^5	7.99×10^5	7.89×10^6

Table D.10. Shock velocities for TSUNAMI simulation of LJUST with air shocks.

Mach #	u_{AB} [m/s]	u_{BC} [m/s]	u_{CD} [m/s]	u_{DE} [m/s]	u_{EF} [m/s]
1.10	378.47	365.69	290.22	330.56	370.37
1.25	428.81	411.15	368.12	350.29	376.83
1.50	515.46	489.58	419.34	380.88	395.90
1.75	600.74	567.72	487.39	420.42	432.72
2.00	684.52	644.55	559.12	450.99	465.30
2.50	857.61	816.43	722.76	529.17	522.34
3.00	1022.09	974.15	854.81	629.96	599.72
3.50	1193.80	1174.32	987.78	778.19	663.63
4.00	1369.04	1343.65	1151.55	809.95	771.07

Table D.11. Mach numbers for TSUNAMI computed shocks in air impacting a cylinder array.

Mach #	M_{AB}	M_{BC}	M_{CD}	M_{DE}	M_{EF}	r
1.10	1.10	1.06	0.84	0.96	1.08	0.0214
1.25	1.25	1.19	1.07	1.02	1.10	0.1212
1.50	1.50	1.42	1.22	1.11	1.15	0.2319
1.75	1.75	1.65	1.42	1.22	1.26	0.2797
2.00	1.99	1.87	1.62	1.31	1.35	0.3202
2.50	2.49	2.37	2.10	1.54	1.52	0.3909
3.00	2.97	2.83	2.48	1.83	1.74	0.4132
3.50	3.47	3.41	2.87	2.26	1.93	0.4441
4.00	3.98	3.90	3.35	2.35	2.24	0.4368

Table D.12. Ratio of p_B/p_R for TSUNAMI simulation of LJUST with air shocks.

Mach #	$p_R(M_{AB})/p_A$	p_B/p_A	p_B/p_R
1.10	1.24	1.16	0.94
1.25	1.60	1.38	0.86
1.50	2.21	1.80	0.81
1.75	2.79	2.22	0.80
2.00	3.33	2.69	0.81
2.50	4.27	3.50	0.82
3.00	5.00	4.19	0.84
3.50	5.57	4.73	0.85
4.00	6.00	5.08	0.85

Table D.13. Shock arrival times for TSUNAMI simulation of LJUST with He shocks.

Mach #	t_A [μ s]	t_B [μ s]	t_C [μ s]	t_D [μ s]	t_E [μ s]	t_F [μ s]
1.10	0.00	67.13	107.03	159.82	199.78	274.31
1.25	0.00	59.68	95.10	136.50	174.60	246.20
1.50	0.00	49.27	79.04	115.47	150.10	212.90
1.75	0.00	42.39	67.83	99.64	129.77	188.95
2.00	0.00	37.00	59.00	88.00	113.30	170.00
2.50	0.00	29.77	47.37	69.15	91.30	138.93
3.00	0.00	24.84	40.02	57.12	76.23	116.80

Table D.14. Shock peak pressures for TSUNAMI simulation of LJUST with He shocks.

Mach #	p_A [Pa]	p_B [Pa]	p_C [Pa]	p_D [Pa]	p_E [Pa]	p_F [Pa]
1.10	1.52×10^5	1.78×10^5	1.36×10^5	1.44×10^5	1.47×10^5	1.79×10^5
1.25	2.05×10^5	2.86×10^5	1.68×10^5	1.50×10^5	1.49×10^5	2.80×10^5
1.50	3.09×10^5	5.48×10^5	2.31×10^5	1.88×10^5	1.83×10^5	4.64×10^5
1.75	4.31×10^5	9.15×10^5	3.23×10^5	2.74×10^5	2.41×10^5	6.24×10^5
2.00	5.51×10^5	1.38×10^6	4.69×10^5	3.79×10^5	3.10×10^5	1.03×10^6
2.50	9.12×10^5	2.71×10^6	7.06×10^5	6.12×10^5	4.17×10^5	2.17×10^6
3.00	1.33×10^6	4.50×10^6	1.05×10^6	8.24×10^5	5.66×10^5	3.79×10^6

Table D.15. Shock velocities for TSUNAMI simulation of LJUST with He shocks.

Mach #	u_{AB} [m/s]	u_{BC} [m/s]	u_{CD} [m/s]	u_{DE} [m/s]	u_{EF} [m/s]
1.10	1111.46	1074.25	842.02	993.18	1086.31
1.25	1250.21	1210.12	1073.67	1041.67	1130.76
1.50	1514.36	1439.79	1220.15	1146.04	1289.21
1.75	1760.14	1685.18	1397.14	1317.21	1368.07
2.00	2016.55	1948.30	1532.76	1568.68	1427.91
2.50	2506.30	2435.37	2040.86	1791.76	1699.82
3.00	3003.72	2823.62	2599.42	2076.79	1995.62

Table D.16. Mach numbers for TSUNAMI computed shocks in air impacting a cylinder array.

Mach #	M_{AB}	M_{BC}	M_{CD}	M_{DE}	M_{EF}	r
1.10	1.099	1.063	0.833	0.982	1.074	0.02
1.25	1.237	1.197	1.062	1.030	1.118	0.10
1.50	1.498	1.424	1.207	1.134	1.275	0.15
1.75	1.741	1.667	1.382	1.303	1.353	0.22
2.00	1.995	1.927	1.516	1.552	1.412	0.29
2.50	2.479	2.409	2.019	1.772	1.681	0.32
3.00	2.971	2.793	2.571	2.054	1.974	0.34

Table D.17. Ratio of p_B/p_R for TSUNAMI simulation of LJUST with He shocks.

Mach #	$p_R(M_{AB})/p_A$	p_B/p_A	p_B/p_R
1.10	1.25	1.17	0.93
1.25	1.62	1.39	0.86
1.50	2.19	1.77	0.81
1.75	2.70	2.12	0.79
2.00	3.14	2.50	0.80
2.50	3.84	2.97	0.77
3.00	4.33	3.39	0.78