Jet Initiation of Deflagration and Detonation

Thesis by

J. Christopher Krok

In Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy



California Institute of Technology Pasadena, California 14 May 1997 To the memory of my father, James Charles Krok, who looked forward to my doctorate even more than I did.

Acknowledgements

I would like to thank the United States Nuclear Regulatory Comission for funding this research, first at Rennselaer Polytechnic Institute, and continuing at the California Institute of Technology. The research presented in this thesis was funded at Caltech by contract number NRC-04-94-044. I would also like to thank the National Science Foundation for awarding me a graduate fellowship covering the first three years of my graduate work, allowing me to concentrate on research.

I would also like to thank the following individuals:

Joe Shepherd, my advisor, for finding diverse and interesting topics, assisting my literature search, and leaving me some spare time to build car parts instead of experiments;

Hans Hornung, G. Ravichandran, Dan Meiron and Joe Kirschvink, for agreeing to serve on my committee and remaining patient through several date, time and venue changes;

My family and friends, for support over the past n years;

Raza Akbar, for providing information and insights related to my research, as well as a few good laughs (Does this mean that Ann-Margaret won't be coming?);

Sensei Tetsuyasu Uekema and my fellow kenshi in Shorinji Kempo, for an awesome budo experience;

Michael Kaneshige, for solving many a Unix problem;

Jamie Guthrie, for administrative and feeding assistance;

Georgia Frueh, for thoughtful insights unrelated to my research;

Karen Cheetham, Katie Gross, Carol Irwin and Jeri Chittum, for their help on administrative matters;

Joe Haggerty, Phil Wood, Larry Fraizer, and Ali Kiani, of the Aero Machine Shop, for free machine shop instruction (free save for the semiannual case of beer);

Pavel Svitek, for mechanical assistance;

Jerry Landry, for the same plus letting me use the wood shop to furnish my apartment; Ron Kibbe and Bob King, of Engineering and Estimating, for their assistance in the design and construction of the laboratory:

Mike Gerfen, of Central Engineering, for work on parts of the facility;

Dave Evans, James Spotila, Liz and John Holt, Donovan Stevens and my other friends in the GPS division for making my Geology minor an enjoyable experience;

Last, but not least, I would like to thank Mr. Van Norman, for innumerable hours of tireless service during the construction of the HYJET facility.

Abstract

We have constructed a facility for the study of jet-initiated deflagration and detonation in hydrogen-air-steam mixtures. The facility is built around two pressure vessels. Mixtures of hydrogen, oxygen and nitrogen are spark-ignited in the driver vessel, generating a hot mixture of combustion products. The pressure rise ruptures a diaphragm, venting the products into the receiver vessel through nozzles of 12.7–92 mm diameter. The receiver is filled with hydrogen-air and hydrogen-oxygen mixtures diluted with either nitrogen or steam.

The deflagration tests studied the lean and maximum-dilution limits of hydrogen-air mixtures ignited by a hydrogen-steam jet. The lean limit of 6% hydrogen was comparable to other studies. The maximum dilution limit for steam was 60%. This is higher than the limit found in spark/glow plug ignition experiments. Shock oscillations in the receiver increased with nozzle size.

Further tests studied the initiation of detonation in both hydrogen-air and stoichiometric hydrogen-oxygen-diluent mixtures. In terms of jet diameter, D, and receiver detonation cell size, λ , we found initiation limits of $2 < D/\lambda < 7$, where other experiments required a D/λ of 11 or more. We propose that the D/λ model does not adequately characterize jet initiation, as it does not reflect the conditions in the driver.

The tests indicated that shock focusing plays an important role, promoting strong secondary explosions with or without prompt initiation of detonation. Mixtures with steam dilution were prone to DDT near the detonation limit, as the slower flame speed allows shock reflection and pressurization to occur before the reactants are consumed. Tests with nitrogen dilution had no DDT regime. Because of DDT and shock focusing, peak pressures were highest in mixtures that were slightly less sensitive than the detonation threshold. Schlieren movies confirmed the formation of a detonation near the nozzle exit.

Contents

A	cknov	wledgements	iii
A	ostra	act	\mathbf{v}
Li	st of	Figures	ix
\mathbf{Li}	st of	Tables	xiii
1	Intr 1.1 1.2 1.3 1.4	roduction The Hydrogen Problem in Severe Accidents	$\frac{1}{3}$
2		JET Experimental Facility	9
	2.1	Pressure Vessels	9
	$2.2 \\ 2.3$	Hydraulic Closure	10 11
	$\frac{2.3}{2.4}$	Gas Handling System	11 12
	$2.4 \\ 2.5$	Firing System	12 12
	2.6	Schlieren System	
	2.0 2.7	Heating System	13
	2.8	Data Acquisition System	13
3	CO	MP and S Series	23
	3.1	Introduction and Background	23
	3.2	Results and Discussion	23
4	\mathbf{SA}	Series	35
	4.1	Introduction and Background	35
	4.2	Results and Discussion	35
5	NП	TRO Series	41
	5.1	Introduction and Background	41
	5.2	Results and Discussion	42

6	BE'	TA Series	61
	6.1	Introduction and Background	61
	6.2	Results and Discussion	65
		6.2.1 Driver Conditions	65
		6.2.2 Critical Dilutions	68
		6.2.3 Sample Pressure Traces	74
		6.2.4 Lead Wave Pressures	88
		6.2.5 Lead Wave Velocities	105
	6.3	Photographic Tests	109
		6.3.1 Tests With Diaphragm Installed	110
		6.3.2 Tests With No Diaphragm	120
		6.3.3 Secondary Phenomena	128
7	Sun	nmary	133
	7.1	COMP and S Series	133
	7.2	SA Series	134
	7.3	NITRO Series	135
	7.4	BETA Series	136
	7.5	Conclusion	138
Bi	bliog	graphy	141
\mathbf{A}	Safe	ety Assessment	145
В	\mathbf{Sys}^{-}	tem Drawings	165
\mathbf{C}	BE	TA Pressure Traces	181
	C.1	Nitrogen Dilution, 298 K	182
	C.2	Nitrogen Dilution, 373 K	194
	С.3	Water Vapor Dilution, 373 K	198
	С.4	Nitrogen Dilution, 298 K, No Diaphragm	204
D	Rur	n Summary	209
\mathbf{E}	RP	I Jet Visualization	221

List of Figures

1.1	Layout of a typical PWR
1.2	Jet diffusion flame resulting from DCH
1.3	Initiation of deflagration in containment atmosphere
1.4	Initiation of detonation in containment atmosphere
1.5	Schematic of detonation cell with shear layers
1.6	Photograph of detonation cells imprinted on soot foil
2.1	Schematic of HYJET facility
2.2	Driver and receiver in mated position
2.3	Driver and receiver, separated
2.4	Threaded nozzle adapter with nozzles, and 3.625" (92-mm) nozzle 17
2.5	Hydraulic closure cross section
2.6	Schematic of gas handling system
2.7	HYJET control system
2.8	Cross section of schlieren system
2.9	Top view of schlieren system
2.10	Window retainer and light/dust boot
2.11	Photo of schlieren exit, with video and framing cameras
3.1	Comparison of RPI and CIT facilities
3.1 3.2	•
3.3	1) -
3.4	I) ·
3.5	COMP pressure traces, 25-mm nozzle
3.6	HYJET pressure traces, 12.7-mm nozzle
3.7	HYJET pressure traces, 25-mm nozzle
3.8	S pressure traces, 12.7-mm nozzle
3.9	Comparison of steam and nitrogen as diluents
4.1	Peak receiver pressure summary, SA series
4.2	SA receiver pressure traces, 12.7-mm nozzle
4.3	SA receiver pressure traces, 25-mm nozzle
4.4	SA receiver pressure traces, 92-mm nozzle
4.5	SA60 receiver pressure traces, showing effect of nozzle size
т.0	SAUD receiver pressure traces, showing effect of nozzle size

5.1	Examples of prompt initiation and secondary explosion in receiver		•	44
5.2	Internal geometry of driver vessel			45
5.3	Constant volume NITRO driver tests			46
5.4	PCB traces from 0N and 25N drivers			47
5.5	Wave diagram for driver detonation interaction			48
5.6	Hugoniot plots for reflected wave in driver and shock in receiver	•	•	49
5.7	Peak pressures and delay time, showing possible focusing	•	•	50
5.8	Initial and highest peak receiver pressures for undiluted driver			51
5.9	Initial and highest receiver pressures for 10% N ₂ driver	•	•	52
5.10	Initial and highest receiver pressures for 20% N ₂ driver			53
	Initial and highest receiver pressures for 25% N ₂ driver			53
	Initial and highest receiver pressures for 30% N ₂ driver			54
	Pressure traces from sting-mounted transducer			55
5.14	Pressure trace with sting at 250-mm station	•	•	56
	Pressure trace at 250-mm station, slow driver pressurization			56
	Geometry of initial shock for ray tracing simulation			57
5.17	Shock focusing found with ray tracing simulation			58
5.18	Expected corner reflections.			59
5.19	Second ray tracing simulation, with corner reflections			60
C 1				<u>co</u>
6.1	Sample driver pressure trace, 25-mm nozzle			63
6.2	Locations of PCB transducers in beta dilution test series			64
6.3	PCB traces from BETA driver			65 67
6.4	Shock Hugoniots for BETA receiver mixtures			67 67
6.5	ZND calculation for H_2 - O_2 - N_2 mixtures			69
6.6	ZND calculation for H_2 -air- H_2O mixtures			70
6.7	Logarithmic correlation of λ and Δ			71
6.8	Plot of initiation results as D/λ			73
6.9	Summary of critical β values.			73
6.10	Comparison of recessed and flush-mount transducers.			77
	Prompt initiation with 92-mm nozzle, N_2 at 298 K			78
	Failure to initiate with 92-mm nozzle, N_2 at 298 K			79
	Secondary explosion with 92-mm nozzle, N_2 at 298 K			80
	Prompt initiation with 25-mm nozzle, N_2 at 298 K			81
	Initiation failure with 25-mm nozzle, N_2 at 298 K			82
	Prompt initiation with 92-mm nozzle, H_2O at 373 K			83
	DDT with 92-mm nozzle, H_2O at 373 K			84
	Running buildup to DDT with 92-mm nozzle, H_2O at 373 K			85
	Initiation failure with 92-mm nozzle, H_2 at 373 K			86
	DDT near T3 with 25-mm nozzle, N_2 at 298 K			87
	T3 trace of DDT with pre-pressurization. \dots \dots \dots			87
	Lead wave pressures, 92-mm nozzle, N_2 at 298 K			90
	Lead wave pressures, 92-mm nozzle, continued			91
6.24	Model of spherical detonation growth	·	·	92

6.25	Regular vs. Mach reflection
6.26	Variation of wall pressure with incidence angle
6.27	Lead wave pressures, 64 and 38-mm nozzles, N_2 at 298 K
6.28	Lead wave pressures, 64 and 38-mm nozzles, continued
6.29	Lead wave pressures, 25-mm nozzle, N_2 at 298 K
6.30	Lead wave pressures, 25-mm nozzle, continued
6.31	Lead wave pressures, 25 and 92-mm nozzles (ND), N_2 at 298 K 98
6.32	Lead wave pressures, 25 and 92-mm nozzles (ND), continued
6.33	Lead wave pressures, 92-mm nozzle, N_2 at 373 K 100
6.34	Lead wave pressures, 92-mm nozzle, continued 101
6.35	Lead wave pressures, 38 and 92-mm nozzles, H_2O at 373 K 103
6.36	Lead wave pressures, 38 and 92-mm nozzles, continued
6.37	V_{2-3} for lead wave, N ₂ -dilution at 298 K
6.38	V_{2-3} for lead wave, N ₂ -dilution at 373 K
6.39	V_{2-3} for lead wave, H ₂ O-dilution at 373 K
6.40	Schematic of detonation shape
6.41	Detonation wave bow leads
6.42	Photos, jet startup sequence
6.43	Photos, jet initiation of deflagration, station 1
	Photos, jet initiation of deflagration, station 2
	Photos, jet initiation of deflagration, station 3
	Photos, jet initiation of detonation, station 1
6.47	Photos, jet initiation of detonation, station 2
6.48	Photos, jet initiation of detonation, station 3
6.49	Photos, jet initiation of deflagration, no diaphragm, station 1
6.50	Photos, jet initiation of deflagration, no diaphragm, station 2
6.51	Photos, jet initiation of deflagration, no diaphragm, station 3
6.52	Photos, jet initiation of detonation, no diaphragm, station 1
6.53	Driver pressure trace, $\beta = 1.7$, no diaphragm
6.54	Photos, jet initiation of detonation, no diaphragm, station 2
6.55	Photos, jet initiation of detonation, no diaphragm, station 3
6.56	Comparison of air vs. nitrogen dilution in driver
6.57	Photos, jet startup with vortex interaction
6.58	Photo sequence, failure to initiate detonation
6.59	Interaction of flame front and vortex ring
H 1	
7.1	Summary of COMP test series
7.2	Comparison of water vapor and nitrogen as diluents
7.3	Summary of SA test series
7.4	Results of constant-volume driver tests. $\dots \dots \dots$
7.5	Summary of critical β values
A.1	Basic layout of experiment, showing both vessels
A.2	Typical driver pressure trace from experiments at RPI

Floor plan, Explosion Dynamics Laboratory	151
Gas Supply system for the Hydrogen Jet Combustion Facility	154
Highest receiver pressure trace recorded at RPI	158
RPI Photos, jet startup in N_2	222
RPI Photos, jet startup in air	223
RPI photos, jet initiation of deflagration.	224
	Gas Supply system for the Hydrogen Jet Combustion Facility.Highest receiver pressure trace recorded at RPI.RPI Photos, jet startup in N2.RPI Photos, jet startup in air.

List of Tables

$3.1 \\ 3.2$	COMP series receiver mixtures	
4.1	SA series receiver mixtures	35
$5.1 \\ 5.2$	NITRO Series driver mixtures	
	Comparison of jet-initiation facilities.	
6.2 6.3	Representative BETA series mixtures Properties of transmitted shocks in receiver	66
$\begin{array}{c} 6.4 \\ 6.5 \end{array}$	Comparison of detonation initiation results	
7.1	Results of NITRO tests	
1.4		100

Chapter 1 Introduction

1.1 The Hydrogen Problem in Severe Accidents

In the event of a severe loss-of-coolant accident (LOCA) in a nuclear power plant, hydrogen gas can be generated by oxidation of the zircalloy cladding on the fuel rods. Figure 1.1 shows the layout of a typical pressurized water reactor (PWR). The LOCA may be the result of a broken pipe, jammed valve, or other related event. As water drains from the reactor cooling system (RCS), steam will fill the open regions. With sufficient loss of coolant, the core may be partially uncovered and the surface temperature can rise enough to start an oxidation reaction between the steam and the zircallov cladding. The steel vessel lining and core support structure may also oxidize, but the zirconium reaction is considered to be the main source of hydrogen. The amount of hydrogen generated depends on the specific accident, and how much of the cladding is involved. If all of the available zirconium reacts, a pressurized water reactor (PWR) could produce 1000 kg of H_2 , and a boiling water reactor (BWR) could produce 2000 kg (Camp et al. 1983). As the hydrogen is generated, a hydrogen/steam mixture fills the open portions of the RCS. Hydrogen dissolved in the liquid water is not a problem; under normal operation, a certain amount of dissolved hydrogen is maintained in the RCS to scavenge oxygen and reduce corrosion in the system.

If the RCS continues to leak, the H_2 - H_2O mixture can enter the containment dome, creating a potentially flammable mixture. If the mixture is ignited, the mode of combustion (deflagration or detonation) will depend on several factors. These include hydrogen concentration, temperature, dilution, ignition source strength, and size of the confined area.

1.2 Combustion Modes

The mixture will not sustain a deflagration unless the hydrogen concentration is above a certain limit, typically taken as 4% (Coward and Jones 1952). Near this lean limit, these flames burn incompletely and only propagate upward. The temperature of the products creates a buoyant flow, which the flame speed can not overcome. For a hydrogen



Figure 1.1: Layout of a typical PWR containment (Camp et al. 1983).

concentration of 8–10%, the flame will burn completely and propagate in all directions (including downward). These flames are expected to place minimal thermal and pressure loads on the containment and equipment. Such a burn took place during the Three Mile Island Unit-2 event in 1979. At 9 hours and 50 minutes into the incident, a 28 psig (1.9 bar) pressure spike was recorded in the containment. For hydrogen concentrations above 10–11%, there can be fast flames and deflagration to detonation transition (DDT). Fast flames can do nearly as much damage as a DDT, due to pre-pressurization by the lead shock, and subsequent shock reflection and focusing.

For a detonation to occur, additional criteria must be satisfied. For a detonation to be "directly initiated," a strong (i.e., explosive) ignition source is required. A strong, impulsive jet of hot gas can also directly initiate a detonation. A detonation can also be the result of flame acceleration. If a flame propagates over obstacles and/or in a confined space, turbulence and shock reflection will accelerate the flame, possibly resulting in a DDT. In addition, detonations will not propagate in a mixture unless it occupies a large enough volume. The less sensitive a mixture is, the larger the volume must be. This means that research can not be scaled-down to a convenient size. The initiation energy must also be increased for less-sensitive mixtures.

There are methods for mitigating a hydrogen release. Hydrogen recombiners are located in the containment, to re-oxidize hydrogen generated by radiolysis of water in the RCS. While these are not designed to handle a large release, efforts are being made to develop large-scale units for this purpose. Water can also be sprayed into the containment; in addition to cooling the reactor components, the evaporated water will increase the steam fraction in the atmosphere and help inert the mixture. If the mixture is flammable, it can be deliberately ignited by glow plugs placed throughout the containment. In the event of an accident, the glow plugs are left on continuously, so the hydrogen will be ignited as soon as it reaches flammable levels. Small containments are inerted with nitrogen, although this can complicate repair efforts in an emergency. All containments in the United States are either inerted or use deliberate ignition as a mitigation method.

1.3 Jet Initiation

In a flammable mixture, the strength of the ignition source can determine the mode of combustion. In most cases, the source will be fairly weak, such as an electrical spark, or deliberate ignition by glow plugs. In the worst case, the reactor core can melt through its vessel, venting a hot jet of hydrogen, steam and molten core particles into the containment atmosphere through pipe and instrument penetrations. This is known as direct containment heating, or DCH. This will heat and pressurize the containment, and can serve as an ignition source. Three possible combustion regimes are shown in Figures 1.2 through 1.4, in order of increasing strength.

If the hydrogen concentration in the containment is too low to support a deflagration, the jet can burn as a diffusion flame. This is shown in Figure 1.2. The jet must be ignited near the release point, before the jet gas is diluted and cooled by entrainment of the containment atmosphere. The hydrogen release must also be sufficiently rapid. If ignition occurs, the resulting plume of combustion products will heat and pressurize the containment. The diffusion flame can also be stabilized and enhanced by entrainment of hydrogen in the containment atmosphere.

If the hydrogen concentration in the containment is above the lean limit, a deflagration can be initiated (Figure 1.3). The lean limit will also be affected by the amount of steam in the containment. If the H_2 concentration is sufficiently high, and the H_2O concentration sufficiently low, flame acceleration and DDT may occur. Diffusion flames and lean-limit ignition were studied previously in a facility at Rensselaer Polytechnic Institute (RPI) (Krok 1992; Ross 1994).

The third and highest-order mode of combustion is a detonation, as in Figure 1.4. In this case, turbulence and heat supplied by the jet cause a local explosion in the contain-



Figure 1.2: Jet diffusion flame resulting from DCH.

ment mixture, which propagates as a detonation wave. The strength of the detonation can be amplified by reflection off of objects and containment surfaces, and through focusing mechanisms.

An in-depth discussion of detonation physics is beyond the scope of this work, but can be found elsewhere (Fickett and Davis 1979; Nettleton 1987). A basic treatment will be provided to lay groundwork for later discussions of results. Briefly, a detonation is a supersonic combustion wave, comprised of a shock and an exothermic chemical reaction. The shock increases the temperature and pressure of the reactants, and after a suitable induction time, the reaction occurs. Energy released by the reaction drives the shock. Thus, the shock and reaction are coupled. While the thickness of a shock is typically a few mean free paths, the finite rate of chemical reaction increases the thickness of a detonation. A detonation can be as much as a centimeter thick, depending on the sensitivity of the mixture. The detonation process is similar in both gaseous fuel-oxidizer mixtures and solid explosives. Chapman and Jouguet independently determined that



Figure 1.3: Initiation of deflagration in containment atmosphere.

flow out of a steady-state detonation is sonic relative to the shock. This sonic condition is required to match the steady-state detonation with the unsteady Taylor expansion behind it. Also, the sonic condition corresponds to the point of minimum entropy in the reaction products (Thompson 1972). Other properties related to a steady detonation are the Chapman-Jouguet velocity, V_{CJ} , and the CJ pressure, P_{CJ} . As the CJ conditions are independent of the internal structure, P_{CJ} , V_{CJ} and other state variables can be evaluated with chemical equilibrium codes, such as STANJAN (Reynolds 1986). The structure of the detonation wave was first modeled by Zel'dovich, von Neumann and Doring, each independently, in the early 1940's. Their model is collectively referred to as the ZND model, and consists of a planar shock followed by a reaction zone.

The one-dimensional, steady detonation model was widely accepted, as the CJ theory predicted velocities fairly accurately. Analytic studies in the 1950's found that the wave structure was not stable, however. The first experimental proof of three-dimensional structure was given by White (1961). Later studies found that the detonation wave



Figure 1.4: Initiation of detonation in containment atmosphere.

contained transverse compression waves. Figure 1.5 shows the transverse wave structure. As the detonation propagates, the transverse waves run back and forth across the incident wave, generating Mach stems when they collide. The junction of the incident wave, transverse wave, and Mach stem is called the triple point. The paths of the triple points can be recorded by running a detonation over a soot-covered metal sheet, called a "soot foil" or "smoked foil." The triple points will remove soot from the sheet, tracing their paths (Figure 1.6). The tracks form irregular parallelograms, called cells. Detonations are thus said to have a cellular structure. The cells are characterized by their width, denoted by λ .

Cell size indicates the sensitivity of a mixture to detonation. As the cells get smaller, the mixture becomes more sensitive. Cell size depends on several parameters of the reactants, including temperature, pressure, stoichiometry, and dilution (both diluent and concentration). Cell size is commonly used to correlate properties of detonations, and to compare different fuel-oxidizer systems. For example, critical initiation energy scales



Figure 1.5: Schematic of detonation cell components, showing wave structures. Cell width is the distance between triple point tracks, measured parallel to wave front. Compare to pseudo-schlieren image of cell generated by numerical simulation (Quirk 1996).



Figure 1.6: Detonation cells imprinted on soot foil.

with λ^3 $(E_C \propto \lambda^3)$. Another important property is the critical diameter, d_C , which is used in detonation diffraction studies. For a detonation to exit a tube (or orifice) and successfully re-establish itself in an open area, the tube diameter must be greater than d_C . Studies have found that $d_C \approx 13\lambda$. This correlation has been carried over to jet initiation experiments, where early studies have found that a jet diameter, D, of 13λ was required for direct initiation of detonation. The use of D/λ will be examined further in Chapters 5 and 6. Much work has been done to measure cell size, but the results are not fully reliable. Within a single detonation, cells recorded on soot foils can have a range of sizes, and their measurement is subjective. Measurements by different members of the same research group can have ranges of $\pm 100\%$ (Tieszen et al. 1986). The particular diluent also affects the regularity of the cellular structure. Mixtures with N₂ dilution have very irregular cells, while Ar dilution results in a more regular pattern.

Attempts have also been made to correlate measured cell size against reaction zone lengths computed with the ZND model. It was first suggested by Shchelkin and Troshin (1965) that λ is proportional to reaction zone length, $\Delta: \lambda \propto \Delta$, or $\lambda = A\Delta$. The value of A is determined by comparison to experimental data, and varies from system to system. Detailed reaction mechanisms are now available for hydrogen-air mixtures with various diluents (e.g., Shepherd (1986)), making computation of Δ quite easy. Several criteria are used to locate the end of the reaction zone; I will use the point of maximum energy release. (Other criteria are M=0.9, M=0.75 or maximum $\partial T/\partial x$.)

1.4 Research Overview

Much work has been done in these areas, but some gaps still exist, primarily in detonation of H_2 -air- H_2O mixtures. Recent examples of small-scale jet initiation research include Carnasciali et al. (1991) and Bezmelnitsin et al. (1997). Large scale tests have been performed by Dorofeev et al. (1995) and Dorofeev et al. (1993). While these tests were mostly unconfined, they did indicate the significance of confinement in initiation of a local explosion. Our goal is to expand the database of these tests by studying a moderate size scale with confinement effects. To that end, we have constructed the Hydrogen Jet Facility, or HYJET. This facility consists of two connected vessels, separated by a diaphragm, and is described in the next chapter.

The first HYJET test series (COMP) revisited the RPI experiments on the effect of igniter strength on the lean flammability limit of diluted hydrogen-air mixtures. These were then expanded (S series) to study the difference in suppression abilities of nitrogen and steam. These tests are described in Chapter 3. Chapter 4 describes the SA test series, which examines jet ignition of constant-stoichiometry H_2 -air mixtures with steam dilution. Examination of jet-initiated detonations begins with the NITRO series in Chapter 5, which studies the effect of driver composition on detonation of H_2 -air mixtures. Chapter 6 covers the BETA series, which fixes the driver composition and determines dilution limits for detonation initiation in stoichiometric H_2 -O₂ mixtures.

Chapter 2 HYJET Experimental Facility

The HYJET facility is located in the GALCIT Explosion Dynamics Laboratory, in the basement of the Guggenheim building. It is built around two pressure vessels, representing the reactor vessel and containment in a nuclear power plant. This is the second-generation redesign of a facility built at Rensselaer Polytechnic Institute in Troy, NY (Krok 1992). A schematic of the HYJET facility is shown in Figure 2.1. As this facility was built in the United States, the majority of its components and support equipment have nominal dimensions given in English units. In the interest of correctness and accuracy, the facility will be described in English units, with conversions where appropriate. In subsequent chapters, information will be given in metric units only.

A copy of the GALCIT Safety Assessment (GSA) for HYJET is provided in Appendix A. The GSA contains an in-depth discussion of the HYJET design considerations, as well as hazards typical of such facilities, and the steps taken to mitigate them. That material will be touched on briefly here.

2.1 Pressure Vessels

The driver vessel, representing the reactor, was constructed at Caltech by the Aeronautics and Central Engineering machine shops. It is shown in Figures 2.2 and 2.3. It is made from 6" OD by 0.5" wall $(152 \times 12.7 \text{ mm})$ seamless 316SS tubing, with stainless steel flanges welded to both ends. Attached to one end is one half of the hydraulic closure mechanism and an extension which brings the overall length of the driver to 92" (2.3 m). The closure and extension create an annular channel near the middle of the driver, which may enhance flame acceleration through generation of turbulence (see Figure 5.2, p. 45). The opposite end of the driver is capped by a blind flange containing instrumentation ports. The volume of the driver is 1 ft³ (0.028 m³). The full assembly was hydrotested in situ to a pressure of 1500 psi (103 bar). Interchangeable nozzles mate to the end of the driver extension. The nozzle retains the diaphragm and incorporates O-rings to seal to the receiver socket. Three nozzles are available with diameters of 1.5", 2.5" and 3.625" (38, 64, and 92 mm, respectively). A fourth unit has a threaded hole that accepts nozzle inserts of 0.25", 0.5" and 1" diameter (6.4, 12.7 and 25 mm), and is equipped with a cruciform diaphragm cutter. Figure 2.4 shows the 3.625" nozzle and threaded nozzle adapter. A threaded plug is also available for the adapter, so either vessel can be used as a constant volume chamber. The diaphragms used in these experiments are 0.005" (0.13-mm) Mylar. Mylar was chosen over aluminum because it was much easier to handle and less expensive. Because of clogging problems, a piece of cellophane tape is used as a diaphragm with the 0.25" nozzle. This works remarkably well, as long as the pressure differential favors the tape during filling.

The receiver is an ASME section VIII pressure vessel built by R. L. Morton Welding, Inc. It is rated for 750 psi at 250 °F (52 bar at 395 K), and carries the ASME U stamp. The vessel is 36" (0.91 m) in outside diameter, and 64" (1.6 m) across the seams, with a total volume of 42 ft³ (1.19 m³). It has a number of through-holes for access and instrumentation. These include: One 10" flange on one end for connection to the driver; one 6" flange on the other end for instrumentation; two 12" flanges for interior access; seven 1" NPT ports along the top for gas and instrumentation connections; two 2" NPT ports for vacuum and mixing; two 1/2" NPT drains; and two Caltech-designed window retainers which hold three windows each. Attached to the 10" flange is the other half of the hydraulic closure, as well as a socket that extends inside the vessel (described below).

Both vessels are mounted on linear bearings and steel rails, allowing them to be moved back and forth. The driver must be moved in order to replace diaphragms. Movement of the receiver allows different window stations to be placed in the path of the schlieren system, illuminating different parts of the jet. The interior walls enclosing the vessels have 0.125" (3.2 mm) steel armor to help contain blown transducers or failed schlieren windows. The exterior walls are concrete foundation and need no additional protection.

2.2 Hydraulic Closure

A hydraulic closure mechanism is used to connect the vessels and seal the diaphragm. This is a modified version of a Caltech-designed closure, used on the GALCIT 6" shock tube. A cross section of the closure is shown in Figure 2.5. (Individual drawings are in Appendix B.) The extensions are designed to align the nozzle exit with the edge of the first schlieren window. The removable ring clamp is the key fastener in the system. It can be seen in Figure 2.3, suspended by counterweights above the juncture point. Figure 2.3 also shows the driver (inner) extension and the two halves of the closure. The diaphragm is placed between the inner extension and nozzle, and the nozzle is secured by two cap screws. The screws are used only to hold the nozzle and diaphragm in place until pressurization. The closure halves are brought together by rolling the driver into the receiver, seating the inner extension in the receiver socket (outer extension). The ring clamp is brought down and latched around the closure flanges. An air-powered hydraulic pump pressurizes the fluid space (Figure 2.5) to 2500 psi (170 bar). Pressure on the annular piston drives the inner extension against the bottom of the socket with a force of over 120 thousand pounds (530 kN). This force is used to crimp the diaphragm and seat the O-rings, which seal all face junctions. The driver, attached to the piston, rolls forward slightly during pressurization. The ring clamp takes the full closure force, keeping the halves from separating. When the system is depressurized, a set of springs (not shown) drive the piston rearward.

2.3 Gas Handling System

Figure 2.6 is a schematic of the gas handling system inside the laboratory. Bottled gases used in the facility are stored in an outdoor bottle farm, while compressed air is plantsupplied. The gases are stored outside as a seismic safety precaution. Supply pressure is controlled by two-stage regulators at the farm, so gas pressures do not exceed 15 psig (1 bar) inside the building. The feed lines are 0.5" x 0.049" seamless SS connected by Swagelok fittings. Special precautions are taken for hydrogen, as it is highly flammable at a wide range of concentrations. The hydrogen line is controlled by a spring-return electropneumatic ball valve, also at the bottle farm. To open this valve, a "dead-man's" switch on the gas handling panel (in the control room) must be held down. This prevents the operator from leaving the panel while hydrogen is flowing, and overfilling the vessel with flammable gas. The spring-return actuator will close the valve if either power or air pressure is lost, blocking the flow of hydrogen in an earthquake or other accident.

Gas handling panels are used to fill the vessels with the desired mixtures. The vessels are filled using the method of partial pressures, via the Heise gauge and metering valves on each panel. All valves at the vessels are Whitey ball valves with electropneumatic actuators. They are controlled from a mimic panel in the control room. Limit switches on the valves activate lights on the mimic panel, showing all valve positions. The switches also signal a logic circuit which only sends power to the firing circuits when all valves are closed.

Gases in the driver vessel are mixed by recirculation with a Senior Flexonics MB-302 bellows pump. In the receiver, gases are mixed by a 12" diameter propeller. The propeller is driven by a Parr Instruments A1180HC magnetically-coupled rotary feedthrough. This feedthrough uses magnets to transfer power from the outer housing to the inner shaft, so there is no need for dynamic shaft seals. It is designed to stir reactants in caloric bomb reactors, so it can withstand high pressures. The feedthrough is cooled by a water jacket at its base. The feedthrough is belt-driven by a universal motor with a variable-speed control.

When steam is used in a mixture, it is supplied by a steam generator (see "Heating System," below). Flow is metered by a preset needle valve. Flow into the receiver is controlled by an electropneumatic ball valve. The system also contains a purge valve, for draining condensate and heating the lines before filling the vessel. Both the purge and fill valves are operated from the control room.

Main vacuum is supplied by a Kinney KTC-112 compound vacuum pump located in the sub-basement Detonation Physics Laboratory. This pump has a free air displacement of 107 cfm, and can pump the facility down to 100 millitorr within 20 minutes under good conditions. This pump has a gas ballast system, enabling it to handle moderate amounts of volatiles, like water vapor. When large amounts of water vapor are present, either from heating or combustion, the Kinney MLR-30 is used for the initial pump-down. This pump displaces gas via an impeller-driven ring of water. It is limited to a minimum pressure of about 150 mbar, but can handle liquid water through the inlet.

2.4 Control Systems

The control and experimental rooms are separated by an armored wall of heavy construction. Once the vessels are joined and the closure pressurized, the experiment is run from the control room. Figure 2.7 shows the layout of the controls. The gas fill panels are on the left. To the right are the mimic panel, heater controls and firing system. The small panel above these is an auxiliary panel with controls for the steam valves, a manifold vacuum gauge, and hydraulic closure indicator. On the far right is the controller for the Cordin camera, and a remote switch for the MLR-30 vacuum pump. Below is the Macintosh IIfx computer, which has since been replaced by a Gateway for data acquisition.

2.5 Firing System

Each vessel has independent primary and secondary ignition systems. The primary system consists of an NGK four-electrode automotive spark plug in a Teflon insulator, mounted in the instrumentation flange. Spark energy is supplied by an EG&G TM-11A high voltage trigger module, which generates a 30 kV pulse. The driver firing button controls a trigger fanout box which distributes signals to the data acquisition boards, video timer, and BNC 7010 delay timer. The delay timer controls the Cordin camera and the driver TM-11A, giving the camera shutter time to open before firing the TM-11A (or, delaying the shutter for slower-burning mixtures). On the receiver, the TM-11A is controlled directly by the firing button. The logic circuit on the mimic panel blocks power to the trigger modules until all valves are closed and the closure is pressurized. In addition, the modules have been modified to include an arming switch, preventing firing by spurious signals.

The secondary system on each vessel consists of a Delco 9G glow plug mounted in the instrumentation flange. These are powered by a Kepco ATE 15-50 power supply, and are used to burn off flammable gas mixtures if the primary system fails.

2.6 Schlieren System

The schlieren system is mounted in two towers straddling the receiver vessel, as shown in Figures 2.8 and 2.9. The sending tower uses a 150 W xenon arc lamp in an Ealing housing, and a 1 mm aperture to provide a point source of light. This is collimated by a 100 mm dia. by 1 m f.l. mirror, and a turning mirror directs the light through the receiver windows. Three window stations are available, for imaging different regions downstream of the nozzle exit. The window ports are 4.6" (117 mm) in diameter, and are bored on 6.125" (156 mm) centers. The windows are made of BK7 glass, and are 150 mm in diameter by 25 mm thick. Windows are only used in one station at a time; the others are filled with steel blanks. One of the window retainers is shown in Figure 2.10, with a light/dust boot on the active window station.

The receiving tower directs the light towards another 100 mm x 1 m mirror, which focuses it on a knife edge. The wood skin on the towers responds to atmospheric changes, and tends to move the focal point off of the knife edge. To compensate for this, lateral motion of the knife edge is controlled by an electric motor and gear drive, which is powered from the control room. The operator can adjust the position of the knife edge until the schlieren image is satisfactory. After passing the knife edge, the light goes through an auxiliary lens, is redirected by a turning mirror, and goes through a second auxiliary lens. These lenses are needed to provide proper image size in the Cordin camera. The light then passes through a Pyrex beamsplitter plate, with approximately 5% of the light going to a Pullnix CCD video camera, and the other 95% going to a Cordin 350-M rotating-drum framing camera.

The CCD camera is used for recording slower burns, and some of the weaker jets. The video system is also used to check system alignment and knife edge position as described above. The Cordin 350-M is a rotating drum camera that uses 35mm film, exposing 224 frames at speeds up to 35,000 frames per second. It is used to film jet startup, rapid deflagrations, and detonations. Camera speed is controlled by a Drive Control Systems MicroSpeed 196 feedback controller. Drive power is supplied by a Kepco ATE 100-10M DC power supply.

2.7 Heating System

The receiver vessel can be heated to a maximum temperature of 383 K, allowing use of water vapor for mixture dilution. Initial heating is provided by a Chromalox CES-48A steam generator. This generator draws 46 kW of electrical power, and can supply up to 139 pounds (63 kg) of steam per hour. Live steam enters the receiver through the steam heating valve (Figure 2.6), heating the vessel walls by condensation. When the receiver reaches the desired temperature, the steam heating valve is closed, and the condensate is pressure-drained through the drain valve. Temperature maintenance is provided by electrical heating pads and tapes affixed to the surface of the vessel. The electrical heaters supply 7.6 kW of heating, split into two zones. Each zone is controlled by an Omega Engineering CN6071A feedback controller, using an SCR73-Z power controller to control 208V, three-phase power. The vessel is insulated by a 2" thick fiberglass blanket, with a Teflon-coated outer surface.

2.8 Data Acquisition System

The data acquisition system used for the first 205 runs was based on a Macintosh IIfx computer. The data acquisition boards and software were manufactured by National Instruments. The boards used were the MIO-16XL-18, the A2000, and the DMA-2800.

The MIO-16 contains 16 single-ended analog input channels, and has an 18 μ s conversion time. The A-2000 has four channels that are sampled simultaneously, with a 1 μ s conversion time. The DMA-2800 allows data to be written directly to memory as it is acquired, and also contains a GPIB interface. LabView software was used to acquire the data.

For runs 206 and on, the data acquisition system was updated by replacing the Macintosh with a Gateway2000 P5-133 PC-compatible. This computer was equipped with two National Instruments 16-channel acquisition boards, an AT-MIO-16E-1 and AT-MIO-16E-10. The 16E-1 board can acquire data up to 1 MHz, and is used for high-speed acquisition from piezoelectric pressure transducers during detonation tests. The 16E-10 board can acquire data at rates up to 500 kHz, and is used for the remaining pressure transducers and thermocouples in deflagration tests. The data from the two boards are displayed on the screen and saved to the hard disk.

Temperature instrumentation consists of a number of type K thermocouples. The driver contains one heavy-duty thermocouple. This does not respond quickly enough to indicate the peak temperature during the driver burn, but does provide initial mixture temperature data. The receiver contains two probes, used primarily for initial mixture temperature, and a rake of seven smaller thermocouples. These are distributed vertically from one of the top instrumentation ports.

To record pressure, both the driver and receiver are equiped with Kulite strain-gauge pressure transducers. The driver uses a model XTC-190-300A, while the receiver uses a XTME-190-250A. The latter model is temperature compensated to 450 °F (500 K), allowing for vessel heating. To protect the diaphragms from combustion temperatures, sintered metal frits are mounted inside the vessels, covering the pressure ports. The frits are 1" in diameter by 0.125" thick. The outer fritt has a pore size of 40 microns, with 20 microns for the inner frit. These serve to quench combustion and absorb heat from the products before they reach the transducers. The Kulites are powered by Dynamics 7600A excitation amplifiers. For faster pressure measurements taken during detonation experiments, the receiver is outfitted with two PCB model 1125A26 piezoelectric transducers. One of these is located in the last instrumentation port on the top of the receiver, and one is in the 6" end flange. The driver also contains a PCB transducer, mounted in the end flange. The PCB transducers are powered by a PCB power supply, and the output is fed through the Trig-Tek amplifiers can be run in attenuating mode for high-pressure tests.







Figure 2.2: Photo of driver vessel mated to receiver. Pneumatic hydraulic pump, TM-11A trigger module and mixing pump are visible on support rack. Support rails can be seen at bottom of photo.



Figure 2.3: Photo of driver separated from receiver, showing driver extension. Cordin high-speed camera is visible in lower left. Clamp ring and counterweight are hanging over juncture point.



Figure 2.4: Threaded nozzle adapter with nozzles, and 3.625" (92-mm) nozzle.



Figure 2.5: Cross section of hydraulic closure; receiver on left, driver on right.



Figure 2.6: Schematic of gas handling system.



Figure 2.7: HYJET control system, showing gas filling panels, mimic panel, heating and firing controls, camera controller and acquisition computer.



Figure 2.8: Cross-sectional view of schlieren system. Cameras and light source are rotated for clarity.


Figure 2.9: Top view of schlieren system.



Figure 2.10: Window retainer and light/dust boot.



Figure 2.11: Exit end of schlieren system, showing auxiliary lens, beamsplitter, and cameras.

Chapter 3 COMP and S Series

3.1 Introduction and Background

The purpose of the COMP test series was to compare the CIT HYJET facility to the original facility at RPI. These tests duplicated the RPI lean limit deflagration tests (Krok 1992). In these tests, the driver mixture was 80% H₂-20% O₂ at 1 bar. When ignited, this vents a mixture of 50% H₂-50% H₂O into the receiver, simulating a DCH jet in a reactor containment. The receiver mixtures contained air and nitrogen in a 1:1 ratio, with 0-10% hydrogen at 1 bar (addition of an inert gas to a flammable mixture is known as "partial preinerting"). Both vessels had an initial temperature of approximately 298 K. The tests used the 12.7 and 25-mm nozzles. It may be argued that diluting the air with nitrogen will raise the lean limit by displacing oxygen. Previous studies have shown that the lean limit in this system is unaffected with up to 70% N₂ in the overall mixture (Kuchta 1985).

In typical flammability limit tests, the gas mixture is ignited by a strong spark at the bottom of an open, vertical tube. These tests have found a lower flammability limit of 4% H₂ in air (Coward and Jones 1952). At these concentrations, however, the flames burn incompletely, and are driven by their own buoyancy. To obtain a deflagration that can propagate in all directions, 9% H₂ is needed for weak ignition sources (Krok 1992). In the COMP series of tests, ignition was supplied by a jet of combustion products. In addition to supplying heat and turbulence to the receiver gas, the jet may burn as a diffusion flame, providing additional energy.

The S series repeated some of the COMP tests using water vapor as a diluent, at 373 K. In this series, only the 12.7-mm nozzle was used. These tests compared the effectiveness of steam and nitrogen as diluents.

3.2 Results and Discussion

The COMP series test matrix is shown in Table 3.1. Figure 3.1 summarizes the results and compares them to those from RPI. The solid points represent tests run at RPI, while the open points are from the CIT COMP tests. The reference line is the adiabatic, isochoric complete combustion pressure (P_{AICC}) calculated by STANJAN (Reynolds 1986). The tests showed that a hot jet of H_2 and water vapor could ignite a deflagration in mixtures containing at least 6% H_2 . The combustion at this concentration was incomplete, however. The hydrogen concentration had to be increased to 8% for complete combustion to occur. Tests in the RPI facility using a glow plug for ignition found that 9% hydrogen was required for any kind of combustion to occur. Glow plug tests were not run in the HYJET facility, but the results should be similar.

Similar results for H₂-air mixtures were found by Benedick et al. (1984) and Marshall (1986), using spark and glow plugs for ignition. These igniters could initiate weak, upward-propagating flames in mixtures with at least 5% H₂, but 8% H₂ was required for complete combustion. The use of mixing fans during combustion was found to increase the degree of completion in the lower concentrations. The tests by Benedick also included 30% N₂ preinerting (30% N₂-70% air); these showed similar results, although some of the tests with 6 and 7% H₂ failed to ignite.

Völkl and Schlamp (1996) studied ignition of H_2 -air mixtures with a hot jet of air, heated by a reflected shock. For a jet temperature of 2550 K, they required a minimum of 10% H_2 to initiate a deflagration in their test chamber. The jet temperature in HYJET has not been measured, but the 12.7-mm jet temperature was measured at RPI (Krok 1992) and estimated to be 1200 K. The jet temperature may be slightly higher in HYJET, owing to differences in the facility design. The combustion-generated jet injects radicals into the receiver, making up for the lower temperature. Also, since the jet contains excess hydrogen, it has the potential to re-ignite as it enters the receiver. The jet can thus maintain temperature as it entrains the cooler receiver gasses.

In the RPI facility, both vessels were of identical size (0.43 m³). Because of the 1:1 volume ratio, the tests were dominated by jet combustion and pressurization. In addition to the influx of mass, the receiver pressure was increased by combustion of hydrogen in the jet. The work by Ross (1994) determined that both the 12.7 and 25-mm jets could produce stable diffusion flames as they vented into the receiver. Thus, as nozzle size is increased, more mass enters the receiver, and more hydrogen burns in the diffusion flame. The 12.7-mm nozzle was small enough to minimize these effects, giving a clear deflagration limit seen in Figure 3.1. The peak pressures remain fairly level until they jump at 6% hydrogen, indicating a deflagration. (This is a marginal case, as evidenced by both high and low points at this concentration.) With the 25-mm nozzle, the receiver pressure repeatedly exceeds the AICC value. The slope in peak pressure is higher between 4 and 6% hydrogen than between the other points, but this would be hard to justify as a deflagration limit without the information from the 12.7-mm nozzle.

In the CIT HYJET facility, receiver pressurization is much less significant. This is illustrated in Figure 3.2, which compares the receiver pressure traces for the 12.7 and 25-mm nozzles venting into 50% air-50% N₂. With the 12.7-mm nozzle, the RPI receiver sees a peak pressure of over 2.5 bar, but the CIT receiver reaches only 1.1 bar. Pressurization is even more pronounced for the 25-mm nozzle, for which the peak pressures reach 3.75 and 1.25 bar, respectively. The lower jet pressurization in HYJET makes deflagrations much easier to detect.

With this in mind, we can examine the full pressure traces from the RPI tests with

Case	% Hydrogen	% Nitrogen	% Air
COMPAIR	0	0	100
COMPN2	0	100	0
COMP0	0	50	50
COMP2	2	49	49
COMP4	4	48	48
COMP6	6	47	47
COMP8	8	46	46
COMP10	10	45	45

Table 3.1: COMP series receiver mixtures.



Figure 3.1: Comparison of RPI and CIT facilities: 0-10% hydrogen in 1:1 air:nitrogen.

the 25-mm nozzle, shown in Figure 3.3 (taken from Ross (1994)). As the hydrogen concentration is increased, the peak pressure continuously rises, with no large jump between 4 and 6%.

By comparison, the onset of deflagration is much clearer in the HYJET facility. In Figure 3.1, the peak pressures for both nozzles are nearly constant for 0-4% hydrogen. At 6%, there is a small but distinct jump. The transition is clearly visible in the full pressure traces, shown in Figures 3.4 and 3.5. With both the 12.7 and 25-mm nozzles, the trace for 6% H₂ climbs well above those for lower concentrations. The slow pressure rise compared to the higher concentrations shows the lower speed of the burn. Also, note that there is a delay in ignition, particularly for the 25-mm nozzle. This may be caused by reverse flow through the nozzle, as shown in Figures 3.6 and 3.7. The driver mixture burns in 4–5 ms, generating hot hydrogen and water vapor as products. The products cool quickly because of the driver's cold walls and large surface to volume ratio, condensing the water.



Figure 3.2: Comparison of RPI and CIT receiver pressurization, driver venting into 1:1 air:nitrogen.



Figure 3.3: Receiver pressure traces for the original COMP-type tests in RPI facility, venting through 25-mm nozzle.

This rapidly drops the pressure to below 1 bar. Now, the pressure drop across the nozzle is reversed, and flow through the nozzle is reversed until the pressures equilibrate. The reverse flow period is shorter with larger nozzles. Figure 3.6 shows pressures for the 12.7-mm nozzle. The traces in Figure 3.6a are from an inert receiver (which is a close approximation to the 6% H₂ case). We see that reverse flow occurs from 0 < t < 1.1 s. Figure 3.6b shows a case with a deflagration in the receiver $(10\% H_2)$. The increased pressure in the receiver extends the reverse flow period to almost t=1.4 s. Figure 3.7 shows the same cases for the 25-mm nozzle, and we see that the driver response is much quicker, shortening the reverse flow period. In terms of weak receiver deflagrations, the flame might not be able to outrun this reverse flow, although it does not get extinguished. In Figure 3.7a, we see that the reverse flow ends at about t=0.25 s. The 6% deflagration in Figure 3.5 doesn't show a pressure increase until t=0.45 s, so it must take some time for the flame kernel to re-establish itself. The 12.7-mm restricts the reverse flow, so the 6% deflagration in Figure 3.4 proceeds immediately. This reverse flow will again be significant in the next chapter (SA test series).

Although the receiver pressure traces indicate when a deflagration occurs, they do not indicate the completeness of combustion. At 10% H₂, combustion should be complete, but may not be for the 8 and 6% mixtures. A simple analysis (Krok 1992) can give a rough idea of the degree of combustion. First, the two vessels are combined into one control volume. Then, the reaction balance is written, weighting the mole (partial pressure) fractions with the vessel volumes. For example, the 6% H₂ mixture gives us:

 $28(0.8H_2 + 0.2O_2) + 1180(0.6H_2 + 0.47N_2 + 0.47(0.79N_2 + 0.21O_2)) \longrightarrow$

$$3.2H_2O + 991.2N_2 + 75.8O_2$$

When the vessel cools after combustion, we assume that all of the water condenses to



Figure 3.4: Receiver pressure traces from COMP series in HYJET facility, venting through 12.7-mm nozzle.

	$\% H_2$	P_f , calculated	$P_f, 12.7$ -mm	P_f , 25-mm
	2	0.985	0.988	0.981
Π	4	0.956	0.988	0.984
I	6	0.926	0.954	0.952
	8	0.897	0.901	0.904
	10	0.868	0.872	0.868

Table 3.2: Comparison of measured and calculated final pressures.

liquid, and makes no contribution to the pressure. Using the ideal gas law, PV=nRT, we note that P/n=RT/V, which is constant (we are bringing T back to the initial value). The result is that $P_f=(n_f/n_i)P_i$, or the final pressure is the original pressure multiplied by the mole ratio across the reaction. In addition to the condensed water, this accounts for mole reduction in combustion. For the 6% H₂ case, this gives us $P_f = 1.0(991.2+75.8)/(93.2+122.4+991.2) = 0.884$ bar. Finally, we account for the condensed water by adding its vapor pressure. The tank is cooled to about 303 K when the final pressure is measured; the corresponding vapor pressure is 0.042 bar. The expected value of P_f for complete combustion of the 6% H₂ mixture is thus 0.926 bar. These final pressures are tabulated in Table 3.2, and compared to representative values from the experiments.

In the real system, not all of the driver hydrogen burns, resulting in higher final pressures. Also, variations in measurement temperature will affect the results. For cases with no deflagration in the receiver, the final pressure is recorded at only 293 K or so. Also, there may not be enough water present to make up the 0.042 bar stated as the vapor



Figure 3.5: Receiver pressure traces from COMP series in HYJET facility, venting through 25-mm nozzle.

pressure. For 2 and 4% H₂, we see that the final system pressure is fairly constant for the two nozzles. It is slightly lower for the 25-mm nozzle, probably because the larger nozzle vents more H₂ into the receiver where it burns as a diffusion flame. At 6% hydrogen, there is a definite drop in P_f , but it is not as low as expected. The conclusion is that combustion was not complete. In the 8 and 10% mixtures, we get final pressures that are very close to the calculated value, indicating complete combustion. Even though we found a deflagration limit at 6% hydrogen, combustion was not complete until 8%. These results agree with those of Benedick et al. (1984) and Marshall (1986), where gas chromatography was used to analyze the post-burn mixtures. Marshall found a combustion fraction of 90% for 6% H₂, although both experimenters experienced difficulties with the chromatograph equipment. Thus, their estimates of burn completion were given for reference only.

The S series of tests duplicated the COMP series, but replaced the nitrogen in the receiver with water vapor. The starting temperature of these runs was approximately 373 K. Only the 12.7-mm nozzle was used in these tests. The results are shown in Figure 3.8. With water vapor, we needed at least 8% H₂ in the receiver to get a deflagration, compared to 6% for N₂ dilution. Water vapor is a more effective diluent than nitrogen, as it has a higher heat capacity ($C_v=0.74$ and 1.41 kJ/kg-K for N₂ and H₂O, respectively, at 300 K). Figure 3.9 directly compares the receiver pressure traces for the COMP8 and S8 tests with a 12.7-mm jet. The nitrogen mixture burns much quicker, giving a sharp peak pressure. The water vapor mixture has a low, broad peak pressure. The presence of water vapor in this mixture reduces the flame speed (Liu and MacFarlane 1983; Liu et al. 1980), allowing heat transfer to occur during the burn, and reducing the peak pressure. The peak pressure seen in the plot is about 2 bar, while $P_{AICC}=2.92$ bar for this mixture. The increase in initial temperature also reduces the peak pressure, but



Figure 3.6: Pressure traces for 12.7-mm nozzle venting into nonflammable and flammable receivers.



Figure 3.7: Pressure traces for 25-mm nozzle venting into nonflammable and flammable receivers.



Figure 3.8: Receiver pressure traces from S series in HYJET facility, using 12.7-mm nozzle.

not to this degree. At the higher temperature, the gas mixture is less dense, reducing the energy density and total energy in the vessel. From STANJAN calculations, P_{AICC} for the COMP8 receiver at an initial temperature of 300 K is 3.75 bar. This drops to 3.17 bar for an initial temperature of 373 K. Marshall (1986) also found that combustion times were increased with the addition of water vapor.

The mole-balance test for complete combustion can not be used for the S series, due to the high water fraction in the receiver and difference in vessel temperatures. Although the receiver is heated, the driver is left at room temperature. As water vapor condenses in the driver (from the initial combustion event), the pressure drops to subatmospheric (see reverse flow discussion on page 27). The reverse flow drives more hot water vapor into the driver, which continues to condense. The result is a constant flow of vapor into the driver, and a buildup of liquid water. With the difference in vessel temperatures, there is some ambiguity in the amounts of condensed and gaseous water. Also, the driver is not equipped with a condensate drain, so cleanup is difficult. As a result, in these experiments, the vessels are evacuated using the liquid ring pump as soon as the system pressure drops below 1 bar. Liu et al. (1980), however, found that there is no significant difference in the degree of combustion between wet and dry mixtures of the same H_2 concentration.



Figure 3.9: Receiver pressure traces showing effectiveness of water vapor as diluent. Mixtures are 8% H_2 in 1:1 air:diluent, with T=300 K for N_2 and 373 K for H_2O .

Chapter 4

SA Series

4.1 Introduction and Background

The SA series of tests examines the effect of ignition source strength on the flammability of H₂-air mixtures with steam dilution. In this series, the hydrogen:air ratio was kept constant at 1:4, or 20% H₂ in air (dry). This mixture was then diluted with 0–60% water vapor. The mixtures are listed in Table 4.1. The initial receiver temperature was approximately 373 K. The driver contained 80% hydrogen and 20% oxygen at 1 bar and 293 K. The 12.7, 25 and 92-mm nozzles were used for receiver ignition.

4.2 **Results and Discussion**

Figure 4.1 summarizes the results of the SA-series tests by comparing the peak receiver pressures to P_{AICC} for the full range of vapor concentrations. As the vapor concentration is decreased from 60 to 50%, the peak pressures rise to the AICC line. From 40% to zero, the peaks for the 12.7 and 25-mm nozzles plot right along the line. (At elevated receiver temperatures, condensation of products at the walls is slower, and the reaction can reach the theoretical peak pressure.) The peak pressures from the 92-mm nozzle lie above the

	Case	% Water Vapor	% Hydrogen	% Air
	SA0	0	20	80
	SA10	10	18	72
Ī	SA20	20	16	64
	SA30	30	14	56
	SA40	40	12	48
	SA50	50	10	40
Ī	SA55	55	9	36
ſ	SA60	60	8	32

Table 4.1: SA series receiver mixtures.



Figure 4.1: Summary of peak receiver pressures for SA-series tests.

AICC line. This is probably due to dynamic effects, such as pre-pressurization of the receiver mixture by the jet startup shock.

Previous experiments by Marshall (1986) used similar mixtures in a condensing-steam environment, with glow plug ignition. The dilution limit was found to be 50% in those tests. Other work cited in that report found maximum limits of 55% H₂O. Djebaili et al. (1994) used a hot jet of 60% H₂-40% Ar to ignite 18% H₂-82% air mixtures with water vapor dilution. With a jet temperature of 2550 K (generated by shock reflection), they found a dilution limit of 48% H₂O. In the present experiments, the 12.7-mm jet was able to initiate a deflagration in a 60% H₂O mixture. Despite the lower temperature (Chapter 3), the radicals in the combustion-generated jet make it a more effective initiator.

The individual tests are illustrated in Figures 4.2–4.4. Figure 4.2 shows the receiver pressure traces for the 12.7-mm nozzle, with vapor concentrations from 0 to 60%. The lowest trace on the plot (from run 68) corresponds to 60% water vapor. A deflagration is seen in this case, but the pressure does not begin to rise until nearly one second after driver ignition. This deflagration takes a long time to ignite, but still progresses. This was also seen in the video recording from the schlieren system. Typically, when a deflagration is initiated in the receiver, it starts when the jet enters the receiver and proceeds down the vessel. In run 68, however, the jet from the driver starts and finishes before any deflagration is seen. At 0.68 seconds after driver ignition, a flame front is seen moving back into the field of view, traveling in the upstream direction. This indicates that the slug of products from the driver ignited the receiver mixture somewhere downstream. Perhaps the mixture was ignited immediately, but the flame speed was so slow that the ignition kernel was convected downstream with the jet gas. Two other tests were run



Figure 4.2: Receiver pressure traces from SA-series tests, 80:20 driver venting through 12.7-mm nozzle.

with this mixture, one producing a burn, and the other failing to ignite. Clearly this is a marginal case, and small differences in the water vapor fraction and quality can affect the results.

Figure 4.3 shows the pressure traces for the 25-mm nozzle. Despite two tests with 60% water vapor (SA60), the 25-mm nozzle was unable to ignite a deflagration at this dilution. We saw from Figure 4.2 that the successful deflagration in the SA60 mixture was very slow, comparable to the 6% H_2 mixture in the COMP tests. In those tests, we speculated that the reverse flow after jet depletion was inhibiting propagation of the flame. In the current tests, the strength of the reverse flow with the 25-mm nozzle may be extinguishing the flame kernel before it can propagate. The tighter obstruction provided by the 12.7-mm nozzle constricts the reverse flow and allows the flame to persist. Also during the 25-mm SA60 tests, condensation was seen forming on the schlieren windows (the windows can not be insulated). Problems with condensation in the steam supply may have created a condensing atmosphere, affecting the results.

Pressure traces from the 92-mm nozzle are shown in Figure 4.4. A 5-point average has been used to reduce the oscillations on these traces. With this nozzle, driver effects dominate the receiver pressure. There is a large jump from 60 to 50% water vapor, so it does not appear that a deflagration occurs at 60%. However, the trace for 60% is above that for 100% air. Also, the 60% trace has a blunt peak, offset from the y-axis, that is indicative of weak combustion (vs. the sharp peak close to the axis for a shock alone). In Figure 4.5, we will see that the long-term pressure trace for 60% H₂O coalesces with that for the 12.7-mm nozzle (see below).



Figure 4.3: Receiver pressure traces from SA-series tests, 80:20 driver venting through 25-mm nozzle.

Figure 4.5 shows receiver pressure traces for the three nozzles used in this series, with 60% water vapor in the receiver. The trace from the 12.7-mm nozzle shows the initial pressurization, followed by a shallow decay as gas flows back into the driver. At t=1 s, the pressure increases again as the deflagration proceeds. The pressure peaks between 3 and 3.5 s, and then decays as the products cool. With the 25-mm nozzle, there is a higher initial peak, but the pressure then decays with no rebound. The higher initial pressure is due to an increased amount of mass venting from the driver before the flow reversal, as well as combustion of hydrogen in the jet. With the 92-mm nozzle, there is a much higher initial pressure. Much of this is from the startup shock. This masks the early stages of the deflagration, but it is evident where the pressure trace joins that from the 12.7-mm nozzle at t=3 s. Also, note the increase in oscillations with nozzle size. This is particularly evident with the 92-mm nozzle. The oscillations are the result of shocks reverberating in the vessel. The soundspeed of the burned SA60 mixture is 740 m/s (STANJAN). The vessel is approximately 2 m long, so an acoustic wave takes 5 ms to make a round trip. The corresponding frequency is 185 Hz, low enough to be resolved by the Kulite sampling at 1 kHz. Expanding the trace for the 92-mm nozzle revealed that the oscillation period was 6 ms, in close agreement with the predicted time. As the mixture cools, the soundspeed decreases, increasing the period. The trace for the 12.7-mm nozzle is smooth in comparison to the other two.



Figure 4.4: Receiver pressure traces from SA-series tests, 80:20 driver venting through 92-mm nozzle. Shock oscillations smoothed by a 5-point average (see Figure 4.5 and discussion).



Figure 4.5: Receiver pressure traces for SA60 mixture, showing effect of nozzle size. Note increase in peak pressure and increase in oscillations as nozzle size is increased.

Chapter 5 NITRO Series

5.1 Introduction and Background

This series of tests began our study of jet initiation of detonation. The work by Knystautas et al. (1979) showed that turbulent mixing of reactants and hot combustion products could initiate a detonation. Those experiments focused on DDT of a flame front venting through an orifice. Two directly connected vessels (with no diaphragm separation) were uniformly filled with an oxy-acetylene mixture. Orifice plates with various hole configurations were mounted in the connection between the vessels. The mixture was spark ignited in one chamber, and vented into the other through the orifice plate. With the proper arrangement of holes, the flame would transition into a detonation shortly after passing through the plate. The best arrangement was found to be an array of holes with a spacing large enough to prevent recombination of the small jets into one large jet. In addition to the orifice plates, wire screens could be installed to generate fine scale turbulence. The results indicated that transition was aided by both large and small scales of turbulence. Large eddies serve to entrain fresh reactants into the hot jet gas, while the fine scales mix the gases together. The use of screens alone would not cause DDT, as there were no large-scale structures to create entrainment. With an orifice plate alone, the detonation appeared to begin in a localized explosion on the surface of the jet. With the addition of the screen, the entire surface of the jet transitioned at once, at a shorter distance from the exit. Finally, if a particular orifice plate could not cause transition, addition of the screen would not help. It is important to note that entrainment has two counteracting effects: While entrainment and mixing heats the receiver mixture, it also dilutes and cools the jet gas, reducing its effectiveness. Ignition occurs when a balance is reached between these two processes.

Other research (Moen et al. 1985; MacKay et al. 1988; Moen et al. 1989) expanded these results to larger scales and less-sensitive mixtures, but in all cases the "driver" and "receiver" chambers were continuously connected, making it difficult to quantify the jet at the time of start-up. (The aim of these experiments was to study DDT in a fueloxidizer cloud containing obstacles, possible in an industrial accident, so attempts were not made to quantify the jet.) The first work to separate the vessels with a diaphragm was that of Carnasciali et al. (1991), followed by Dorofeev et al. (1993), Bezmelnitsyn et al. (1995), Dorofeev et al. (1995) and Bezmelnitsin et al. (1997). The work of Carnasciali et al. (1991) and Bezmelnitsin et al. (1997) will be further addressed in the next chapter, which describes the BETA test series. The work by Dorofeev has some connection to the present NITRO series, as their driver and receiver chambers used hydrogen-air mixtures. In many works, what we refer to as the "driver" is named the "jet" or "flame" chamber. Likewise, the receiver is named the "detonation" or "explosion" chamber. I will use the "driver" and "receiver" terms throughout for clarity.

5.2 **Results and Discussion**

The present NITRO test series began with a driver mixture of 80% H₂-20% O₂, and went on to study the effect of a slower driver flame speed. The flame speed was reduced (see Figure 5.3) by diluting the H₂-O₂ mixture with nitrogen, to a maximum of 50%. Since the diluent displaces reactants, it also reduces the peak driver pressure. To correct for this, the initial driver pressure was increased with the amount of dilution, in a way that would keep the peak pressure constant (9.7 bar, corresponding to no N₂). The required initial pressures were calculated with STANJAN. The resulting driver mixtures are shown in Table 5.1. Unforeseen dynamic effects raised the peak pressures, however (discussion below).

Driver	% Nitrogen	% Hydrogen	% Oxygen	P_i , mbar
0N	0	80	20	1000
5N	5	76	19	1018
10N	10	72	18	1036
15N	15	68	17	1057
20N	20	64	16	1083
25N	25	60	15	1114
30N	30	56	14	1152
35N	35	52	13	1198
40 N	40	48	12	1254
45N	45	44	11	1322
50N	50	40	10	1405
55N	55	36	9	1506

Table 5.1: NITRO Series driver mixtures.

All of the tests used the 92-mm nozzle. The receiver mixtures consisted of 0-30% hydrogen in air at one bar and room temperature. The objective of the tests was to determine the lean limit of receiver detonation initiation for each driver dilution. We did not expect direct initiation of detonation in the receiver; previous tests have indicated (Dorofeev et al. 1993) that a minimum jet diameter of 13λ is required to directly initiate a

detonation via a turbulent jet. Cell-size measurements for stoichiometric (30%) hydrogenair range from 11 mm (Bull et al. 1982; Stamps and Tieszen 1991) to 15 mm (Guirao et al. 1982). Based on these values, the 92-mm nozzle in HYJET has a D/λ ratio of only 6.1–8.4 for this mixture. However, the tests showed that we were able to initiate detonations in mixtures with as little as 24% hydrogen, or $D/\lambda=4.3$ (Guirao et al. 1982). The current experiments used the PCB transducers mounted on the end flange (reflected pressure) and the last top port of the receiver vessel (static pressure). These are the E and T3 locations shown in Figure 6.2 on page 64. Data was acquired at 250 kHz for 32 ms.

The results were surprising. Some of the tests showed high pressure peaks after the initial shock wave, even with no detonation evident. In order to better separate the results, we use a criteria called "prompt" initiation. Initiation is prompt when both the static and reflected pressure traces show the passage of a detonation. Figure 5.1a shows a prompt detonation. Both of the pressure traces show the sharp rise in pressure and peak values characteristic of a detonation. Figure 5.1b shows a trace from a failed initiation. The lead wave on both transducers is small, but strong secondary explosions are evident shortly after passage of the lead wave. The secondary explosions in Figure 5.1b probably occur in the precompressed mixture at the end of the vessel. We later determined that this was the result of shock focusing (described below).

Due to the D/λ limitations of our driver, we originally thought that the "prompt" cases were the result of a DDT occurring between the jet exit and the T3 transducer. However, the results of the BETA test series (in the next chapter) showed that the detonations were directly initiated by the jet. It appears that the D/λ criteria is not appropriate for this type of experiment, as it does not reflect the driver composition or exit geometry. The initiation process is probably similar to that described by Knystautas: Large eddies from the jet entrain reactants and small-scale turbulence mixes them with the hot products. The startup structure of impulsively generated jets (i.e., from diaphragm rupture) was photographically studied by Lacerda (1986). Photographs show that the jets have a large head, enclosing a vortex ring. The jet head is preceded by a bow shock. Both the shock and the jet head travel downstream, and the jet assumes a quasi-steady structure at the nozzle exit. Photographic tests in the RPI facility (Appendix E) showed the jet head to be highly turbulent, a result of the violent rupture process. In the current initiation experiments, the bow shock will sensitize the reactants before they are entrained by the vortex ring. Once entrained, small-scale turbulence in the head mixes the reactants with the hot jet gas. After a suitable induction time, one or more local explosions will occur, initiating the detonation. Typically, jet initiation is attributed to the SWACER mechanism (shock wave amplification by coherent energy release), first proposed by Lee et al. (1978). This requires an induction time gradient in the reactants, which is provided by turbulent diffusion at the reactant-jet boundary in the large eddies. (If the induction time is uniform, the whole body explodes simultaneously, only reaching the constant-volume pressure. The gradient allows pressure waves to build into a detonation.) Additional vortex combustion studies include Chan et al. (1990), Yip et al. (1985) and McCormack et al. (1972).

The results of the NITRO tests are summarized in Table 5.2. The undiluted driver was able to initiate a detonation in 26% hydrogen, and we expected the diluted drivers to require higher hydrogen concentrations. This was not the case. Drivers with 30% or more N₂ were unable to initiate detonations in any H₂-air mixture. All drivers with 25% and less N₂ initiated detonations in H₂-air mixtures with at least 26% H₂. The "25N" mixture was the most effective, giving a prompt initiation in only 24% hydrogen. Despite the small difference in hydrogen concentrations, the results were repeatable.

$\% N_2$	Minimum $\%$ H ₂ for Detonation	$\% N_2$	Minimum $\%$ H ₂ for Detonation
0	26	25	24
10	25	30	No detonation
20	26		

Table 5.2: Results of NITRO tests.



b: Prompt initiation failure with secondary explosion.



The first step was to determine why the 25% nitrogen driver was more effective than the others. Using the nozzle plug, I ran a series of constant-volume driver tests with the full range of dilutions. The results, shown in Figure 5.3, indicated that the peak pressures in the driver were not constant as planned. While the flame speed did go down (represented by the burn time, from ignition to peak pressure), the peak pressure increased to a broad plateau of nearly 13 bar. This can only be a dynamic effect of the confinement geometry. When P_{AICC} is calculated by STANJAN, it is strictly an equilibrium calculation. The reactants immediately turn to products, with no consideration for dynamic effects. This is best approximated by rapidly-burning mixtures in a spherical vessel with central ignition. In our case, the vessel is a long tube ignited at one end. Shock waves, such as the one generated at ignition, have time to run to the end and reflect back, compressing the reactants. Furthermore, turbulence can be generated by the annular channel at the driver-extension junction (Figure 5.2), promoting flame acceleration. This would generate further waves and precompression. Also, as the initial pressure is increased, the effects of the shock will multiply. As the N₂ fraction is increased beyond 30%, the decrease in flame speed overcomes these effects, and the peak pressure is reduced by heat transfer during the burn.



Figure 5.2: Internal geometry of driver vessel. Annular channel (166 mm dia. by 102 mm long) is formed by the hydraulic closure and extension.

The idea of driver enhancement by dilution is not unheard of. In Carnasciali et al. (1991), a driver with stoichiometric H_2 - O_2 and 46% N_2 was more effective than one with only 12% N_2 . This was attributed to increased radical concentration in the jet with less dilution. They argued that the response time of the receiver mixture must be short enough (i.e., more sensitive) to accept the higher concentration of radicals.

To study the possibility of transition in the driver, I installed a PCB transducer in the instrumentation flange, next to the spark plug. In this location, the transducer can not record the actions near the diaphragm. However, shock waves reflected from the diaphragm or generated by local explosions at the end of the driver can be seen. The reflected pressure ratio is much higher for shocks than for detonations (approx. 7 vs. 2.5, see p. 75), so the shock reflections seen here over-represent the conditions in the driver. The pressure traces from two drivers, with zero and 25% N₂ dilution, are shown in Figure 5.4 (P_{CJ} =18.22 and 18.58 bar, respectively). The 0N driver shows a peak of 15 bar, while the 25N reaches nearly 25 bar. The higher pressure in the 25N driver is a result of the lower flame speed. In this case, there is time for shock reflection and flame acceleration to induce transition to detonation. Without dilution, most of the reactants are consumed before transition can occur. From the pressure traces, it is likely that



Figure 5.3: Peak pressures and burn times (time to peak pressure) for nitrogen dilution mixtures burned in plugged driver. The peak pressures were expected to fall around 9.7 bar, as calculated with STANJAN.

detonation occurred in the 25N driver, but not in the 0N driver, as the peak reflected pressure in that case is below even P_{CJ} .

If a detonation does occur, our problem becomes one of a stronger impulsive jet, or of detonation transmission and direct initiation. The effect of detonation in the driver can be evaluated with an appropriate wave analysis. Figure 5.5 shows a wave diagram for this system. If a detonation occurs in the driver, it will generate reflected and transmitted waves at the mixture interface (i.e., the diaphragm). Wether the reflection is a shock or an expansion depends on the detonation conditions and the properties of the receiver mixture. When the diaphragm ruptures, it is replaced by a contact surface between the two gases. The pressure and velocity must be matched across this surface (i.e., $P_2=P_3$, $u_2=u_3$). The conditions in region 1 are the CJ detonation conditions, and can be computed with an equilibrium code such as STANJAN. The conditions in regions 2 and 3 are computed by shock and expansion relations that calculate pressure change as a function of velocity change across the wave. Typically, ΔP is calculated for a range of Δu across the waves (i.e., the shock Hugoniot), and the matching condition is found graphically. The equations can be found on page 417 of Thompson (1972).

The results of the wave calculations are shown in Figure 5.6. The reflected wave conditions are plotted for both drivers. For the receiver Hugoniot, a representative mixture of 25% H₂-air was chosen. In the figure, the solid lines on the reflected wave indicate a reflected shock, and the dashed lines indicate a reflected expansion. The CJ points are also shown on both curves. If the receiver mixture is tailored, its Hugoniot will pass through the CJ point, and a shock will be transmitted with no reflected wave in the driver. In our case, we see how the character of the reflected wave is affected by the



Figure 5.4: PCB traces from NITRO drivers, venting into air. 25N driver shows stronger reflected shock. PCB is located at ignition end of driver.

driver mixture. The high H_2 fraction in the 0N driver results in a high soundspeed, CJ velocity, and gas velocity following the detonation. The receiver mixture is much denser than the combustion products in the driver, and a reflected shock is the result. This drives a stronger shock into the receiver than the 25N driver, where increased driver density allows a reflected expansion to occur.

The Mach numbers of the shocks in the receiver can be determined from the Hugoniot matching conditions. For the 0N driver, the receiver shock has M=4.31, and a post-shock temperature of 1242 K. The 25N driver generates a M=3.98 shock, with a corresponding temperature of 1107 K. To determine the consequences of these shocks, we need to determine the induction time of the shocked mixture. This can be estimated by calculations with thermodynamic data and kinetic mechanisms. I calculated the induction times with a constant-volume combustion program ("CV"), that uses thermodynamic data and chemical kinetics to determine temperature and pressure profiles over time. For the M=4.31 shock (0N driver), the induction time is 27 μ s. In this time, the shock moves 45 mm. A typical detonation is less than 1 cm thick, so it is unlikely that a detonation in the 0N driver would directly initiate the 25% H₂-air receiver mixture. In addition, the PCB pressure traces indicated that a detonation was unlikely in this driver, so this shock process may not apply.

The M=3.98 shock generated by the 25N driver leads to an induction time of 0.457 ms, much longer than with the 0N driver. In this time, the shock moves 0.7 m, which would clearly decouple it from the reaction zone. As these shocks leave the nozzle exit, they diffract into the larger receiver vessel, rapidly reducing their strength. Thus, we conclude that neither driver is creating direct initiation conditions.

We will now examine the combustion events in the receiver. In many cases, even with



Figure 5.5: Wave diagram for reflection of detonation at end of driver.

prompt initiation, the highest peak pressure did not occur at the lead wave, but some time later. Some of these were very strong. Two of the 25N tests had late peak reflected pressures of just over 100 bar, despite receiver hydrogen fractions of only 22 and 23%. A repeat of the 23% H₂ case obtained a peak pressure of 50 bar, which is half the previous value but still more than the reflected CJ pressure of 33 bar. Clearly, the geometry and dynamics of a confined system is important in any type of combustion analysis. In an attempt to analyze these results, Figure 5.7 plots the highest peak pressure in each test versus the delay time from the initial wave (excluding 8 points with delays over 3 ms). Some of the points fall along t = 0, showing that the lead shock or detonation was the strongest wave in the train. Many of the tests, however, had a highest peak near 0.3 ms, as shown by the points clustered around the reference line. This indicated a regular wave phenomena, later determined to be shock focusing.

To summarize the results for the various driver dilutions, Figures 5.8 through 5.12 plot the initial and peak wave pressures (recorded at the end of the vessel) against receiver hydrogen percentage. In all cases, the solid points indicate prompt initiation, and the open points represent all other cases. As these values are taken from the end-mounted transducer, where reflection occurs, only the reflected CJ pressure is shown for comparison. The 25% dilution case (Figure 5.11) has the most data points, and its description can be applied to the other cases. At low H₂ concentrations, <10%, we see that both the lead and delayed-peak waves are small. In the 15–20% range, we begin to see significant secondary explosions, approaching 20 bar. Above 20%, the secondary explosions get quite strong. In these cases, even though the mixture is not sensitive enough to detonate promptly, it is sensitive enough to undergo a local explosion or DDT after it has been sensitized by the lead shock. As we pass the initiation threshold, the peak pressures are relieved to some degree, because the detonation is proceeding into



Figure 5.6: Hugoniot plots for reflected wave in driver and shock in receiver. On reflected wave Hugoniot, solid line indicates reflected shock; dashed line indicates reflected expansion.

undisturbed reactants. In terms of industrial or reactor scenarios, this means that the greatest potential for damage may be found in mixtures below the detonation threshold.

To study the shock focusing problem, the E transducer was mounted on a sting penetrating the end flange, aligned with the axis of the vessel. A series of tests were run using a stoichiometric H_2 -air driver to generate a shock in the receiver, which was filled with air. One run was made with the sting at each of 16 positions, ranging from 100 to 475 mm from the end of the vessel, in 25 mm increments. The results are shown in Figure 5.13, as a sort of x-t diagram. To account for variations in diaphragm rupture time, each trace was time-adjusted to make the lead shock correspond to a shock of M=1.09 running along the sting. This Mach number was selected based on the lead shock reflected pressure of 1.33 bar. While Figure 5.13 does show focused waves, with peak pressures reaching 2.5 bar and more, no distinct structure is seen. The curved line connects small waves that have a pattern consistent with the results of the ray tracing simulation (described below). Based on calculations of round-trip times, the first large shock after the lead (labeled "initial focus") is not the reflection from the end flange. At the 100-mm station, the delay between the initial shock and this initial focus shock is 0.3 ms, consistent with the characteristic time found in Figure 5.7. This is the focus responsible for secondary explosions, which we will try to model below.

In addition to the timing problems, it seemed remarkable that the lead shock could be amplified to this degree. I wondered if the small shock was not from the diaphragm rupture, but an artifact of driver combustion. To study this, I ran a test wherein the diaphragm was ruptured by slowly pressurizing the driver with air. The sting was placed at the 250-mm station, where it would be outside the flange pipe. As evident from



Figure 5.7: Highest peak receiver pressure seen in receiver versus time from lead shock. Note cluster of points around t=0.3 ms.

Figures 5.14 and 5.15, the lead and focused shocks follow the same pattern. Thus, we conclude that the small lead shock is in fact the diaphragm rupture shock, and the following shocks are the result of focusing.

In a final attempt to expose the focusing, an acoustic wave study was performed using a ray tracing program ("raytrace") written by Joe Cates and Danny Howard of GALCIT (Cates and Howard 1993). This program is written in PV-Wave command language, and uses displacement potential functions to track acoustic longitudinal and shear waves. The program can calculate reflections and transmissions at fluid, solid and fluid-solid interfaces.

The ray tracing program uses a unit square as a domain. The inside diameter of the vessel is 0.86 m, so the dimensions were scaled by 1.16. The interior contour of the end flange connection was measured and scaled, and was input with a 4:1 ellipse matching the interior surface of the head. (Previously, the facility has been shown with the receiver on the left and the driver on the right; this has been reversed for simplicity in the calculations.) A curved shock was used as the starting condition, and was generated with 146 rays, each specified by the coordinates of the initial point and the launch angle. The outer ends of the shock start at x=0.05 in model space, and the associated rays were calculated assuming that they radiated from a point source behind the nozzle (see Figure 5.16). The location of this point was chosen so that the rays grazing the edge of the 92-mm nozzle would meet the edge of the elliptical head. The resulting half angle is 14.5° . Rays were launched at 0.2° increments.

The results are shown in Figure 5.17, where t=0 is arbitrarily taken as point of first contact. The extra line segments connecting the waves at t=0.668 ms are artifacts of the program. We clearly see the formation of a focus region at t=1.158 ms, where the



Figure 5.8: Initial and highest peak receiver pressures for undiluted driver.

shock fronts collide and cross over, after reflecting from the end of the tank. The point of collision is about 325 mm from the face of the end flange. The portion of the original shock reflecting from the end flange will also enter this region and shock it further. Local explosions may occur in this region. It has been difficult to reconcile this with the map of pressure traces shown in Figure 5.13, although one similar structure is shown, centered at 280 mm. Nonlinearities in the real system will alter the timing and shape of the wavefronts.

A second attempt was made to find the origin of the first strong focus in Figure 5.13. When the shock reaches the end of the vessel, we expect a reflection from the corners of the flange extension, as shown in Figure 5.18. This may not have been seen in the first ray tracing simulation because the corners were sharp (zero radius). If we modify the surface definition and angle the corners, we see the focus generated in Figure 5.19. This is a rough approximation, as the corners are only modeled with two surfaces. Unfortunately, time constraints prevented me from adding rounded corners to the surface definition. Such a simulation would give results similar to Figure 5.18. At a later time, the parts of the shock reflected from the elliptical head form a second focus, as shown in the first simulation (Figure 5.17). This simulation also explains the nature of the (apparently) erroneous shock fronts shown at t=0.668 ms in the first simulation. These were an attempt by the program to account for the corner, but as it had an infinitesimal radius, a large number of starting rays would have been needed to resolve it.

The existence of focal regions was shown in the experiments of Sturtevant and Kulkarny (1976). In that study, shocks of various strengths (1.005 < M < 1.5) were reflected by different concave forms. The focus region seen in Figure 5.17 is similar to those of weak shocks (M=1.1, 1.2) reflected from parabolic reflectors. Even for weak shocks, nonlinear effects were found to dominate the focal region. Because of these nonlinearities,



Figure 5.9: Initial and highest peak receiver pressures for driver with 10% N₂ dilution.

the focus problem would be much better modeled by Amrita (Quirk 1996) or a CFD (computational fluid dynamics) code.

In the HYJET receiver, reflected shocks and focal regions can sensitize reactive mixtures, promoting local explosions and DDT (Chan 1995). The result is the presence of strong secondary explosions as seen in Figure 5.1. Strong reflections can occur even when a detonation is initiated promptly.



Figure 5.10: Initial and highest peak receiver pressures for driver with 20% N₂ dilution.



Figure 5.11: Initial and highest peak receiver pressures for driver with 25% N₂ dilution. This was the strongest driver, initiating prompt detonations at 24% H₂ in receiver, and high peak pressures just below that threshold.



Figure 5.12: Initial and highest peak receiver pressures for driver with 30% N₂ dilution. No prompt detonations were initiated by this mixture. P_{CJ} not shown.



Figure 5.13: Pressure traces from sting-mounted PCB transducer, positioned at 25 mm intervals from 100 to 475 mm from face of end flange. Position of lead shock is adjusted for M = 1.09. Driver is 30% H₂-air, receiver is 100% air.



Figure 5.14: Pressure trace with sting at 250-mm station. Driver mixture was stoichiometric hydrogen in air, and gave a peak pressure of 6.14 bar. Receiver is filled with air.



Figure 5.15: Pressure trace with sting at 250-mm station. Diaphragm was ruptured by quasi-static driver pressurization. Rupture occurred at 6.78 bar. Receiver is filled with air.


Figure 5.16: Geometry of initial shock for ray tracing simulation.



Figure 5.17: Results from ray tracing simulation, showing development of focus region at far end of receiver vessel.



Figure 5.18: Shock reflections expected from corners of flange extension. The reflections coalesce to create a focus region near the face of the flange.



Figure 5.19: Results from second ray tracing simulation, showing reflections from (truncated) corners. If corners were modeled with a radius, results would be similar to Figure 5.18.

Chapter 6 BETA Series

6.1 Introduction and Background

The purpose of this test series was to study jet initiation of detonation in comparison with previous experiments (Carnasciali et al. 1991; Bezmelnitsin et al. 1997). Those experiments used stoichiometric mixtures of the form $H_2 + 0.5(O_2 + \beta N_2)$. The degree of dilution is represented by β , the ratio of diluent to oxygen. The objective is to find the maximum value of β (β_{CRIT}) for which a detonation can be initiated in the receiver vessel. The present experiments differ from the previous ones mainly in facility size and location of the jet with respect to the receiver gas. A comparison of the three facilities is given in Table 6.1. In addition to the listed differences, the previous facilities used eight spark plugs distributed throughout the driver for a rapid pressure rise and consistent peak pressure. The HYJET facility has only one spark plug at the end of the driver. The peak pressures remain fairly consistent, however. An analysis of 14 runs used for photographic shots gave an average peak pressure of 13.84 bar, with a standard deviation of 0.26. The time from ignition to peak pressure was 11.23 ms on average, with a deviation of 0.15. (The driver Kulite pressure was recorded at 4 kHz, so the peak time has an accuracy of ± 0.13 ms.) A sample driver pressure plot is shown in Figure 6.1. These peak pressures are for the 25-mm nozzle; pressures are similar for the 38-mm nozzle. The 64 and 92-mm nozzles have peak pressures of 10-11 bar, due to the increased venting area. The peak pressure recorded with the 25-mm nozzle is much higher than the P_{AICC} of 8.62 bar, and is fairly close to the CJ pressure of 16.8 bar. A PCB transducer was later installed in the driver, and the pressure signals indicated that the driver mixture was transitioning to detonation somewhere down the tube. An analysis (described below) showed that a detonation in the driver is not adequate to directly initiate a detonation in the receiver, but our jet is better described as strongly impulsive, vs. a jet generated by constantvolume combustion. The jets in the previous facilities entered flush with the end of the receiver vessel. In the present facility, the driver vessel extends into the receiver by about 0.5 m. The effect of this extension has not been determined.

The first reported data was from Carnasciali, where the effect of diaphragm material and driver composition were also studied. These tests used glass diaphragms for clean

	Carnasciali	Bezmelnitsin	Krok
Driver diameter, m	0.2	0.2	0.13
Driver length, m	0.66	0.66	2.36
Driver volume, ℓ	21	21	28
Receiver diameter, m	0.48	0.52	0.86
Receiver length, m	0.78	0.72	1.98
Receiver volume, ℓ	141	154	1180
Receiver/driver volume ratio	6.8	7.3	42
Orifice diameter, mm	76, 102, 119	120	25, 38, 64, 92

Table 6.1: Comparison of jet-initiation facilities.

rupture and consistent peak pressure. They found an optimum driver mixture of $\beta = 2.6$, proposing that this created the ideal radical concentration. This mixture was used in the HYJET experiments. Carnasciali also found little dependence on orifice diameter, using ethylene as a fuel and orifice diameters of 76, 100 and 120 mm.

The experiments of Bezmelnitsin et al. sought to duplicate Carnasciali's experiments, and then relate them to initiation in unconfined mixtures. To do this, the driver vessel was attached to a polyethylene bag 1.5 m in diameter by 3.5 m long. The bag was hung vertically to avoid any surface reflections from ground contact. As they expected, confinement played a strong role in detonation initiation. Unfortunately, a table in Carnasciali et al. (1991) contained a typo, stating that the optimum driver β was 7.6, instead of the 2.6 quoted in the body of the text. J. Shepherd discovered the typo after we were unable to rupture our mylar diaphragm with the $\beta = 7.6$ mixture. Bezmelnitsin had occasional diaphragm rupture problems (with copper diaphragms), but was able to complete the tests. They found a maximum dilution of $\beta = 2.1$ for detonation in confinement, and $\beta = 1.5$ for the unconfined case. They were able to show that confinement plays a strong role in the initiation of detonation. However, the effect of their weak driver mixture is unclear. From pressure traces, they determined that initiation was due to interaction of the jet's bow shock with the vessel wall, thus relying on confinement. In the HYJET facility, photographic evidence shows the detonation propagating directly from the jet, initiating within 100–150 mm of the jet exit. Furthermore, the receiver vessel diameter is larger in HYJET, requiring a longer time for the rupture shock to reflect and return to the jet region.

The present experiments first duplicated the mixtures of Carnasciali and Bezmelnitsin, to compare the effect of HYJET's geometry to the other facilities. With nitrogen dilution as a reference, the experimental series was then expanded to include N₂ and H₂O dilution at 373 K. In addition, nozzle sizes of 25, 38 and 64-mm were used to study the effect of jet diameter. The PCB transducer configuration is shown in Figure 6.2. The early tests with nitrogen (runs 312 through 318) used only the E and T3 transducers, as in the NITRO series. For the remainder of the tests, two more transducers were installed at the T1 and T2 stations. The four transducers are spaced at 0.51 m intervals.



Figure 6.1: Sample driver pressure trace (25-mm nozzle), from Kulite (slow) transducer. Run 406.

The variety of phenomena observed in this series requires use of terminology similar to that in the NITRO series. A "prompt" initiation is one in which a detonation is initiated in the region of the nozzle exit. A DDT occurs when there is evidence of a slow pressure rise followed by detonation-like waves, or when shock waves traveling down the vessel build into a detonation. A "secondary" explosion occurs shortly after the primary wave train has passed. These are typically found in the end of the vessel, where focusing occurs, but have been seen elsewhere. A related phenomena is a "late" explosion, which occurs some time after the lead waves have passed, and is usually localized to a single transducer. Finally, any weaker combustion event will be termed a deflagration. A deflagration will show no significant wave action on the PCB transducers. The Kulite transducer was used to record deflagration pressure rises, but the data are not presented here. Two Kulites were destroyed during tests with H_2O ; after the second one was destroyed, it was not replaced. In jet initiation terminology, only a prompt initiation is considered a "GO." All other cases are "NO-GOs." The broader terminology is used here as a reminder that significant events can occur, even when a detonation is not initiated.



Figure 6.2: Locations of PCB transducers in beta dilution test series.

Table 6.2: Mixture compositions for representative values of β in the system $H_2 + 0.5(O_2 + \beta X)$.

β	%X	$\%O_2$	$\%\mathrm{H}_{2}$	β	%X	$\%O_2$	$\%\mathrm{H}_2$
1.0	25.0	25.0	50.0	3.6	54.5	15.2	30.3
1.2	28.6	23.8	47.6	3.8	55.9	14.7	29.4
1.4	31.8	22.7	45.5	4.0	57.1	14.3	28.6
1.6	34.8	21.7	43.5	4.2	58.3	13.9	27.8
1.8	37.5	20.8	41.7	4.4	59.5	13.5	27.0
2.0	40.0	20.0	40.0	4.6	60.5	13.2	26.3
2.2	42.3	19.2	38.5	4.8	61.5	12.8	25.6
2.4	44.4	18.5	37.0	5.0	62.5	12.5	25.0
2.6	46.4	17.9	35.7	5.2	63.4	12.3	24.7
2.8	48.3	17.2	34.5	5.4	64.3	11.9	23.8
3.0	50.0	16.7	33.3	5.6	65.1	11.6	23.3
3.2	51.6	16.1	32.3	5.8	65.9	11.4	22.7
3.4	53.1	15.6	31.3	6.0	66.7	11.1	22.2

6.2 **Results and Discussion**

6.2.1 Driver Conditions

With driver pressures of 14 bar indicated by the Kulite transducer, a PCB was installed in the driver to record shock wave data, as in the NITRO series. The receiver was filled with air, and the driver was vented through the 25 and 92-mm nozzles. The pressure traces are shown in Figure 6.3. As the transducer is at the ignition end of the vessel, it can not directly detect events near the nozzle. We can only see reflected shocks that result from local explosions or detonation there. With the 92-mm nozzle, we see a peak pressure well below that for a reflected detonation. The 25-mm trace shows a much higher peak, which is likely the result of a detonation reflecting off of the nozzle adapter. Thus, local explosions appear with the increased confinement of the smaller nozzles. We will still do the detonation transmission analysis for all cases.



Figure 6.3: PCB traces from driver venting into air. Transducer located on instrumentation flange, adjacent to spark plug.

The procedure for generating a shock Hugoniot and matching the reflected detonation was given in the NITRO analysis (page 46), and will not be repeated here. In the BETA series, we have one driver mixture, and a number of receiver mixtures. The resulting Hugoniots are plotted in Figure 6.4. The intersection of the Hugoniots for the receiver and the reflected driver wave indicates both the pressure/velocity jump across the shock in the receiver, and the nature of the reflected wave in the driver. In the BETA tests, all of the receiver mixtures result in a reflected expansion in the driver. With the shock conditions for the receiver determined, we can again calculate the shock temperatures and induction times. The results are tabulated in Table 6.3.

From Table 6.3, we see that none of the receiver mixtures are subject to direct initiation. The 373 K N_2 -dilution mixture has the shortest induction time, at 0.27 ms. In this

Diluent	T_R, \mathbf{K}	β	M_{CJ}	M_S	P_S , bar	T_S, \mathbf{K}	t_{IND} , ms
N ₂	298	4.3	4.90	3.62	14.7	971	11.8
N_2	298	3.0	5.05	3.58	14.4	958	15.0
N ₂	298	2.6	5.10	3.56	14.2	951	17.2
N_2	373	5.2	4.17	3.38	13.5	1130	0.27
H_2O	373	1.1	4.45	3.10	11.3	972	13.1
H ₂ O	373	0.55	4.56	3.06	11.0	973	10.9

Table 6.3: Results of analysis on transmitted shock in receiver, initiated by detonation in driver.

time, the shock will move 0.4 m, so there is no chance of shock-reaction coupling. All of the other induction times are on the order of 20 ms, which is enough time for the receiver to deflagrate from jet ignition before spontaneous explosion would occur. So, while our driver does not directly initiate detonation, it does provide a stronger impulse than the Carnasciali (constant-volume combustion) driver. Previous research (Inada et al. 1992) has further indicated that interaction of a detonation with a diaphragm will destroy the cellular structure. The volume of the HYJET driver is 30% larger than the others, and has a total energy equivalent of approximately 9 g Tetryl. This energy is not released instantaneously, but over 1 ms or so. The HYJET driver also has a much larger aspect ratio (length divided by diameter) than the others (18 vs. 3). This increases the acoustic resonance time and the "piston" effect of work done on the receiver gas. In the future, we will minimize the potential for transition by moving the spark plug to the midpoint of the driver (Üngüt and Shuff 1989) or by adding more spark plugs, distributed throughout the driver.



b: Receiver at 373 K

Figure 6.4: Shock Hugoniots for BETA receiver mixtures, with reflected driver wave Hugoniot. Upper plot is for mixtures at 298 K, lower plot for mixtures at 373 K. For reflected wave Hugoniot, solid line indicates reflected shock; dashed line indicates reflected expansion.

	Maximum β for detonation				
Receiver	Carnasciali	Bezmelnitsin	Krok		
$N_2, 298 K$	2.6	2.1	4.3		
$N_2, 373 \ K$			5.2		
$H_2O, 373 K$			1.0		

Table 6.4: Comparison of detonation initiation results.

6.2.2 Critical Dilutions

In the HYJET experiments, β_{CRIT} was determined to a resolution of 0.1, with the exception of the steam runs. At higher values of β (above, say, 3.76, the value for air), this means a difference of only one half of one percent in diluent, and less in the reactants. This approaches the accuracy of the pressure gauges used to fill the vessels, resulting in a "fuzzy" (i.e., uncertain) determination of β_{CRIT} in some cases. For example, in the series of shots with N₂ at 298 K, one run with $\beta=4.4$ was a prompt initiation, but subsequent runs were not. The reverse occurred with nitrogen at 373 K, where one of the runs with $\beta=5.2$ failed to initiate, when the others were prompt.

Note that the initial temperatures of 298 K and 373 K are "nominal;" they represent the average/typical receiver temperature of the series. In the tests at 298 K, the true initial temperatures ranged from 294 to 304 K. In the N₂-dilution tests at 373 K, the temperature range was from 372 to 378 K. In the H₂O tests at 373 K, the temperature range was from 374 to 378 K. The initial conditions for each run are listed in Appendix D. The digital thermometers used to measure temperature have an accuracy of ± 0.5 K.

After the β_{CRIT} tests were completed, a few tests were done without a diaphragm separating the two chambers, using the 92 and 25-mm nozzles. These runs were done as a link to the work by Knystautas et al. (1979). The plumbing system was rerouted to allow circulation between the two vessels.

The results with the 92-mm nozzle are summarized in Table 6.4, to provide a quick comparison with the other facilities. The BETA tests in the HYJET facility found considerably higher values of β_{CRIT} than the previous studies. This will be examined in more detail below.

In jet initiation experiments, results are typically presented as the ratio of jet diameter to detonation cell size in the receiver mixture, or D/λ . In the present experiments, the detonation only takes place in the receiver mixture. Since the driver composition is not reflected in λ , the D/λ criterion may not be applicable here. Carnasciali did a brief study of the effects of driver composition. For a driver with $\beta=2.6$, they obtained receiver initiation at $D/\lambda\approx11.7$ ($\beta_{CRIT}=2.6$). For a driver with $\beta=0.4$, they found $D/\lambda\approx59$ ($\beta_{CRIT}=0.4$). (The critical receiver dilutions for H₂ matched the driver dilutions. This was not true for other fuels.) A smaller effect of driver composition was seen in the H₂-air system in the NITRO series, as well as in the work of Dorofeev et al. (1993).

Regardless, D/λ will be presented here for completeness and comparison to other work. Cell sizes are thus needed for the values of β_{CRIT} found for each nozzle and dilu-



Figure 6.5: ZND estimation of cell sizes for N₂ dilution at 298 K (A=70). Data points are from Knystautas et al. (1982) and Bull et al. (1982).

ent. The cell sizes can be estimated from computed reaction zone lengths, as described in Chapter 1. For the BETA mixtures, Δ was calculated for each β_{CRIT} using the program "ZND" (Shepherd 1986). Typically, the correlation is $\lambda = A\Delta$, where A is assumed constant for a given system and determined by comparison to experimental data. Data for stoichiometric H₂-O₂ with N₂-dilution is available from Knystautas et al. (1982) and Bull et al. (1982), and is plotted in Figure 6.5 against the ZND computation for A=70. No previous studies have been done on the H₂-O₂-H₂O system, but data for H₂-air-H₂O is available from Stamps et al. (1991) and Ciccarelli et al. (1994). The effect of the N₂ is unclear, but the data is plotted in Figure 6.6 against the ZND curve for A=30.

We see from Figures 6.5 and 6.6 that a constant A does not accurately reflect the measured values of λ , particularly at high and low values of β (Figure 6.5) and low steam concentrations (Figure 6.6). To overcome this, and better adapt the steam data to mixtures without nitrogen, a different correlation can be used. Recently, Shepherd and Kaneshige (unpublished) have found that a power-law correlation can be used to account for the change in A. In Figure 6.7, the data from the previous figures are plotted as $\log \lambda$ versus $\log \Delta$. The data can be correlated by the relation $\lambda=39\Delta^{0.68}$ (fitted by least squares). Unfortunately, this relation is not dimensionally meaningful, but this form has proven useful in several fuel-oxidizer systems. The data show increased scatter for some of the Knystautas N₂ data; this is considered acceptable, as cell irregularities can lead to measurement uncertainties. The power-law correlation was used to calculate the required values of λ .

The results are listed in Table 6.5, and plotted in Figure 6.8. With the exception of one case, the values fall roughly within the range $2 < D/\lambda < 7$, well below the previously quoted value of 13. The exception is the 92-mm nozzle with N₂ and no diaphragm



Figure 6.6: ZND estimation of cell sizes for stoichiometric H_2 in air with steam dilution at 373 K (A=30). Data points are from Stamps et al. (1991) and Ciccarelli et al. (1994).

 $(D/\lambda=10.7)$. The tests with no diaphragm are not directly comparable to the other tests, though.

In the similar work by Knystautas et al. (1979), D/λ was not computed for the mixtures, as the geometry of the orifice between the vessels was the main factor. (Degree of turbulence was also found to be important by MacKay et al. (1988) and Moen et al. (1989).) Knystautas proposed that the minimum size of the large eddies must be at least of the order of the detonation kernel, or λ , for initiation to occur. This means that, with the right exit conditions, initiation could be seen in mixtures with $D/\lambda \rightarrow 1$. Carnasciali et al. (1991) suggested that minimum kernel size could be defined by the critical tube diameter, $d_c \approx 13\lambda$, but the BETA results indicate that a smaller kernel is possible. Again, we see that the D/λ criterion is not well-suited to jet initiation experiments, even when the same mixture is used in both vessels.

As shown in Figure 6.9, the results correlate much better when plotted as β_{CRIT} vs. nozzle area. First, we see that the points for nitrogen dilution at 298 K fall on a regular trend. With the two largest nozzles, the curve seems to be approaching an asymptote, which represents a physical limitation of the driver. Perhaps increasing the driver volume (length or diameter) would shift the asymptote upward. The size of the receiver vessel may also play a role in these experiments. While larger jets can initiate more dilute mixtures, these mixtures have longer induction times, leading to delayed initiation. A strong jet, entraining reactants, may reach the end of the vessel before initiation can occur. As nozzle size decreases, the curve must have a very sharp drop-off, as a nozzle with zero area can not initiate combustion. Thus, it would be possible to find a nozzle area for which even straight H₂-O₂ could not be promptly initiated. Unfortunately, lack of time prevented using the 12.7 and 6.4-mm nozzles in the HYJET tests. Instead of



Figure 6.7: Plot of $\log \lambda$ vs. $\log \Delta$, with power law correlation.

using D/λ , perhaps it would be better to model the driver as an initiation energy (which scales with λ^3). The problem is to determine the key parameters. Figure 6.9 indicates that D^2 would be useful. Other possibilities would be the peak pressure, P_P , and energy density of the driver mixture. For exit geometries other than a circular nozzle, a factor would be needed to reflect turbulence generation, as shown by Knystautas et al. (1979).

A critical energy approach was taken by Üngüt and Shuff (1989) in their experiments on jet-initiated DDT. As their experiments used a uniform mixture in both vessels, they found that D/λ still represented the normalized energy release of the jet. They also used the Damköhler number, τ , defined in this case as the ratio of vortex entrainment time to reaction induction time. If τ is large, the reaction will go to completion before the entrainment process is complete (and initiate a deflagration). The results indicated that D/λ must be greater than 5 for initiation to occur, and that if τ was above a critical value, initiation would not occur for any D/λ . Üngüt and Shuff related this to a minimum jet velocity requirement. Urtiew and Tarver (1979) studied the transmission of a detonation from a tube to a hemisphere and modeled the process in terms of work done by the driver on the receiver gas. In the future, we will examine and combine ideas from both analyses to generate a model for our case, where different mixtures are used in the vessels.

The work of Knystautas et al. (1979) showed that obstructions in the jet enhance turbulence and can aid in transition. To see if increased turbulence would affect the HYJET results, β_{CRIT} was determined for the 25-mm nozzle with the diaphragm cutter installed. As shown in the plot, this raised β_{CRIT} by a small but significant amount. I expected that the cutter would develop only small-scale turbulence, as it is upstream of the nozzle exit, and the four quadrants of the jet can easily recombine. However, the results of Knystautas et al. (1979) (discussed in Chapter 5) found that addition of smallscale turbulence would not help a particular orifice initiate a detonation when it could

D, mm	Diluent	T	β_{CRIT}	ZND Δ , mm	D/λ
92	N_2	$298 \mathrm{~K}$	4.3	0.222	6.6
64	N_2	$298 \mathrm{K}$	4.2	0.213	4.7
38	N_2	$298 \mathrm{K}$	3.0	0.133	3.8
25	N_2	$298 \mathrm{K}$	2.6	0.114	2.8
$25, \mathrm{w/c}$	N_2	$298 \mathrm{K}$	2.9	0.128	2.6
92, ND	N_2	$298 \mathrm{K}$	3.3	0.149	10.7
25, w/c, ND	N_2	$298 \mathrm{K}$	1.8	0.088	3.3
92	N_2	$373 \mathrm{K}$	5.2	0.293	5.4
92	H_2O	$373~{ m K}$	1.1	0.479	3.9
38	H_2O	$373~{ m K}$	0.55	0.114	4.3

Table 6.5: Summary of D/λ results. (w/c, with cutter; ND, no diaphragm.)

not before. The diaphragm cutter must be adding some amount of large-scale turbulence.

Other comparisons can be made from Figure 6.9. One set of runs was done with nitrogen dilution at 373 K and the 92-mm nozzle to provide a link between the nitrogen and steam runs. Higher temperatures increase a mixture's sensitivity to detonation, and we see from the figure that β_{CRIT} follows this trend. We also see the effectiveness of steam as a detonation supressant. The points for steam dilution lie well below those for nitrogen. Below $\beta=1$, the resolution of the tests was increased to 0.05 to keep the change in diluent near 1%. In a few of the tests, the vessel was overfilled with steam because of condensation problems in the supply. This resulted in an initial pressure error of +3% or so, but β was recalculated so it would be correct. The excess of vapor in these tests placed them outside of the area of β_{CRIT} , so they did not affect the limit determinations.

In the tests with no diaphragm, the mixture had to be much more sensitive for prompt initiation to occur. Without a diaphragm, the driver continuously vents reactants ahead of the flame front, lowering the peak pressure. The resulting flow field in the receiver may reduce the strength of the jet head vortex when the flame front reaches the nozzle and products are vented. High-speed photography (discussed below) of detonation initiation with the 25-mm nozzle showed no evidence of pre-flow leading the jet into the receiver, so these mixtures had probably detonated before reaching the nozzle. However, β_{CRIT} for this system gives $D/\lambda=3.3$. Critical tube diameter experiments have shown a fairly reliable correlation of $d_C=13\lambda$, so there is virtually no chance of detonation transmission through this nozzle. With the 92-mm nozzle, $\beta_{CRIT}=3.3$, with $D/\lambda=10.7$. This is much closer to d_C , but in this case the nozzle diameter is nearly the diameter of the driver, so only a small surface is available for shock reflection. While flame acceleration will still occur, transition to detonation in the driver is unlikely. These tests were only done to a resolution of $\beta=0.25$ or so, to roughly characterize the results with respect to the other tests.



Figure 6.8: Plot of initiation results as D/λ .



Figure 6.9: Summary of critical beta values.

6.2.3 Sample Pressure Traces

Pressure traces from selected runs are shown in Figures 6.11 through 6.21, representing borderline values of β . (Pressure traces from all BETA runs are shown in Appendix C.) Typical examples are shown of prompt initiation, secondary and late explosions, and deflagration. Examples are given of both the 92 and 25-mm nozzles, to show the weaker shocks of the small nozzles in deflagrations. These shocks decay by the end of the vessel.

Interestingly, the tests with nitrogen showed no DDTs, although there were some secondary and late explosions. This result led me to reassess the NITRO experiments. In the NITRO tests, I originally thought that the detonations we saw at the end of the vessel were the result of DDT, because of our low D/λ in those tests (see Chapter 5). The additional instrumentation in the BETA tests showed that all of the mixtures with N₂-dilution are either promptly initiated or do not detonate. Thus, I concluded that the detonations in the NITRO tests were the result of prompt initiation. (The receiver mixtures in the NITRO series are very close to the BETA mixtures with $\beta=3.76$.) DDT was seen in the tests without diaphragms, although these are not directly comparable. The DDTs may result from the pre-existing, turbulent flow field generated by driver venting, before the flame reached the nozzle.

In contrast, the water vapor tests had a region of DDTs between deflagration (β =2.0) and prompt detonation (β =1.1). The presence of water vapor reduces the flame speed (Liu et al. 1980; Liu and MacFarlane 1983). This may allow shock reflection and focusing to occur before all of the reactants are consumed. With only nitrogen, the flame burns fast enough to consume the reactants before the onset of DDT.

In some cases, noise is evident on one or more of the transducers. The PCB transducers use Microdot connectors, which are prone to loosening under vibration. Since the transducers run on constant current, a break in the circuit results in a (theoretically) infinite voltage from the power supply, causing a spike in the data. Attempts were made to minimize this, but the problem can only be resolved by removing the transducers from their mounts and tightening the connections. This required a tool that was not always available. Fortunately, the lead wave is always clean, and the noise only occurs after a strong wave passes.

In the early runs, the T-station transducers were mounted in pipe plugs that thread into fittings along the top of the vessel. I did not realize that this left a long cavity between the transducer and the vessel, about 25 mm in diameter and 50 mm deep. For runs 354 and on, new mounts were installed that brought the transducers to the inner surface of the receiver. Fortunately, the results indicate that the antechamber had little effect on the pressure traces, other than adding some noise from shock reflections. This is shown in Figure 6.10, with recessed transducers in run 353, and flush-mounted units in run 356.

Figures 6.11 through 6.13 represent runs with nitrogen dilution at 298 K. Figure 6.11, β =4.3, is a typical rendition of prompt initiation in this facility. No shock waves appear before the detonation. The small amount of noise immediately preceding the detonation, particularly on T3, is believed to be stress waves traveling through the vessel. This has also been seen in the GALCIT 11-inch Detonation Tube. Immediately behind the

reflected detonation on the E transducer, there is a three-pronged peak as strong as the detonation (this form is seen often). I believe this is the result of focusing at the end of the vessel, as described in Chapter 5. In this case, the second peak follows the detonation by 0.28 ms, which agrees with the 0.3 ms characteristic time of the focusing process. The traces show a pressure pulse traveling back up the vessel from this explosion. Reflected detonations have recently been studied by Shepherd et al. (1991). When a detonation undergoes normal reflection, the pressure is approximately $2.5P_{CJ}$. For the BETA mixtures, $M_{CJ} \approx 5$. By comparison, a M=5 shock in air has a reflected pressure of nearly seven times its incident pressure. The complex geometry of HYJET will yield different reflection traces than those from a simple tube, but the basic pattern is the same. Figure 6.12, $\beta = 4.4$, shows a failure to initiate. The deflagration process is much slower than the leading waves, so it does not appear on these traces. There is a significant secondary explosion on T2, near 13.6 ms. The cause of this is unknown, although it is occasionally seen in other runs. It is highly localized; the only corroboration is provided by the shock oscillations on T1. Figure 6.13 shows the same mixture with a secondary explosion at the end of the vessel. This appears to be a DDT, as there are waves building behind the lead shock as it moves down the tank, but the peak pressure delay corresponds to shock focusing.

Figures 6.14 and 6.15 represent runs using the 25-mm nozzle (with cutter) with nitrogen dilution at 298 K. Figure 6.14 is a prompt initiation, similar to that with the 92-mm nozzle. The wave traveling shortly behind the detonation on T1 appears on many prompt initiations. I believe that this may result from detonation of material behind the nozzle exit, and reflection off the upstream head of the vessel. Figure 6.15 is a deflagration with no explosive phenomena. Note that the lead shock is much smaller, and decays to a continuous compression by the end of the vessel.

Figures 6.16 through 6.19 are from runs using H₂O dilution at 373 K, with the 92mm nozzle. Figure 6.16 is a prompt initiation, with the same structure as the previous examples. Figure 6.17 is the next increment of dilution, $\beta=1.2$. This shows a small shock running down the vessel, with a closely coupled secondary explosion at the end. This appears to act too quickly for shock focusing to occur. A wave then runs back up the vessel. This is probably a detonation, as there would not have been enough time for a deflagration to consume the reactants. Also, the peak pressure and sharpness of the wave are consistent with prompt detonations. Figure 6.18 is for $\beta=1.6$, and shows a "running" transition to detonation. As the lead shock moves down the vessel, a stronger wave builds immediately behind it, and the wave reflects off the end of the vessel as a detonation. This sends another wave back up the vessel. Finally, Figure 6.19 shows initiation of deflagration, with a moderate explosion in the reflection, and a localized late explosion on T1.

Figures 6.20 and 6.21 are from one of the runs with the 25-mm nozzle and no diaphragm, allowing a flow field to be set up before combustion reaches the receiver. This is a classic DDT. Figure 6.20 shows the complete set of traces, while 6.21 is a closeup of the T3 trace, showing the pre-pressurization. We see that the initial wave reaches T3 at 8.5 ms, and gradual pressurization occurs from venting and deflagration. About 4.5 ms after the initial wave, an explosion occurs near T3. This explosion travels both up and down the vessel as a detonation. This wave is fairly weak at the upper end of the tank (T1 and T2), as some of the reactants have already been consumed in the deflagration.



Figure 6.10: Comparison of recessed (run 353) and flush-mount (run 356) transducer signals.



Figure 6.11: Prompt initiation with 92-mm nozzle, N₂ at 298 K, β =4.3. Note upstream propagation of reflection. Run 338.



Figure 6.12: Failure to initiate detonation with 92-mm nozzle, N₂ at 298 K, β =4.4. Note late explosion on T2. Run 337.



Figure 6.13: Failure to initiate detonation with 92-mm nozzle, N₂ at 298 K, β =4.4. Secondary explosion on E presumed to be in focal region. Run 339.



Figure 6.14: Prompt initiation with N₂ at 298 K, β =2.9, using 25-mm nozzle with cutter. Run 369.



Figure 6.15: Failure to initiate detonation with 25-mm nozzle (with cutter), N₂ at 298 K, β =3.0. Run 368.



Figure 6.16: Prompt initiation with H₂O at 373 K, β =1.1. Run 380.



Figure 6.17: DDT at end of vessel, with H₂O at 373 K, β =1.2. Run 382.



Figure 6.18: Running buildup to DDT, with H₂O at 373 K, β =1.6. Run 351.



Figure 6.19: Failure to initiate detonation, with H₂O at 373 K, β =2.0. Run 348.



Figure 6.20: DDT near T3, 25-mm nozzle with no diaphragm, with N₂ at 298 K, β =1.8. Run 409.



Figure 6.21: Pressure trace from T3 in previous plot, enlarged to show pre-pressurization before detonation.

6.2.4 Lead Wave Pressures

Figures 6.22 through 6.36 are a study of the lead wave pressures at each transducer. Reference pressures on each plot (shock wave, CJ detonation, and reflected detonation) were calculated with STANJAN. The choice of M=1.33 as a shock Mach number is based on two runs (numbers 319 and 320) with an air-filled receiver. The standard ($\beta=2.6$) driver mixture was used with the 92-mm nozzle, and the amplifier gains were turned up to minimize noise. The tests showed the lead shock moving at 450 m/s between T2 and T3, with a pressure of 1.8 bar. STANJAN gave the sound speed of the air as 388 m/s, and the pressure from a M=1.33 shock to be 1.82 bar. Although this is only used as a reference in the graphs, it gives good agreement in most of the tests with no prompt initiation. The 92-mm nozzle gives slightly higher pressures when there is hydrogen in the gas mixture.

In all prompt initiation cases, we see a pressure at T1 that is near the reflected CJ pressure. As the wave proceeds down the vessel, the pressure decreases at T2 and T3, but is still above the static CJ pressure. At transducer E, the pressure is again near the reflected CJ value, as expected. The T_i pressures can be explained by Figures 6.24–6.26, which model the detonation growth. In the case of an unconfined spherical detonation, the wave locally becomes flatter as the radius of curvature increases. The initial process in the vessel is similar, with the addition of reflections from the vessel walls. The reflections will not interfere with the detonation as it propagates, but determine the pressure measured at the wall.

In Figure 6.24, the detonation is initiated a short distance from the nozzle exit. It is unlikely that the detonation could be initiated immediately at the exit, as the reactants are being pushed downstream by the jet and time is needed for entrainment and ignition. Using the spherical initiation model, the wave flattens as it proceeds down the vessel. As the wave flattens, the angle between the wave and the wall (θ in Figure 6.25) changes from zero (normal reflection above point of initiation) to the limit of 90° (planar detonation). The change in θ leads to a change in the reflection mode and wall pressure. The two modes of reflection are regular and Mach reflection, and are shown in Figure 6.25. The associated wall pressures are shown in Figure 6.26. The pressures in Figure 6.26 were calculated by Raza Akbar of GALCIT (work in progress) from two- and three-shock theory with heat release. The data presented is not for the BETA mixtures, but illustrates the typical variation of pressure expected for reflected detonations (see also Nettleton (1987)). For $\theta = 0$, normal reflection occurs, and the pressure is approximately 2.5 P_{CJ} . When the detonation is planar, $\theta = 90^{\circ}$ and there is no reflected wave, yielding a wall pressure of P_{CJ} . A cusp occurs in the region of Mach wave formation. Pressure data from the BETA experiments follows this trend. A similar effect is seen in blast waves generated by explosives detonated above the ground (Glasstone and Dolan 1977).

The 92-mm nozzle (Figures 6.22 and 6.23) tends to give high pressures (reflected detonation) at nearly every transducer in a prompt initiation, with the exception of the runs with no diaphragm. Note that some of these traces were clipped by the acquisition system, so the true peak pressures may be higher. This may indicate that the large nozzle is able to initiate a detonation further into the vessel than the other nozzles. A

second possible reason for these high pressures is the combination of driver mass flow and receiver induction time. The 92-mm nozzle was able to initiate detonation in the least sensitive mixtures, but as a consequence, the induction time (for the receiver mixtures) was the highest. The detonation will be initiated further into the vessel, as the reactants are being driven downstream by the jet flow. In comparison, the T2 and T3 pressures were lower for the tests with $\beta=2.6$. This mixture is considerably more sensitive than the other mixtures used ($\beta \geq 3.76$), and the reduced induction time may allow initiation to occur before the reactants are driven far downstream by the jet flow.

Figures 6.27 and 6.28 show the detonation growth for the 64 and 38-mm nozzles. The same trend occurs here as for the 92-mm nozzle, but the results are more pronounced. The pressures at T1 are at or above the reflected CJ value, so the detonation is initiated near that axial location. The pressures drop progressively at T2 and T3, indicating flattening of the wave, and again jump to the reflected CJ value as they reflect off the end of the vessel.

Figures 6.29 and 6.30 show the peak pressures from the 25-mm nozzle, both with and without the diaphragm cutter. The pressures at T1 fall further below the reflected CJ line than those for the larger nozzles, indicating that the detonation is initiated closer to the nozzle. The 25-mm nozzle will have a lower mass flowrate than the other nozzles, so the reactants will not be convected as far downstream before initiation as with the other nozzles. In addition, the mixtures are more sensitive, so the induction time is reduced, bringing initiation closer to the jet exit. The photographic tests support this, showing that detonation was initiated within 100–200 mm of the nozzle exit. The peak pressures follow the decreasing trend at T2 and T3. At the end of the vessel, the pressures approach the reflected CJ value but fall short; the larger nozzles typically met or exceeded this value. The data for the 25-mm nozzle is particularly well clustered; perhaps the increased sensitivity of this mixture provides more repeatable initiation (i.e., initiation across most of the jet head vs. local initiation at the edge of one of the larger jets).

The tests with no diaphragm (and a uniform mixture in both vessels) are represented in Figures 6.31 and 6.32. The 92-mm nozzle gives high pressures at T1, typical of the other cases. The pressures at T2 and T3 follow the usual trend. In the tests using the 92-mm nozzle with diaphragm, the points were often near the reflected CJ line at all three T transducers. The mixtures used in the no-diaphragm tests were more sensitive, however, and the reduced induction time may allow initiation closer to the nozzle exit, as mentioned previously. This is most evident with the 25-mm nozzle, for which the T1 pressures fall far below the reflected CJ pressure. These were the most sensitive mixtures used in the BETA series, and have the shortest induction times.

The lead wave pressures for the N₂-dilution tests at 373 K are shown in Figures 6.33 and 6.34. These tests used the 92-mm nozzle only, and the results are similar to those for the 92-mm tests at 298 K (Figures 6.22 and 6.23). The pressures at the T-transducers are all high near β_{CRIT} , but the T2 and T3 pressures drop as β is decreased. The induction time reasoning applied to the other cases can be used here as well.



Figure 6.22: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with 92-mm nozzle. Three points on T1 plot at 36 bar are at the maximum transducer level; true values will be somewhat higher.



Figure 6.23: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with 92-mm nozzle, continued.



Figure 6.24: Model of detonation growth as sphere. Wave flattens as detonation proceeds down vessel, and angle between detonation and wall approaches 90° .



Figure 6.25: Schematics of Mach and regular reflection. If θ is small enough, regular (two-shock) reflection occurs. For θ larger than about 60° (Figure 6.26), a Mach wave is generated to match the flow behind the detonation to the boundary.


Figure 6.26: Calculated values of wall pressure using two- and three-shock theory with energy release.



Figure 6.27: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with 64- and 38-mm nozzles. Solid points are for 64-mm nozzle, open points for 38-mm.



Figure 6.28: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with 64- and 38-mm nozzles, continued. Solid points are for 64-mm nozzle, open points for 38-mm.



Figure 6.29: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with 25-mm nozzle. Solid points are for nozzle with diaphragm cutter.



Figure 6.30: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with 25-mm nozzle, continued. Solid points are for nozzle with diaphragm cutter.



Figure 6.31: Lead wave pressures for nitrogen-diluted mixtures at 298 K, with no diaphragm. Mixture is same in both vessels. Solid points are for 92-mm nozzle, open points for 25-mm nozzle with diaphragm cutter.



Figure 6.32: Lead wave pressures for nitrogen-diluted mixtures at 298 K, no diaphragm, continued.



Figure 6.33: Lead wave pressures for nitrogen-diluted mixtures at 373 K, 92-mm nozzle.



Figure 6.34: Lead wave pressures for nitrogen-diluted mixtures at 373 K, continued.

Figures 6.35 and 6.36 show the process of DDT in the H₂O dilution cases. As β is decreased, the lead wave pressures begin to rise, especially on T3. They finally take a large jump at the transition point. The pressures at the E transducer are especially high in the DDT region. This is to be expected. As β is decreased, the mixture becomes more sensitive, but not enough for prompt initiation. When β is slightly above β_{CRIT} , the mixture is most susceptible to transition. This results in the highest pressures (up to 80 bar in this set of tests), because the mixture is shocked before the transition. Once the prompt limit is reached, the pressures are relaxed, because the detonation is proceeding into unshocked reactants.

Shepherd (1992) studied combustion-generated loading in H₂-air-H₂O mixtures, and found similar results. Severe loadings occurred when slow-burning, lean or dilute mixtures burned almost to completion before transitioning to detonation. The combustion compresses the unburned mixture, leading to hot spots and localized explosions that can coalesce and detonate the remaining reactants. This is analogous to knock in an internal combustion engine. Estimated pressures from this condition reach 165 bar. The worst DDT case occurs under unique conditions, when a detonation forms in shocked reactants very close to a confining surface. If the precursor shock reflects just before the detonation overtakes it, the surface will receive an impulse from both waves (i.e., shock piling). Reflected pressures in this regime were predicted to be in the range of 300–600 bar. However, the conditions and timing required for this scenario are highly improbable.

Combustion modeling by Breitung (1993) predicted peak DDT pressures of over 100 bar in realistic mixtures and conditions. Boyack et al. (1992) determined that detonation focusing by edges and corners created pressures higher than that for normal detonation reflection. Reflected pressures can also be increased if a layer of inert gas lies between the detonation and the surface.



Figure 6.35: Lead wave pressures for steam-diluted mixtures at 373 K. Solid points are for 92-mm nozzle, open points for 38-mm nozzle.



Figure 6.36: Lead wave pressures for steam-diluted mixtures at 373 K, continued.

6.2.5 Lead Wave Velocities

The final study is into the lead wave velocities. The wave arrival times were recorded at each transducer, and the wave speed was calculated between transducers T2 and T3. Between T1 and T2, wave curvature and the startup process will introduce timing differences over and above those due to acceleration or decay. Transducers T3 and E are at different radial locations, so the shape of the wave would affect the apparent velocity. This effect will be used to estimate wave curvature.

The lead wave velocity, V_{2-3} , is shown in Figures 6.37 through 6.39. Transition is clear in the N₂-dilution plots; the points either lie near the shock line, or above the CJ line. The excess velocity of the detonations may be due to overdrive, or may be the result of wave obliquity at the edges of the vessel (Figure 6.24). In the H₂O case (Figure 6.39), the evolution of the lead wave from shock, through DDT to detonation, is evident from $\beta=3$ to β_{CRIT} . When detonation occurs, we see that the velocity is a bit higher than the CJ value, for the reasons cited above.



Figure 6.37: Leading wave speed measured between transducers T2 and T3, for N₂diluted mixtures at 298 K. Diamonds, 92-mm nozzle; squares, 64-mm; circles, 38-mm; triangles, 25-mm; open triangles, 25-mm w/c.

The velocity between the T3 and E transducers can not be measured accurately, because the transducers are at different radial locations, and the wave is bowed. The center of the wave arrives before the edges, and the velocity between T3 and E will appear to be higher. We can, however, measure the amount of lead that the center of the wave has over the edges. Figure 6.40 shows a simplified schematic of the wave, relative to the transducers. If we assume that the wave velocity is constant at V_{2-3} , the lead, L, is equal to the distance between the transducers minus the "apparent" distance traveled. In short, $L=0.51 - V_{2-3}(t_E - t_{T3})$, where t_i is the arrival time at transducer *i*. The leads



Figure 6.38: Leading wave speed measured between transducers T2 and T3, for N_2 -diluted mixtures at 373 K (92-mm nozzle).

calculated from the detonation arrival times varied from 1 to 12 cm, with a few negative values. The negative values indicate that the wave was decelerating between the T3 and E transducers. As shown in Figure 6.37, the detonations are still overdriven at station T3, so deceleration is expected. The lead calculation is only a rough estimate. For comparison, we can look at the ray trace simulation of Chapter 5. In the simulation, the initial wave (Figure 5.16, page 57) had a radius of curvature of 1.72 m. The horizontal distance from the wave origin to the edge of the wave was 1.66 m. This results in a lead of 6 cm, so at least the magnitude is comparable. On the final run of the BETA series, the sting from the shock focusing study (Chapter 5) was installed in the end flange and aligned with T3. A detonation was initiated with the 92-mm nozzle in a mixture of $\beta=2.6$ (N₂), and the lead was calculated. The velocity was measured at 2320 m/s. The arrival time difference was 0.04 ms, giving a lead of 9.3 cm. This is considered to be the "correct" measurement.



Figure 6.39: Leading wave speed measured between transducers T2 and T3, for H_2O diluted mixtures at 373 K. Solid points, 92-mm nozzle; open points, 38-mm.



Figure 6.40: Simplified schematic of wave shape relative to transducer positions. Note that as wave travels, center arrives before edges. L is lead distance, App is apparent distance traveled.



Figure 6.41: Detonation leads computed from V_{2-3} and arrival times at T3 and E. Solid points are for N_2 (298 and 373 K), open points for H_2O (373 K).

6.3 Photographic Tests

In the final set of tests, the schlieren system and Cordin camera were used to film the startup and ignition phenomena. In these runs, the camera was run at 34 kfps using 3200 ASA Kodak T-Max black-and-white film. At this framing rate, the frame-to-frame time is 29.412 μ s, and the exposure time for each frame is 3.9 μ s. A total of 224 frames is written per run, give or take a few frames lost to capping shutter synchronization. At 34 kfps, this gives a total write time of 6.6 ms. The film was not pushed in developing, but the camera writes in such a way that image on the negative is only 7.6 mm in diameter. (The frames are rectangular, placed two across on 35-mm film. The system was adjusted to get the largest possible circle within that frame size.) This means that the negative must be enlarged by 11x to make a printed image 85 mm in diameter (which fills a standard 4x5-inch print). As a result, the pictures are fairly grainy. The actual diameter of the area imaged is that of the light path, 100 mm. Square tabs are seen at the edges of the field; these are retention brackets from the collimating and focusing mirrors.

The camera speed is more than adequate for a deflagration, but is fairly slow for capturing jet startup and detonations. The images do show some interesting phenomena, however, and indicate that the detonations are initiated by the time they enter the second window station. Good images of jet-initiated detonations, taken at higher speeds, can be found in Inada et al. (1992).

Unfortunately, we have no fiducial reference for the time of diaphragm rupture, or the time delay for shutter opening. As a result, the times shown on the figures are for frame-to-frame reference purposes, and are not tied to the ignition time. Some velocities are calculated from the photos, but the boundaries are not always clear because we are looking at the entire thickness of a 3-dimensional phenomena in 2 dimensions. The wave position measurement is accurate to about ± 6 mm (after scaling), which can result in more than 10% error in waves that move 50 cm between measurements. (Detonations and jet heads tend to be visible on only two frames, which generates this amount of error. Slower moving features can be measured over several frames, reducing the relative error.) Also, the detonations move a significant distance during the exposure, so this adds some smear. The reported velocities given in the subsequent discussion should be considered rough estimates.

One run was taken at each of the three window stations for two different regimes: Prompt initiation, and deflagration. In addition, these cases were run both with and without a diaphragm. The 25-mm nozzle was used (with cutter) in all cases, to minimize the radial extent of the jet and keep the phenomena in the field of view. The windows are on 156-mm centers. In the cases with a diaphragm, the driver always uses the standard (β =2.6) mixture. In cases without the diaphragm, the mixture is the same in both vessels. In the deflagration tests, β =3.76 in the receiver. During the detonation tests, a problem was encountered. To minimize the possibility of initiation failure, a receiver mixture of β =2.6 was used in the receiver tests, adequately below the β_{CRIT} of 2.9. In the first two detonation runs, 407 and 408, this mixture underwent prompt initiation as expected. On subsequent runs, the mixture could not be detonated, and β had to be reduced to 2.4 for prompt initiation to occur. Similarly, the dilution had to be reduced (to $\beta=1.5$) for the no-diaphragm runs. After run 414, the hydrogen supply bottles were replaced. While gas contamination seems highly unlikely, this is being investigated, as nothing else seems to be suspect.

6.3.1 Tests With Diaphragm Installed

Figures 6.42 through 6.48 are from runs using a diaphragm. Figure 6.42 shows the jet startup process in an air-filled receiver, as a reference. In frame 1, we see a vortex ring leaving the nozzle, with a faint lead shock moving out ahead of it. In frame 5, another shock is passing through the vortex. This shock was measured at 330 m/s, which is subsonic; the true speed must be a little faster than sonic (340 m/s). The vortex ring is traveling at 40 m/s. It is difficult to directly relate this to the driver pressure trace (Figure 6.1), as the Kulite transducers (with thermal protection) do not respond quickly enough to show shock waves in the driver. However, we can deduce that some event in the driver is pulsing the diaphragm without breaking it, like hitting a drum. This displaces gas that is between the diaphragm and nozzle exit, forming the vortex ring. Other wave actions in the driver will cause the other shock waves. The initial lead shock in frame 1 may be formed when the driver is ignited. Also, the driver inner surface has an annular channel (Figure 5.2, p. 45) where the body of the driver mates to the extension, and this may generate turbulence and flame acceleration. In frame 62, the jet begins to emerge from the nozzle. Note that the vortex ring is just exiting the field of view. The jet head rapidly expands into the driver, at a speed of 1700 m/s. Experiments with the camera run at a slower speed for a longer time show that this jet assumes a quasi-steady structure once the initial expansion head leaves the field of view. In the final experiments of the former RPI facility (Appendix E), startup of a 12.7-mm jet was filmed at 6.72 and 13.44 kfps. The smaller nozzle reduced the radial extent of the flowfield, and a highly turbulent vortex head was visible, leading the flow downstream. Lacerda (1986) did an in-depth photographic study of jet startup, varying the pressure and density ratio across the orifice. In Figure 6.42, gas density is 0.68 kg/m^3 in the driver, and 1.18 kg/m^3 in the receiver. This falls between the $N_2 \longrightarrow N_2$ and $He \longrightarrow N_2$ cases in Lacerda. Lacerda found that lateral expansion was enhanced when a light gas vented into a heavier one $(e.g., Ne \longrightarrow N_2.).$

Initiation of a deflagration is shown in Figures 6.43-6.45, taken from stations 1-3, respectively. In 6.43, we see the jet emerging in frames 1-3. The jet head velocity measured here is 1500 m/s. The vortex ring has already left the field of view. In frame 3 it appears that material is being entrained into the jet from the right. (The face of the inner extension is 230 mm in diameter, more than twice the size of the window, so flow must move radially inward as it is entrained.) In frames 4 and 5, the beginning of a fine flame structure is visible. As the turbulence from the jet subsides, the flame surfaces join and form larger cells (frame 41), but the cells become fine and elongate by frame 51. In frame 61, the cells seem to be hitting the window, which flattens and smoothes them. By frame 91, the flame is fully against the window, with only the two

large structures remaining. The long arc structure that bisects the frame moves to the upper right in later frames, while the other branch disappears. The flame structure again becomes turbulent around frame 120. This alternate smooth and rough structure is seen in many of the deflagration runs. A possible explanation is that jet-induced motion of the receiver atmosphere is convecting the flame fronts to different regions of the vessel. Also, the initial flame front will move downstream with the jet, leaving a volume of unburned gas in the head of the vessel upstream of the nozzle exit. It is important to remember that the schlieren system is looking through the entire width of the vessel, so we may be seeing flame fronts at different depths, while the flames hitting the window have quenched.

In Figure 6.44 we move to station 2. In frames 1–4, we see the vortex ring (moving at 100 m/s) being rapidly overtaken by the bow shock of the jet (740 m/s). Remarkably, the vortex is still visible in frame 4, despite interference from jet gas. By frame 20 the flame structure is visible, and large pieces of the diaphragm are passing in frame 28. In the remaining frames, we see the alternating smooth/rough structure seen in the previous figure.

The deflagration photos from station 3 (Figure 6.45) are very interesting. In the first frame, we see that the lead shock from the jet startup has had time to advance away from the body of jet gas. At the same time, particles from the diaphragm are overtaking the lead shock. The small particle visible in the first few frames is moving at 680 m/s, while the larger ones that come later are moving at 760 m/s. (The sound speed in the receiver gas is 400 m/s). The Mach angle of the small particle was measured at 35° , yielding 700 m/s, in good agreement with the previous value. As the large particles go past, we see that they are acting as flameholders, dragging the flame fronts behind them, in their wakes. By frame 20, this region of the vessel is fully involved in combustion, and at frame 120 we see the flame front hitting the window.

Figures 6.46–6.48 show the jet initiation of detonation, at stations 1–3. The pressure traces from these runs confirm a prompt initiation. At the first station, Figure 6.46, I believe that the regions of self-light in frames 2 and 3 are the initiation region. The head of the jet is moving at 1500 m/s, consistent with previous measurements. In this run, the frames after 5 were obliterated by self-light. For subsequent runs, I added more baffles to the schlieren system, which seemed to solve the self-light problem. We would not expect much of the detonation to be visible at this station, as the reactants are being driven downstream by the jet. Unfortunately, the windows were also "sandblasted" by the detonation. The wave loosened rust particles from the sides of the tank, and drove them into the windows. I was able to clean the windows to some extent, but the surface was still pitted from the impacts. From the damage pattern, it appears that the particles had hit the downstream side of the window port in the vessel wall, and then bounced back into the windows. The mounting pad in the vessel wall for the window retainer is about 60 mm thick, with a 120 mm diameter hole for the light path; see Figure 2.8 for a cross section. For future runs, when I moved the windows to a new station, I sanded and cleaned the inner surface of the port. This greatly reduced the damage in future runs. A separate set of fresh windows was used for deflagration tests, to improve picture quality.

Figure 6.47 shows the detonation passing station 2. Here, the wave is highly curved, and has a measured speed of 1400 m/s. These observations are better correlated to the previous jet heads, but in the original print of frame 3, cellular structure is visible in part of the field. This did not come out in reproduction. In Figure 6.48, however, we see that the detonation has begun to flatten out by station 3. The measured velocity at this station is 1950 m/s, and with the measurement error, this corresponds well to the CJ velocity of 2100 m/s for this mixture. At this velocity, the wave moves about 1 cm during the 3.9 μ s frame exposure, adding to the uncertainty. In measuring the photographs, I took the sharpest part of the leading edge as the reference. In frames 2, 3 and 5, cellular structure characteristic of a detonation is visible in the original prints. This did not reproduce well, but is visible in the figure. It is important to not look at the figure too closely, and just try to see the overall texture of the image. The cells are composed of a grid of lines that are nearly orthogonal, rotated about 45° from horizontal. The cell size for this mixture is approximately 8 mm. A few other waves are seen in frames 54 and 55, but since the curvatures are different, they don't seem to be the same waves. Thus, their direction can't be determined.



6 (0.147 ms)





64 (1.853 ms)

65 (1.882 ms)

Figure 6.42: Jet startup sequence for standard driver ($\beta = 2.6$), with 25-mm nozzle. Run 406.



- $-3 \,\,(0.059\,\,{
 m ms})$
- 2 (0.029 ms)

1(t=0)





Figure 6.43: Jet initiation of deflagration by 25-mm nozzle, window station 1. Receiver $\beta{=}3.76.$ Run 416.



- 1(t=0)
- 2 (0.029 ms)
- 4 (0.088 ms)



- 82 (2.382 ms)
- 92 (2.676 ms)

134 (3.912 ms)

Figure 6.44: Jet initiation of deflagration by 25-mm nozzle, window station 2. Receiver $\beta{=}3.76.$ Run 419.



3 (0.059 ms)



2 (0.029 ms)

1(t=0)





Figure 6.45: Jet initiation of deflagration by 25-mm nozzle, window station 3. Receiver $\beta{=}3.76.$ Run 425.



1(t=0)

2 (0.029 ms)

3 (0.059 ms)



Figure 6.46: Jet initiation of detonation by 25-mm nozzle, window station 1. Receiver β =2.6. Run 407.



1(t=0)

2 (0.029 ms)

3 (0.059 ms)



 $4~(0.088~{\rm ms})$

Figure 6.47: Jet initiation of detonation by 25-mm nozzle, window station 2. Receiver $\beta = 2.4$. Run 424.



2 (0.029 ms)



54 (1.559 ms)



55 (1.588 ms)



6.3.2 Tests With No Diaphragm

Figures 6.49–6.55 are from runs with no diaphragm between the vessels. The lack of a diaphragm allows a flow field to start before the flame exits the driver. The venting also decreases the peak pressure in the driver. Figures 6.49–6.51 show the initiation of a deflagration. In Figure 6.49, the first frame is from run 412, which failed to catch the deflagration because the shutter timing was still being adjusted. We see the shock structure typical of underexpanded jets. (The nozzle is a simple orifice, so we expect choked flow.) In frame 0, we see that the pre-jet flow has nearly died out by the time the product jet arrives in frame 1. The leading edge of the jet is moving at 2000 m/s in the photo, but this mixture has a higher hydrogen fraction and hence a higher sound speed. Flame structure is beginning to form in frame 4, and by frame 11 the field is filled by a turbulent flame front. This goes on to hit the windows at frame 111.

Moving to station 2 in Figure 6.50, we see that the lead shock has pulled away from the jet head. The lead shock was photographically measured at 840 m/s, while the jet head has a velocity of 700 m/s. The field remains filled with jet flow structure through frame 5, and a flame structure is formed by frame 11. As the flame progresses, the structure goes from fine to coarse until the flame hits the window at frame 111. Figure 6.51, at station 3, is essentially the same. The lead shock is further separated from the jet (velocities of 590 and 500 m/s, respectively), and the flame front is well-established by frame 22. One interesting feature is seen in frame 120, where a wrinkled band about 1 cm thick is seen. This band is just right of center, and arcs in a way that connects the shadows of the mirror retention tabs. The nature of this form is unknown. In the adjacent frames on the negative, it doesn't appear to be moving, but simply fades in and fades out over 6–10 frames.

Figures 6.52–6.55 show the initiation of a detonation with no diaphragm. Station 1, Figure 6.52, is basically the same as in the diaphragm case, Figure 6.46. No distinct wave is seen at startup, but there is a region of intense self-light at the jet head that is not seen in the deflagration cases. Oddly, no precursor flow was seen in this case, as there was in the deflagration. Either the flame is quick enough to stay close to the shock, or the mixture has transitioned to detonation inside the driver. The nozzle diameter is less than one-third of the critical tube diameter for this mixture, so it is unlikely that a detonation would pass through the nozzle without failing. The driver pressure trace (β =1.7, Figure 6.53) is similar to that of the standard driver (β =2.6), except the peak pressure is reached about 4 ms sooner in this case. Since the Kulite doesn't respond quickly enough to show a detonation, it is not possible to discern transition in the driver. The jet head in this case (leading edge of the self-light) is moving at 1300 m/s. In frames 11–13, we see a round wave developing. This may be the detonation reflecting off of the windows. This phenomena was seen at all three window stations.

At station 2, Figure 6.54, the capping shutter opened just as the detonation was passing, so vignetting occurred in the early frames. However, in frame 1 we can see the distinct dark front seen in Figure 6.48. There is some cellular structure visible in the original print, but the cell size is much smaller due to the decreased dilution, so it is not visible in reproduction. In frame 10, we again see the circular wave pattern. Figure 6.55

is from station 3, and here we see the wave passing in the first two frames. The velocity here is 2200 m/s, which compares well with the CJ value of 2280 m/s. Cellular structure is visible in the originals, but the cell size for this mixture is only 6 mm, so the pattern is hard to see. The circular form is again seen in frame 7.





Figure 6.49: Jet initiation of deflagration by 25-mm nozzle, no diaphragm, window station 1. In both vessels, $\beta = 3.76$. First frame, showing jet, is from run 412, which was a camera timing test using the same mixture. Run 417.



1(t=0)





Figure 6.50: Jet initiation of deflagration by 25-mm nozzle, no diaphragm, window station 2. In both vessels, β =3.76. Run 418.



5 (0.118 ms)

120 (3.500 ms)



Figure 6.51: Jet initiation of deflagration by 25-mm nozzle, no diaphragm, window station 3. In both vessels, β =3.76. Run 426.

80 (2.324 ms)

50 (1.441 ms)



Figure 6.52: Jet initiation of detonation by 25-mm nozzle, no diaphragm, window station 1. In both vessels, β =1.7. Run 411.



Figure 6.53: Driver pressure trace, $\beta = 1.7$, no diaphragm.



1(t=0)

10 (0.265 ms)





Figure 6.55: Jet initiation of detonation by 25-mm nozzle, no diaphragm, window station 3. In both vessels, β =1.5. Run 431.

6.3.3 Secondary Phenomena

This section contains photographs that were not part of the main analysis, but showed interesting phenomena nonetheless. Figure 6.57 is from a camera timing run that used air as the driver diluent instead of nitrogen. The change in stoichiometry increased the flame speed, so the peak driver pressure occurred 2 ms earlier than usual (Figure 6.56). In the first frame, we see the bow shock and vortex ring produced by the diaphragm. By frame 4, we see a second vortex ring formed by the initial flow of jet gas, indicating that the diaphragm must have already ruptured. In frame 6, the rings have combined, and the jet gas is beginning to run through the vortex. We see fluid entrainment proceed through frame 8, and fast jet material is evident in frame 9. It appears that the diaphragm ruptured before the flame front reached it, as the gas venting before frame 9 is moving slower than it would for a typical jet.



Figure 6.56: Driver pressure traces showing effect of diluent. Data from Kulite (slow) transducer.

Figure 6.58, from station 2, is from a no-diaphragm run that was expected to undergo prompt initiation, but did not. The flame later underwent DDT. Again, we see no precursor flow as we did in the deflagration cases. In the first few frames, we see a shock front, followed by the flame. The shock speed is about 770 m/s, while the flame speed is only 400 m/s. In between the two waves, weak shocks are visible as thin lines. The DDT probably occurs after the lead shock reflects from the downstream end of the vessel, when the flame front hits the twice-shocked reactants. This is similar to run 409; the pressure traces from that run are shown in Figures 6.20 and 6.21 on page 87. The DDT occurs much later than the initial flame, so the capping shutter closes before the returning wave passes. In the remaining frames shown, however, we see the alternating smooth-rough flow field that occurred in the previous deflagration cases. The early images in this
sequence are similar to those seen by Inada et al. (1992) in a failed initiation, although their case was with a diaphragm.

Figure 6.59 is another initiation failure sequence viewed from station 2, but in this run a diaphragm was used. This run resulted in a deflagration only. These photos show the interaction of the flame front with the vortex ring. In the first frame, the lead shock has just passed over the vortex. In frames 2 and 3, note the bubble forming around the lower part of the vortex. This is a flame, and indicates that ignition occurs at the leading edge of the jet. In these photos, the lead shock is moving at 760 m/s, and the flame at 400 m/s, nearly identical to the previous example.







- 10 (0.321 ms)
- 11 (0.357 ms)
- 12 (0.393 ms)

Figure 6.57: Jet startup sequence, with initial vortex rings due to diaphragm-piston action. Driver mixture was diluted with air instead of nitrogen. Camera run at 28 kfps for this sequence. Run 403.





Figure 6.58: Failure to initiate detonation with 25-mm nozzle, no diaphragm, station 2. In both vessels, $\beta=1.7$. This flame later transitioned to a detonation. Run 422.



1(t=0)

2 (0.029 ms)



Figure 6.59: Failure to initiate detonation with 25-mm nozzle, using diaphragm, station 2. In the receiver, $\beta = 2.6$. Note flame/vortex interaction in frames 2 and 3. Run 421.

Chapter 7 Summary

The HYJET facility was constructed to study hydrogen combustion phenomena related to severe accidents in nuclear power plants. Jet-initiated deflagration and detonation have been studied in H₂-air and H₂-O₂ mixtures with N₂ and H₂O dilution. The mixtures are contained in an 1180 ℓ receiver vessel that can be maintained at temperatures up to 383 K. The jet ignition source is supplied by a 28 ℓ driver vessel that is filled with H₂-O₂-N₂ mixtures. These mixtures are spark ignited and the products are vented through nozzles of 12.7–92 mm diameter. The resulting event in the receiver depends on the receiver composition, driver composition, initial temperature, and jet (i.e., nozzle) diameter. The tests were divided into several series, based on objective.

7.1 COMP and S Series

The COMP series compared the HYJET facility to a similar facility previously used at Rensselaer Polytechnic Institute. These tests examined the effect of igniter strength on the lean flammability limit of diluted H₂-air mixtures. The receiver mixtures consisted of nitrogen and air in a 1:1 ratio, with 0–10% hydrogen. The driver was filled with 80% H₂-20% O₂, producing a hot jet of 50% H₂-50% H₂O upon ignition to simulate a DCH jet. The initial conditions in both vessels were 1 bar and 298 K. The driver was vented through the 12.7 and 25-mm nozzles. The results are summarized in Figure 7.1, which compares the peak receiver pressures to P_{AICC} .

Both the RPI and CIT facilities were able to ignite deflagrations in mixtures with at least 6% H₂. Previous studies in the RPI facility found that at least 9% H₂ was required for ignition via glow plug. Initiation of deflagration was easy to detect in HYJET, for either nozzle diameter. In the RPI facility, tests with the 25-mm nozzle were dominated by receiver pressurization and combustion of the jet gas as a diffusion flame. Receiver deflagration would not have been indicated without data from the 12.7-mm nozzle. Finally, a simple mole-balance method was used to estimate completeness of combustion in the HYJET tests. The results indicated that combustion was incomplete for 6% H₂, but complete for 8 and 10%. A reverse-flow period was also seen that had the potential to delay or suppress deflagration with the 25-mm nozzle.



Figure 7.1: Summary of COMP test series.

The S series duplicated the COMP mixtures, using water vapor for dilution instead of nitrogen. The initial receiver temperature for these tests was 373 K, and only the 12.7-mm nozzle was used. The tests showed that H_2O is a more effective suppressant than N_2 , owing to its higher heat capacity. With H_2O dilution, the H_2 concentration had to be increased to 8% for a deflagration to occur. The pressure traces for 8% H_2 with N_2 and H_2O dilution are shown in Figure 7.2.

7.2 SA Series

While the previous series examined deflagration at the lean limit, the SA series fixes the stoichiometry and varies the fraction of water vapor to study deflagration suppression. In this series, the hydrogen-air ratio in the receiver was kept constant at 20% H₂ in air (dry). The mixture was diluted with 0–60% water vapor. Initial conditions in the receiver were 1 bar and 373 K. The driver mixture was 80% H₂-20% O₂ at 1 bar and 298 K, as in the previous series. The 12.7, 25 and 92-mm nozzles were used for receiver ignition. The results are shown in Figure 7.3, which plots the peak receiver pressures against P_{AICC} .

The 12.7 and 92-mm nozzles were able to initiate deflagrations in mixtures with up to 60% water vapor. Previous studies, using glow plug ignition, were only able to ignite mixtures with 55% H₂O. Reverse flow with the 25-mm nozzle may have extinguished the flame kernel before it could propagate in the 60% mixture. It was able to initiate a deflagration in mixtures with 50% H₂O.

As nozzle diameter was increased, receiver pressure traces became increasingly noisy, owing to shock oscillations. With the 92-mm nozzle, jet effects dominate. In the 60% mixture, deflagration with the 92-mm nozzle was evident when the long-term pressure trace was compared to that of the 12.7-mm nozzle.



Figure 7.2: Comparison of water vapor and nitrogen as diluents.

7.3 NITRO Series

The NITRO series studied jet initiation of detonation, and the effects of driver strength. The receiver was filled with 0-30% H₂ in air, at 1 bar and 298 K. The driver used a fixed ratio of 80% H₂-20% O₂, which was diluted with 0-50% N₂ to reduce the flame speed. To compensate for the displaced reactants, the initial pressure was increased to keep the peak pressure constant at approximately 9.7 bar. Unforeseen dynamic effects raised the peak pressure to nearly 13 bar for 20-35% N₂. The flame speed was successfully reduced, as indicated by the burn time. Peak driver pressures for a plugged driver are shown in Figure 7.4.

The results for jet initiation are shown in Table 7.1. Drivers with 30% or more N_2 were unable to initiate a detonation in any H₂-air mixture. Drivers with less dilution were able to initiate detonations in mixtures containing at least 26% H₂. The driver with 25% N₂ was the most effective, requiring only 24% H₂ for detonation in the receiver. It appears that, although the peak pressures were similar for 30% nitrogen, the decrease in flame speed subdued the driver.

$\% N_2$	Minimum $\%$ H ₂ for Detonation	$\% N_2$	Minimum $\%$ H ₂ for Detonation
0	26	25	24
10	25	30	No detonation
20	26		

Table 7.1: Results of NITRO tests.

Previous studies by other researchers indicated that a minimum jet diameter-cell size ratio of $D/\lambda \approx 11-13$ was required for direct initiation of detonation. With the 92-mm



Figure 7.3: Summary of SA test series.

nozzle, HYJET has a $D/\lambda \approx 8$ for 30% H₂-air, so we thought that our "detonations" were actually the result of DDT between the nozzle exit and the transducers. Additional instrumentation in the BETA series showed that these detonations were initiated promptly at the jet exit. Since the D/λ criteria does not take into account the energy in the driver, its usefulness in jet initiation is questionable. Other research has shown that jet initiation is dependent on both large and small-scale turbulence, for entrainment and mixing, respectively.

Effects of confinement were also evident in the NITRO tests. When the receiver hydrogen concentration was just below the detonation threshold, strong secondary explosions were seen. Secondary explosions were also seen following the detonations. Many of these occurred approximately 0.3 ms after the lead wave reflection. We found that the secondary explosions were the result of shock focusing from the elliptical head of the vessel. An attempt to experimentally map the focus zone showed strong focusing, but was unable to clearly determine the shape of the region. Acoustic simulations indicated the presence of two focusing regions, one in the flange extension and one at the focus of the elliptical head.

7.4 BETA Series

The BETA series continued our study of jet initiation. The receiver was filled with stoichiometric H₂-O₂ mixtures of the form H₂ + 0.5(O₂ + βX), where X represents N₂ or H₂O dilution. The initial conditions were 1 bar at 298 and 373 K for N₂, and 373 K for H₂O. The objective was to find the maximum value of β (β_{CRIT}) for which a detonation could be initiated. The driver used this mixture with N₂ and β =2.6, at 1 bar and 298 K. The 25, 38, 64 and 92-mm nozzles were used. Combustion regimes were determined by



Figure 7.4: Results of constant-volume driver tests.

examination of pressure traces.

The results are summarized in Table 7.2. Earlier research with these mixtures required $D/\lambda \ge 11$ for detonation to occur. In the BETA series, we found $2 < D/\lambda < 7$ (with one exception at 10.7). Again, it appears that D/λ is of limited use in jet initiation experiments. We propose that a critical energy model may be more suitable. The results correlate well when plotted as β_{CRIT} vs. nozzle area, shown in Figure 7.5. We see that β_{CRIT} decreases with nozzle area for all systems. For the 298 K N₂ case, which used all of the nozzles, we see β_{CRIT} approaching an asymptote as nozzle size is increased. This indicates a physical limit for the HYJET facility. As nozzle size is decreased, we expect a sharp drop below 25 mm, as a nozzle size must exist for which no detonation will occur with $\beta=0$. The effect of jet turbulence is also seen, as adding the diaphragm cutter to the 25-mm nozzle increases its effectiveness by a small amount.

Other trends can be seen by fixing the nozzle size at 92-mm. Mixtures become more sensitive as temperature is increased, and we see that β_{CRIT} is higher for N₂ at 373 K than at 298 K. Water vapor is a more effective suppressant, and β_{CRIT} is much lower for H₂O at 373 K. The tests with no diaphragm are not directly comparable to the others, but we still see the change in β_{CRIT} with nozzle size.

Analysis of the peak pressures recorded at each transducer indicated that the detonation initiation was spherical in nature, with the 92-mm nozzle initiating a detonation further into the vessel than the smaller ones. Even direct initiation must take place downstream of the nozzle exit, as the jet fluid is displacing the reactants. Initiation will also be delayed by the induction time, which will vary as β is changed.

For each run, the velocity of the lead wave was calculated near the end of the vessel. The difference between initiation and failure was clearly indicated. If a detonation occurred, the wave velocity was slightly above the CJ value, indicating either overdrive or

D, mm	Diluent	T	β_{CRIT}	% Diluent	ZND Δ , mm	D/λ
92	N ₂	298 K	4.3	58.9	0.222	6.6
64	N_2	298 K	4.2	58.3	0.213	4.7
38	N_2	298 K	3.0	50.0	0.133	3.8
25	N_2	298 K	2.6	46.4	0.114	2.8
25, w/c	N_2	$298 \mathrm{K}$	2.9	49.2	0.128	2.6
92, ND	N_2	298 K	3.3	52.4	0.149	10.7
25, w/c, ND	N 2	298 K	1.8	37.5	0.088	3.3
92	N_2	373 K	5.2	63.4	0.293	5.4
92	H_2O	373 K	1.1	26.8	0.479	3.9
38	H_2O	373 K	0.55	15.5	0.114	4.3

Table 7.2: Summary of D/λ results. (w/c, with cutter; ND, no diaphragm.)

an oblique incidence. If the jet failed to initiate a detonation, the lead wave typically corresponded to a shock of M=1.33, although shocks from the 92-mm nozzle were slightly stronger. The degree of wave curvature was also calculated, but the vessel geometry affects the wave structure at the end of the vessel. The bow leads for detonations fell in the range 1 < L < 12 cm. One "correct" measurement was taken with a sting installed, indicating a lead of 9 cm.

A photographic analysis of the 25-mm nozzle showed that the detonations were initiated downstream of the nozzle exit, by the second or third window station. Deflagrations were highly turbulent, as expected. We also found that wave action in the driver "thumps" the diaphragm like a drum, generating a small ring vortex at the exit. This travels nearly 100 mm before the diaphragm ruptures and the main jet flow begins. The vortex does not appear to have any effect on detonation initiation.

7.5 Conclusion

The HYJET facility has proved useful in studying jet-initiated combustion phenomena. Combustion-generated jets with radicals were more effective igniters than shockgenerated hot jets of air or hydrogen. Lean-limit ignition tests found a 6% hydrogen-air limit for combustion to occur, with 8% required for complete combustion. This agrees with previous tests using sparks and glow plugs. Tests with steam dilution of a 20% H₂-air mixture achieved ignition with 60% H₂O, while previous tests with glow plugs found a limit of 50–55%.

In detonation tests, we found that shock focusing is very important in mixtures immediately below the detonability limit. If a mixture is not detonated promptly, focusing, DDT and shock reflection can generate pressures up to and even over 100 bar. This is over twice the reflected CJ pressure ($\approx 2.5 P_{CJ}$), which can no longer be considered an upper limit for design considerations. DDT was also much more likely in mixtures containing H₂O than in those with N₂ dilution.



Figure 7.5: Summary of critical beta values.

The tests also found that detonation limits (in jet initiation) are strongly dependent on driver strength and geometry. While previous studies required a minimum jet diameter of $11-13\lambda$ for initiation, we were able to initiate detonation with $2 < D/\lambda < 7$. The results indicate that jet energy is a more meaningful parameter than D/λ .

Future experiments in this facility will continue to study jet initiation of detonation. To suppress transition in the driver, we will add more spark plugs, or move the existing one to the middle of the vessel. We will then vary driver parameters, such as dilution (i.e., P_{AICC} and flame speed) and length, in an attempt to model the initiation process. Ideally, "unconfined" tests would be useful to remove receiver size effects, but this is not feasible with the HYJET facility. The final tests will study detonation initiation with particles in the jet gas. These particles, simulating molten core material in a DCH event, will enhance heat transfer to the reactants and accelerate the onset of detonation.

Bibliography

Anon. (1984, September). Military Explosives. Department of the Army. TM 9-1300-214.

- Benedick, W. B., J. C. Cummings, and P. G. Prassinos (1984). Combustion of hydrogen:air mixtures in the VGES cylindrical tank. Report NUREG/CR-3273 SAND83-1022, Sandia National Laboratories.
- Berman, M. (1985, august). A critical review of recent large-scale experiments on hydrogen-air detonation. In 23rd ASME/AIChE/ANS National Heat Transfer Conference, Denver, Colorado.
- Bezmelnitsin, A. V., S. B. Dorofeev, and Y. G. Yankin (1997). Direct comparison of detonation initiation by turbulent jet under confined and unconfined conditions. Russian Research Centre Kurchatov Institute, Moscow, Russia.
- Bezmelnitsyn, A. V., S. B. Dorofeev, and V. P. Sidorov (1995, June). Large scale turbulent jet initiation experiments in KOPER facility, test series 4. Technical report, Russian Research Center Kurchatov Institute, Moscow, Russia.
- Boyack, K. W., S. R. Tieszen, and D. W. Stamps (1992). Loads from the detonation of hydrogen-air-steam mixtures. Technical Report SAND92-0541, UC-741, Sandia National Laboratories.
- Breitung, W. (1993). Conservative estimates for dynamic containment loads from hydrogen combustions. *Nuclear Engineering and Design* 140, 95–109.
- Bull, D. C., J. E. Elsworth, P. J. Shuff, and E. Metcalfe (1982). Detonation cell structures in fuel/air mixtures. *Combustion and Flame* 45(1), 7–22.
- Camp, A. L., J. C. Cummings, M. P. Sherman, C. F. Kupiec, R. J. Healy, J. S. Caplan, J. R. Sandhop, and J. H. Saunders (1983). Light water reactor hydrogen manual. Report SAND82-1137 (NUREG/CR-2726), Sandia National Laboratories.
- Carnasciali, F., J. H. S. Lee, R. Knystautas, and F. Fineschi (1991). Turbulent jet initiation of detonation. *Combustion and Flame 84*, 170–180.
- Cates, J. and D. Howard (1993). Ray tracing program. Documentation for Ae 237 class project.
- Chan, C. K. (1995). Collision of a shock wave with obstacles in a combustible mixture. Combustion and Flame 100, 341-348.
- Chan, C. K., D. Lau, and D. Radford (1990). Transition to detonation resulting from burning in a confined vortex. In *Twenty-Third Symposium (International) on Combustion*, pp. 1797–1804. The Combustion Institute.
- Ciccarelli, G., T. Ginsburg, J. Boccio, C. Economos, C. Finfrock, L. Gerlach, K. Sato, and M. Kinoshita (1994). High-temperature hydrogen-air-steam detonation experiments in the bnl small-scale development apparatus. Report NUREG/CR-6213 BNL-NUREG-52414, Brookhaven National Laboratory.

- Coward, H. F. and G. W. Jones (1952). Limits of flammability of gases and vapors. Bulletin 503, United States Bureau of Mines.
- Djebaili, N., R. Lisbet, C. Paillard, and G. Dupre (1994). Comparison between the ignition of H₂-air-CO₂ and H₂-air-H₂O mixtures by hot gas jet. In *Twenty-Fifth Symposium (International) on Combustion*, pp. 1539–1545. The Combustion Institute.
- Dorofeev, S. B., A. V. Bezmelnitsyn, A. A. Efimenko, A. S. Kochurko, V. P. Sidorov, J. G. Yankin, and I. D. Matsukov (1993, June). Experimental study on the combustion behavior of hydrogen- air mixtures with turbulent jet ignition at large scale. Technical Report RRCKI-80-05/3, NUGEG/CR-6072, Russian Research Center Kurchatov Institute.
- Dorofeev, S. B., A. V. Bezmelnitsyn, and V. P. Sidorov (1995, December). Large scale turbulent jet initiation experiments in KOPER facility, test series 4 and 5. Technical report, Russian Research Center Kurchatov Institute.
- Fickett, W. and W. C. Davis (1979). Detonation. Berkeley: University of California Press.
- Glasstone, S. and P. J. Dolan (1977). *The Effects of Nuclear Weapons* (third ed.). United States Department of Defense.
- Guirao, C. H., R. Knystautas, J. Lee, W. Benedick, and M. Berman (1982). Hydrogen-air detonations. In 19th Symposium (International) on Combustion, pp. 583-590. The Combustion Institute.
- Inada, M., J. H. Lee, and R. Knystautas (1992). Photographic study of the direct initiation of detonation by a turbulent jet. In A. R. Seebass (Ed.), Dynamic Aspects of Detonations, Volume 153 of Progress in Astronautics and Aeronautics, pp. 253-269. American Institute of Aeronautics and Astronautics.
- Knystautas, R., J. H. Lee, and C. M. Guirao (1982). The critical tube diameter for detonation failure in hydrocarbon-air mixtures. *Combustion and Flame* 48(1), 63– 83.
- Knystautas, R., J. H. Lee, I. Moen, and H. G. Wagner (1979). Direct initiation fo spherical detonation by a hot turbulent gas jet. In Seventeenth Symposium (International) on Combustion, pp. 1235–1244. The Combustion Institute.
- Krok, J. C. (1992). Hydrogen combustion facility and experiments. Master's thesis, Rensselaer Polytechnic Institute, Troy, New York, USA.
- Kuchta, J. M. (1985). Investigation of fire and explosion accidents in the chemical, mining, and fuel-related industries—a manual. Bulletin 680, United States Bureau of Mines.
- Lacerda, N. L. (1986). On the Start Up of Supersonic Underexpanded Jets. Ph. D. thesis, California Institute of Technology.
- Lee, J. H., R. Knystautas, and N. Yoshikawa (1978). Photochemical initiation of gaseous detonations. Acta Astronautica 5, 971–982.

- Liu, D. D. S., L. J. Clegg, D. Bell, and D. C. Marek (1980). The effect of steam on the combustion of hydrogen-air mixtures near the lower flammability limit. Technical Report CONT-H-7, Whiteshell Nuclear Research Establishment, Pinawa, Manitoba, Canada.
- Liu, D. D. S. and R. MacFarlane (1983). Laminar burning velocities of hydrogen-air and hydrogen-air-steam flames. *Combustion and Flame* 49, 59–71.
- MacKay, D. J., S. B. Murray, I. O. Moen, and P. A. Thibault (1988). Flame-jet ignition of large fuel-air clouds. In 22nd Symposium (International) on Combustion, pp. 1339– 1353. The Combustion Institute.
- Marshall, Jr., B. W. (1986). Hydrogen:air:steam flammability limits and combustion characteristics in the FITS vessel. Report SAND84-0383 (NUREG/CR-3468), Sandia National Laboratories.
- McCormack, P. D., K. Sheller, G. Mueller, and R. Tisher (1972). Flame propagation in a vortex core. *Combustion and Flame 19*, 297.
- Moen, I. O., D. Bjerketvedt, T. Engerbretsen, A. Jenssen, B. H. Hjertager, and J. R. Bakke (1989). Transition to detonation in a flame jet. *Combustion and Flame* 75, 297–308.
- Moen, I. O., D. Bjerketvedt, A. Jenssen, and P. A. Thibault (1985). Transition to detonation in a large fuel-air cloud. *Combustion and Flame 61*, 285–291.
- Nettleton, M. A. (1987). Gaseous Detonations: Their Nature, Effects and Control. Chapman and Hall.
- Quirk, J. J. (1996). An introduction to Amrita. Technical report, California Institute of Technology. For information, see http://www.galcit.caltech.edu/~jjq/.
- Reynolds, W. C. (1986, January). The element potential method for chemical equilibrium analysis: Implementation in the interactive program STANJAN, version 3. Technical report, Dept. Mechanical Engineering, Stanford, CA.
- Ross, M. C. (1994). Transient jet diffusion flames in hydrogen-air-nitrogen atmospheres. Master's thesis, Rensselaer Polytechnic Institute, Troy, New York, USA.
- Shchelkin, K. I. and Y. K. Troshin (1965). *Gasdynamics of Combustion*. Mono Book Corp.
- Shepherd, J. E. (1986). Chemical kinetics of hydrogen-air-diluent detonations. In J. Bowen, J.-C. Leyer, and R. Soloukhin (Eds.), *Dynamics of Explosions*, Volume 106 of *Progress in Astronautics and Aeronautics*, pp. 263–293. American Institute of Aeronautics and Astronautics.
- Shepherd, J. E. (1992, September). Pressure loads and structural response of the BNL high-temperature detonation tube. Prepared for Brookhaven National Laboratory.
- Shepherd, J. E., A. Teodorczyk, R. Knystautas, and J. H. S. Lee (1991). Shock waves produced by reflected detonations. In *Progress in Astronautics and Aeronautics*, Volume 134, pp. 244–264.

- Stamps, D. W., W. B. Benedick, and S. R. Tiezen (1991). Hydrogen-air-diluent detonation study for nuclear reactor safety analyses. Report NUREG/CR-5525, SAND89-2398, Sandia National Laboratories.
- Stamps, D. W. and S. R. Tieszen (1991). The influence of initial pressure and temperature on hydrogen-air-diluent detonations. *Combustion and Flame* 83(3), 353–364.
- Sturtevant, B. and V. A. Kulkarny (1976). The focusing of weak shock waves. J. Fluid Mech. 73, 651-671.
- Thompson, P. A. (1972). Compressible-Fluid Dynamics, pp. 347–358. McGraw-Hill.
- Tieszen, S. R., M. P. Sherman, W. B. Benedick, J. E. Shepherd, R. Knystautas, and J. H. S. Lee (1986). Detonation cell size measurements in hydrogen-air-steam mixtures. *Progress in Astronautics and Aeronautics 106*, 205–219.
- Ungüt, A. and P. Shuff (1989). Deflagration to detonation transition from a venting pipe. Combustion Science and Technology 63, 75-87.
- Urtiew, P. A. and C. M. Tarver (1979). Effects of cellular structure on the behavior of gaseous detonation waves under transient conditions. In *Progress in Astronautics and Aeronautics*, Volume 75, pp. 370–384. Proceedings of the 7th International Colloquium on Gas Dynamics of Explosions and Reactive Systems.
- Völkl, T. and S. Schlamp (1996). Ignition of a hydrogen-air mixture by a hot air jet. Ae104 Final Report.
- White, D. R. (1961). Turbulent structure of gaseous detonations. *Physics of Fluids* 4(4), 465.
- Yip, T. W. G., R. A. Strehlow, and A. I. Ormsbee (1985). An experimental investigation of two dimensional flame-vortex interactions. In 20th Symposium (International) on Combustion, pp. 1655. The Combustion Institute.