N89-14162 53-28 174727

1988

NASA/ASEE SUMMER FACULTY RESEARCH FELLOWSHIP PROGRAM

JOHN F. KENNEDY SPACE CENTER
UNIVERSITY OF CENTRAL FLORIDA

FT466751

ON THE HAZARD OF HYDROGEN EXPLOSIONS AT SPACE SHUTTLE LAUNCH PADS

Prepared By:	John M. Russell
Academic Rank:	Associate Professor
University and Department:	Florida Institute of Technology Department of Aerospace and Mechanical Engineering
NASA/KSC:	
Division:	Mechanical Engineering
Branch:	Propellants and Gases
NASA Counterpart:	W. I. Moore
Date:	August 19, 1988
Contract No.:	University of Central Florida NASA-NGT-60002

ON THE HAZARD OF HYDROGEN EXPLOSIONS AT SPACE SHUTTLE LAUNCH PADS

by

John M. Russell
Florida Institute of Technology

ABSTRACT

This report was prepared in support of efforts to assess the hazard of accidental explosions of unburned hydrogen at space shuttle launch pads. It begins with a presentation of fundamental detonation theory and a review of relevent experiments. A scenario for a catastrophic explosion at a KSC launch pad and a list of necessary conditions contributing to it is proposed with a view to identifying those conditions which, if blocked, would prevent the catastrophe. The balance of the report is devoted to juxtaposition of reassuring and disquieting facts, presentation of a set of recommendations for further work, and listing of three main conclusions. One conclusion is that ignition of hydrogen-air mixtures by weak ignition sources in unconfined geometries may produce a detonation, provided the effective flame area in the initial fireball is rapidly increased by turbulent mixing. Another conclusion is that detonability limits can be different from and narrower than flammability limits only if one restricts the rate of work that can be done on a flammable gas by mechanical agencies acting on its boundaries.

Key words: Deflagration-to-detonation transition, spherical explosions, detonation, hydrogen-air explosions, flame trench

SUMMARY

The space shuttle main engines discharge hundreds of pounds of unburned hydrogen into the launch pad environment during shutdown from rated power level during an abort sequence and at the end of a flight readiness firing. Numerous personnel at KSC and elsewhere have conducted a variety of studies to determine whether this unburned hydrogen exposes the flight or launch hardware to the risk of damage from accidental explosions. Most of these studies were concluded or cancelled in late 1987. This report is the result of a one-man ten-week effort undertaken in the summer of 1988 by a NASA/ASEE faculty research fellow. The main purpose of this effort was to make sense out of the results now in hand and to indicate areas in which future efforts might be especially valuable.

In pursuing this goal, I found that few, if any, of the previous studies directed specifically to the problem of unburned hydrogen at space shuttle launch pads presented any kind of primer on the basic principles of mechanics, thermodynamics, and chemistry that govern the phenomena of detonation in gases. After some early discussions with my KSC contact (W.I. Moore of the Propellents and Gases Branch, DM-MED-4, KSC), we agreed that the preparation of a document which describes the basic ingredients of a detonation, comments on the relevence of certain experiments on the origin of gaseous explosions to the conditions at KSC launch pads, presents definitions of all the relevent technical terms in related areas of combustion and detonation theory, and assembles a select bibiography would be worthwhile.

This report begins with a definition of the problem and a description of the kinds of boundary conditions to which flow in the flame trenches at KSC shuttle launch pads are subject. After this, a connected account of the essential elements of the theory of gaseous detonations is presented. In this section, I review three older studies by G.I. Taylor on the theory of explosions with spherical symmetry. As in the elementary theory of gasdynamics, much insight can be gained by considering the response of a gas to motion of a piston in contact with it, or to the analog of a piston in three dimensions (*i.e.* an expanding sphere). If a shock wave is sent through any flammable gas by movement of a piston or expanding sphere, then by moving the piston or expanding sphere fast enough, one may produce an arbitrarily large temperature rise across the shock and may thus cause the shocked gas to ignite. If, in addition, the motion of this piston or expanding sphere is sustained for a long enough time interval, then one can ensure complete combustion of the shocked gas. Such a zone of complete combustion following a lead shock amounts to a detonation wave. Overpressure produced by such detonation waves may easily reach tens of atmospheres, which illustrates their destructive potential.

If a flammable mixture of gases is ignited at a point by a weak source, the thermal expansion of the resulting fireball may exert an action on the un-

burned gas around it similar to that of the expanding sphere described above. If the gas is a mixture of hydrogen and air, and if the flame front produced by weak ignition remains spherical, then according to results of a 1960 study by the Arthur D. Little Company the gas will not detonate. If, however, the effective area of the flame front is abruptly increased by turbulent mixing or by other mechanisms, then detonation may occur, as is indicated by several more recent experimental studies.

After this discussion of fundamentals, the report proceeds to describe a scenario for a catastrophic explosion at a KSC shuttle launch pad and the necessary conditions contributing to it. The idea is that if a necessary contributing condition is blocked then the sequence of events would be interrupted and no catastrophe would occur. After a discussion of this catastrophe scenario, I juxtapose various reassuring facts with disquieting ones. The report then takes up the matter of recommentations and ends with a short list of conclusions. The recommendations are, first, to consider the list of necessary contributing conditions for a catastrophe discussed earlier and try to identify those that can be blocked most easily. The second recommendation is to exploit (and, if necessary, develop) simple models of selected flow details to inform one's thought on the phenomena most likely to relate to these necessary conditions.

There are three conclusions. In abbreviated form, they are, first, that detonations in unconfined hydrogen-air mixtures can be produced without blasting caps or other high energy detonators provided there is a mechanism for rapidly increasing the effective flame area in a local fireball. Secondly, detonability limits can be different from, and narrower than, flammability limits only if restrictions are imposed on the rate that work can be done on a flammable mixture of gases by adjacent boundaries. In the absence of such restrictions, all flammabe mixtures are detonable. Thirdly, there are realistic prospects for ruling out accidental detonations of hydrogen at KSC shuttle launch pads. One promising approach is to establish a well-founded list of necessary contributing conditions for a catastrophe and to consider, through the use of simple models of selected flow details, the credibility or lack of credibility of each such condition. The results of such an effort would either certify the safety of existing equipment and operating procedures or identify changes that would lead to such a certification.

TABLE OF CONTENTS

Figure Title

ORIGINAL PAGE IS
OF POOR QUALITY

1. INTRODUCTION

The main engines of the space shuttle orbiter discharge hundreds of pounds of unburned hydrogen into the launch pad environment during some modes of operation. Two such modes of operation are engine shutdown from rated power level in a flight readiness firing (FRF) and an abort. Millions of dollars have been spent by the U.S. Air Force and by NASA to assess the risk of a catastrophic accident resulting from explosions of this gas. Some of these efforts will be described in the following sections. As of July 1988, however, no one has demonstrated that clouds of explosive gases near the shuttle orbiter either definitely do or definitely do not constitute a credible hazard.

In view of the importance of the unburned hydrogen problem, W.I. Moore of the Propellants and Gases Branch, Mechanical Engineering Division, Kennedy Space Center, NASA suggested to the present author that the preparation of a general review of the unburned hydrogen problem would be a worthwhile project to work on during the author's NASA/ASEE Faculty Summer Research Fellowship. This report is the result of this one-man ten-week effort.

1.1 HISTORY

According to internal NASA documents made available to the author, an acoustic signature characteristic of a gaseous detonation was detected in the exhaust duct of a space shuttle launch facility at the Vandenburg Launch Site in California sometime during (or before) November 1984. This event prompted a series of studies involving Rockwell International, Martin Marietta, Lockheed Missles and Space Corporation, and technical personnel at several NASA and Air Force facilities (Vandenburg, Johnson Space Flight Center, Marshall Space Flight Center, the National Space Technology Laboratories, Kennedy Space Center, *etc.*) which resulted in the design of a hydrogen disposal system for the exhaust duct at the Vandenburg facility [*cf.* Breit & Elliott (1987)[1]] The design featured a system to inject superheated water into the duct. The specifications call for a system in which the superheated water quickly turns to steam and is delivered in sufficient quantities to render the gases in the exhaust duct inert. Installation of this system was postponed indefinitely after the Challenger disaster.

The questions raised during the study of the Vandenburg facility raised similar questions regarding the safety of the shuttle launch pads at the Kennedy Space Center. Unlike the Vandenburg facility (from which no space shuttles have yet been launched) the KSC facilities have a distinguished performance record. In twenty five launches, six flight readiness firings and two aborts, no alarming pressure signatures have been reported The confidence one might derive from this observation is tempered, however, by the results of an elementary calculation due to F. Howard (1987)[2] at KSC. He noted that an explosion can damage the shuttle orbiter if it causes a shock wave to strike the orbiter with an overpressure in excess of 1.32 psi. The explosive yield of a spherical blast that produces this overpressure at the orbiter is, of course, dependent upon the distance from the orbiter to the center of the blast. Taking this distance to be 200 feet (which represents the distance from the base of the orbiter to the most remote part of the flame trench at pads 39A and 39B at KSC) only six pounds of hydrogen are needed to fuel a blast that produces a damaging overpressure.

During a shutdown from rated power level, by contrast, the amount of unburned hydrogen discharged by the space shuttle main engine (after all hydrogen burn off ignitors have ceased to burn) is on the order of 400 pounds. One may not, therefore, dismiss the problem out of hand on the grounds that the *amount* of unburned hydrogen is too small to do harm. At this juncture, one should also remark that the figure 400 pounds refers only to the unburned hydrogen *outside* the space shuttle fuel tank. If detonation of that gas caused a breach of the shuttle fuel tank, the potential for harm could be far greater.

Previous efforts to assess the hazard presented by unburned hydrogen have included:

a. A statistical study of previous firings of hydrogen-oxygen rocket engines in the U.S. [Littlefield (1987)[3]]. Among its results was the reassuring observation that only six confirmed detonations have taken place out of over 16,000 firings.

b. Testing of a model of the exhaust duct at the Vandenburg Launch Facility into which exhaust gases from an H_2-O_2 rocket were discharged in a controlled fashion. This work was done by the Lockheed Missles and Space Corporation in Santa Cruz in support of the hydrogen disposal system for the Vandenburg Launch Site.

c. Measurements of gas properties in the exhaust plume produced by firing a full-scale space shuttle main engine at the National Space Technology Laboratory in Mississippi.

d. Numerical simulation of the exhaust plume of a space shuttle main engine in various modes of operation. These calculations were performed by the Rocketdyne Corporation in September and October 1986.

e. Preparation to install instruments in the flame trench at pad 39B at KSC to measure gas properties during the flight readiness firing in the summer of 1988.

f. Commissioning of a study by Bransford and Voth of the National Bureau of Standards to assess the problem of unburned hydrogen at KSC and make recommendations [*cf.* Bransford & Voth (1987)[3]].

g. Consultation with personnel at Combustion and Explosives Research in Pittsburgh, Pennsylvania. This effort resulted in a recommendation to install long-burning hydrogen burn-off ignitors in upcoming flight readiness firings.

h. A study by E.E. Zukoski at the California Institute of Technology titled 'Flow into the SSME exhaust duct' (Aerospace Memorandum number 5 , February, 1987) and a reply by Shelby Kurzius (NASA MSFC)

1.2 GUIDING QUESTIONS

The author's efforts this summer have been guided by two questions, namely

Q1 Is there a *set of events* common to all credible scenarios leading to a catastrophic explosion near the orbiter? Such a set of events might include:

- formation of a suitably large cloud of explosive gas suitably close to the orbiter
- initiation of a detonation in the cloud

Q2 Is either of the above events *precluded* by present hardware and operating procedures at KSC?

All other questions addressed in this report are stimulated by the two questions just listed.

1.3 OVERVIEW OF THE REMAINDER OF THIS REPORT

In section 3, I will discuss the boundary conditions to which fluid in the exhaust plume of the SSME is subject. Discussion of the physical phenomena that relate to gaseous detonations in the flame trench at KSC shuttle launch pads is not feasible without some background in the theory and observation of detonations. To this end, section 3 is devoted to an elementary discussion of the physical principles that govern detonation phenomena and to a discussion of some of the most instructive examples from the theory of spherical explosions. Section 4 is devoted to a discussion of detonation experments. In section 5, I propose a scenario involving eleven events that lead to a catastrophic explosion. Certain necessary conditions must contribute to these events and nine such conditions are listed in the same section. In section 6, I juxtapose various reassuring and disquieting facts. Sections 7 and 8 are devoted to recommendations and conclusions, respectively.

2. BOUNDARY CONDITIONS TO WHICH FLUID IN THE EXHAUST PLUME IS SUBJECT

2.1 FIXED BOUNDARIES

The fixed boundaries to which the exhaust plume from the SSME is subject consist of the mobile launch platform (with its exhaust duct), the blast deflector, the flame trench, and, in the case of flight readiness firings and on-pad aborts, the placement of the SSME nozzles. Figures 1 and 2 illustrate these boundaries and their placement relative to each other.

2.2 TIME-DEPENDENT BOUNDARIES

The time-dependent boundaries to which the exhaust plume is subject consist of the hydrogen burn off ignitors, the sound supression water spray (SSWS), the time dependent flow rates, chemistry, and thermodynamic state of the gases discharged by the SSME, and, in the case of a launch, the placement of the SSME exhaust nozzles. Plots of the time-dependent cumulative discharge of unburned hydrogen from the SSME during various firing sequences are presented in Breit & Elliott (1987)[1] and Bransford & Voth (1987)[4] (to name two sources). The case of an on-pad abort appears to result in the greatest cumulative discharge of unburned hydrogen. Bransford and Voth give the figure 800 pounds of total discharge, though this figure does not take account of the action of the hydrogen burn off ignitors. If one assumes that all of the H_2 discharged by the SSME during the burn period of the ignitors is ignited and safely disposed of by ordinary burning, then the more relevent figure for hazard assessment is the total discharge after the ignitors are spent. The latter figure in the case of an on-pad abort is on the order of 400 pounds.

None of the studies I have encountered presents reliable quantitative information on the state of the gas beneath (*i.e.* downstream of) the SSWS, though some authors have stated conjectures about it. Dr. E.E. Zukoski of Caltech, writing as a consultant to the Aerospace Corporation, prepared a document titled 'Flow into the SSME Exhaust Duct' , Aerospace Memorandum number 5 Febrary 12, 1987, in which he addresses this question. I have not yet succeeded in obtaining a copy of this document, but I have read a review of it by Dr. Shelby Kurzius at MSFC. According to Zukoski and Kurzius, the SSWS discharges enough water so that, if thoroughly mixed with the exhaust gases from the SSME, there will be enough to extinguish the exhaust flame by cooling. It remains an open question whether the exhaust flame is really extinguishable in practice and whether the downstream mixture of gases and water droplets is sufficiently diluted with water vapor to render it nonflammable.

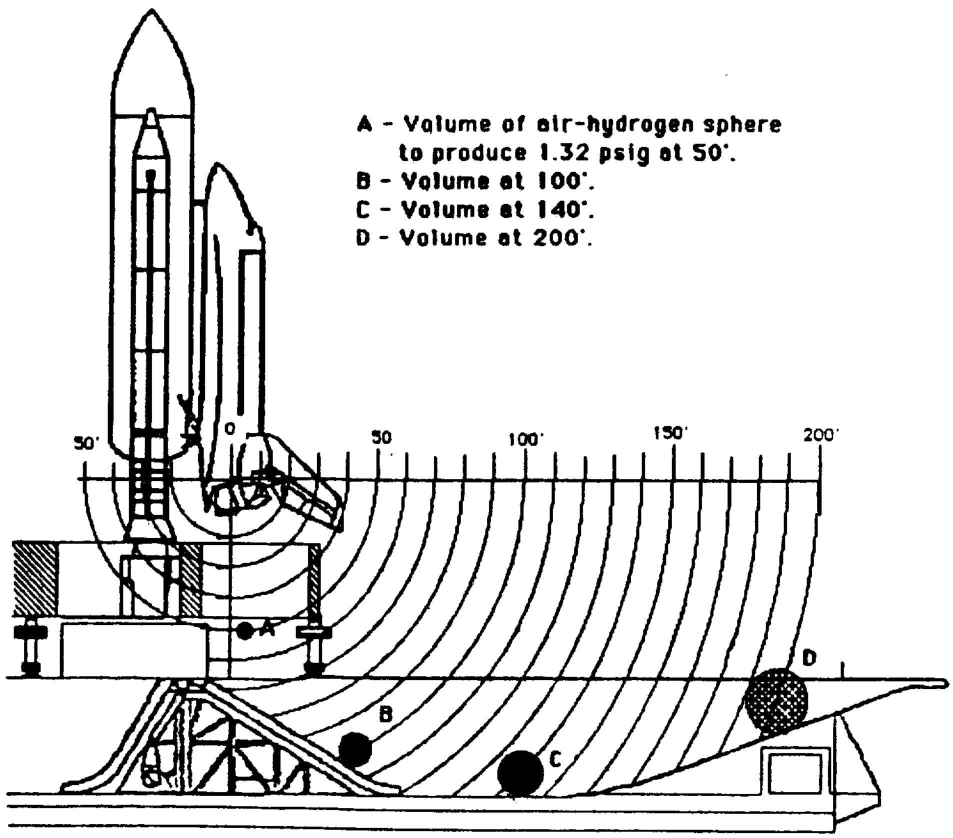

Figure 1. Space shuttle on the launch pad, viewed in a direction perpendicular to the flame trench [from Howard (1987)[2]] showing relative placements of the exhaust nozzles, exhaust duct in the mobile launch platform, and the flame trench. Also shown are the results of some of Howard's calculations described in the text.

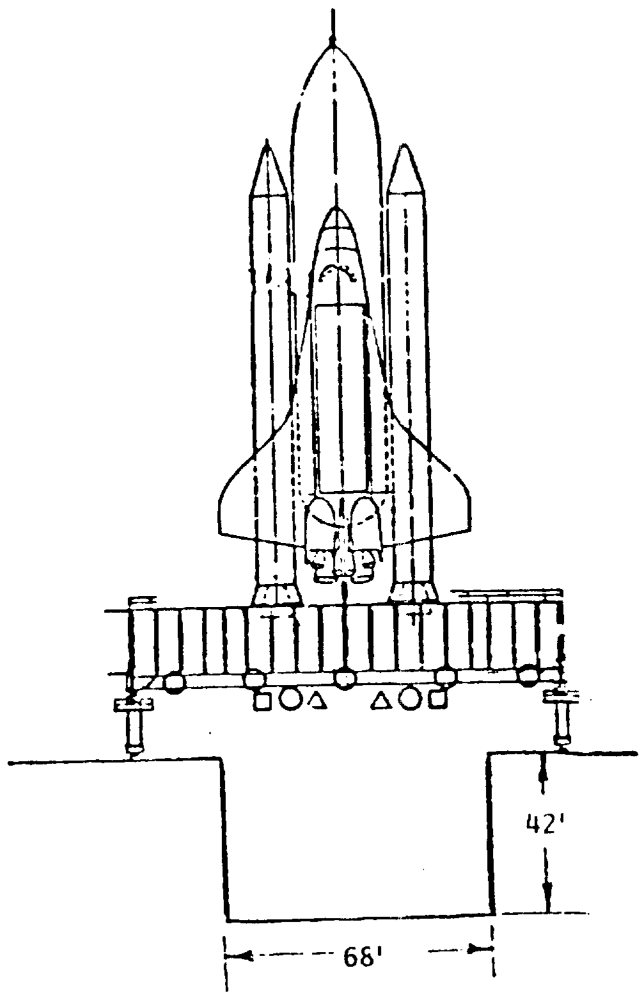

Figure 2. Space shuttle on the launch pad, viewed in a direction parallel to the flame trench.

3. BACKGROUND ON DETONATION THEORY

As was stated in the Introduction, one can not discuss the specific issues relating to the hazard of detonations at KSC shuttle launch pads without having some working vocabulary on detonation phenomena. The present section furnishes two kinds of background that will be useful to this end, namely an analytical glossary of technical terms and a select catalog of some classical solved problems in gas dynamic and detonation theory that seem to be particularly informative. By 'analytical glossary', I mean a glossary of terms arranged in logical rather than alphabetical order starting with the concepts that are most fundamental.

3.1 UNIDIRECTIONAL PROBLEMS

3.1.1 INERT SHOCK WAVES. Consider a fluid flow in which the streamlines are parallel and the fluid speed does not vary in the cross-stream direction. Suppose, further, that the flow is steady. Let x be a spatial coordinate measured positive in the direction of the fluid velocity vector and let u be the component of the fluid velocity in this direction. Let p, ρ, and e denote the pressure, mass density, and specific internal energy of the fluid. A *shock wave* is a discontinuity or step change in p, ρ, e, u, and other quantities that separates two regions in which these quantities are smoothly varying. The changes in p, ρ, e, u, *etc.* across a shock must be compatible with the basic laws of mechanics and thermodynamics including the law of conservation of mass, the equation for the rate of change of translational momentum, and the equation for the rate of change of energy. Let the subscrips '0' and '1' denote the conditions on the upstream and the downstream side of the shock, respectively. Then the three laws just mentioned may be expressed in the form

$$\rho_0 u_0 = \rho_1 u_1 \equiv \dot{m} \tag{1}$$

$$p_0 + \rho_0 u_0^2 = p_1 + \rho_1 u_1^2 \tag{2}$$

$$e_0 + \frac{p_0}{\rho_0} + \frac{u_0^2}{2} = e_1 + \frac{p_1}{\rho_1} + \frac{u_1^2}{2} \quad , \tag{3}$$

respectively. Here, $\dot{m}$ denotes the rate of transport of fluid mass per unit area (measured perpendicular to the streamlines). The parameters in these equations must be compatible with the thermodynamic equation of state of the substance. If the substance undergoes no chemical reactions in the shock itself, this equation may be represented by

$$e = f(p, \frac{1}{\rho})$$

on either side of the shock. If the substance is a thermally and calorically perfect gas, then we may write

$$e + \frac{p}{\rho} = \frac{\gamma}{\gamma-1}\frac{p}{\rho} \quad , \tag{4}$$

in which γ is a shorthand for the ratio c_p/c_v. Here, c_p and c_v are the specific heats of the substance at constant pressure and at constant volume, respectively. When equation (4) holds, equation (3) may be replaced by

$$\frac{\gamma}{\gamma-1}\frac{p_0}{\rho_0} + \frac{u_0^{\,2}}{2} = \frac{\gamma}{\gamma-1}\frac{p_1}{\rho_1} + \frac{u_1^{\,2}}{2} \quad . \tag{5}$$

The eariest discussion of shock waves appears to be due to George Gabriel Stokes [Stokes (1848)[5]]. The foregoing equations are associated with the names of Rankine [Rankine (1870)[6]] and Hugoniot [Hugoniot (1887)[7]] and are often called *the Rankine-Hugoniot shock conditions*.

In a typical problem in shock wave propagation, the value of γ is a given constant. Also given are data specifying the thermodynamic state of the gas upstream of the shock, including the values of ρ_0 and p_0. There are four unknowns, namely (u_0, u_1, p_1, ρ_1) whose values are constrained by the three equations (1), (2), and (5). As one might then expect, exactly one parameter is left undetermined by the equations written so far.

One convenient choice of parameter, in terms of which the family of solutions of (1), (2), and (5) may be expressed is the Mach number based on the fluid speed u_0 and sound speed a_0 upstream of the shock, *i.e.*

$$M = \frac{u_0}{a_0} \quad , \tag{6}$$

in which

$$a_0^{\,2} = \gamma\,\frac{p_0}{\rho_0} \quad . \tag{7}$$

The fractional changes in all the relevent flow quantities across the shock may then be expressed in terms of M, *e.g.*

$$\frac{p_1}{p_0} = 1 + \frac{2\gamma}{\gamma+1}(M^2 - 1) \tag{8}$$

$$\frac{\rho_1}{\rho_0} = \frac{u_0}{u_1} = \frac{(\gamma+1)M^2}{(\gamma-1)M^2 + 2} \tag{9}$$

as is shown in all elementary books on gas dynamics [*cf.* Liepmann & Roshko (1957)[8],§2.13]. One may regard M as a measure of the *shock strength* (stronger shocks having higher M).

Now consider a plane which is oriented parallel to the shock and is situated downstream of it. Suppose, moreover, that this plane moves with the fluid.

Let $x_p(t)$ be the time-dependent position of this plane. Then the action exerted on the fluid in the region where $x > x_p(t)$ (*i.e.* the region containing the shock) by the fluid in the region where $x < x_p(t)$ is indisttinguishable from the action of a rigid body such as a piston that drives the flow. If one imagines that the flow is *in fact* driven by a piston and that the motion of this piston is prescribed, then a suitable boundary condition for the problem would assert that the velocity of the fluid in contact with the piston equals the (prescribed) velocity of the piston. Only when such boundary data are prescribed can one determine M (or any other measure of the shock strength) uniquely.

3.1.2 DETONATION WAVES. Let T denote the local instantaneous absolute temperature in a gas. From the equation of state of an ideal gas, *i.e.*

$$p = (c_p - c_v)\rho T \quad ,$$

it follows that

$$\frac{p_1}{p_0} = \frac{\rho_1 T_1}{\rho_0 T_0} \quad .$$

Substituting (8) and (9) to eliminate p_1/p_0 and ρ_1/ρ_0, one obtains (after some rearrangement)

$$\frac{T_1}{T_0} = \frac{p_1/p_0}{\rho_1/\rho_0} = 1 + \frac{2(\gamma-1)}{(\gamma+1)^2}\,\frac{\gamma M^2+1}{M^2}\,(M^2-1) \tag{10}$$

[*cf.* Liepmann & Rosko, equation 2.49]. If a gas is flammable and if a shock of sufficient strength passes through it, then either the abrupt rise in temperature, the abrupt rise in velocity, or both may initiate combustion of the gas. A definition of combustion will be furnished in section 3.1.3 below. If such a combustion takes place and is completed in a finite distance behind the shock, then the localized reaction zone and the shock that leads it is called a *detonation wave*. Detonation waves always propagate supersonically (*i.e.* $M > 1$) relative to the fluid upstream of them. A *deflagration wave*, by contrast, is a flame front that propagates subsonically relative to the unburned gas.

Let the subscript '2' denote the conditions at the downstream extremity of the reaction zone of a detonation wave. The flow quantities upstream of the lead shock are related to those at the downstream end of the reaction zone by a set of equations similar to (1)-(3), *i.e.*

$$\rho_0 u_0 = \rho_2 u_2 = \dot{m} \tag{11}$$

$$p_0 + \rho_0 u_0^2 = p_2 + \rho_2 u_2^2 \tag{12}$$

$$e_0 + \frac{p_0}{\rho_0} + \frac{u_0^2}{2} = e_2 + \frac{p_2}{\rho_2} + \frac{u_2^2}{2} \quad . \tag{13}$$

Here, the specific internal energy e includes not only the usual thermal part (which, for a calorically perfect gas equals $c_v T$) but also a chemical part. If one assumes that the fluid on either side of the detonation is a thermally and calorically perfect gas and if one denotes by $q > 0$ the chemical energy per unit mass that is converted to thermal energy during the chemical reaction one may take

$$e_0 = (c_v)_0 T_0 + q \tag{14}$$

$$e_2 = (c_v)_2 T_2 \tag{15}$$

in (13). By manipulations similar to those which led to (5) above, equation (13) may be written

$$\frac{\gamma_0}{\gamma_0 - 1}\frac{p_0}{\rho_0} + q + \frac{{u_0}^2}{2} = \frac{\gamma_2}{\gamma_2 - 1}\frac{p_2}{\rho_2} + \frac{{u_2}^2}{2} \quad . \tag{16}$$

If values of $(p_0, \rho_0, \gamma_0, \gamma_2, q)$ are given and (p_2, ρ_2, u_0, u_2) are sought, then the system (11), (12), (16) consists of three equations for the four unknowns. As was the case with inert shocks, the family of solutions of this system will have one free parameter and again one may take this parameter to be the Mach number $M = u_0/a_0$ based on the fluid velocity and sound speed upstream of the lead shock.

If one substitutes $u_0 = \dot{m}/\rho_0$ and $u_2 = \dot{m}/\rho_2$ into (12) and (16) to eliminate u_0 and u_2, one obtains

$$(\dot{m})^2 = \frac{p_2 - p_0}{\dfrac{1}{\rho_0} - \dfrac{1}{\rho_2}} \tag{17}$$

and

$$\frac{(\dot{m})^2}{2}\left(\frac{1}{{\rho_0}^2} - \frac{1}{{\rho_2}^2}\right) + q = \frac{\gamma_2}{\gamma_2 - 1}\frac{p_2}{\rho_2} - \frac{\gamma_0}{\gamma_0 - 1}\frac{p_0}{\rho_0} \tag{18}$$

after some rearrangement. If one factors the expression $({\rho_0}^{-2} - {\rho_2}^{-2})$ in (18) and eliminates $(\dot{m})^2$ by means of (17), one obtains, after simplification,

$$\frac{1}{2}\left(p_2 - p_0\right)\left(\frac{1}{\rho_0} + \frac{1}{\rho_2}\right) + q = \frac{\gamma_2}{\gamma_2 - 1}\frac{p_2}{\rho_2} - \frac{\gamma_0}{\gamma_0 - 1}\frac{p_0}{\rho_0} \tag{19}$$

which involves only two of the four unknowns, namely p_2 and ρ_2. A *Hugoniot curve* is a graph of (19) with p_2 as the ordinate and $1/\rho_2$ as the abscissa. This curve is a hyperbola [*cf*. Strehlow (1968)[9], §5-4].

Now the speed of sound a_0 in the unburned gas is given by ${a_0}^2 = \gamma_0 p_0/\rho_0$. It follows that

$$(\dot{m})^2 = (\rho_0 u_0)^2 = (\rho_0 a_0 M)^2 = {\rho_0}^2\gamma_0 \frac{p_0}{\rho_0} M^2 = \gamma_0 p_0 \rho_0 M^2 \quad .$$

Thus, (17) can be written

$$\frac{p_2 - p_0}{\frac{1}{\rho_0} - \frac{1}{\rho_2}} = \gamma_0 p_0 \rho_0 M^2 \quad . \tag{20}$$

If p_0, ρ_0, γ_0, and M are all specified, then a graph of (20) (with p_2 as the ordinate and $1/\rho_2$ as the abscissa) is a straight line called the *Rayleigh line*.

If a detonation wave is to exist, there must be at least one intersection between the Rayleigh line and the Hugoniot curve. Depending on the strength of the lead shock (as characterized by the parameter M), there may be no intersection, one intersection, or two intersections of the Rayleigh line with the Hugoniot curve.

I have already remarked that the strength of the lead shock (as characterized by the value of M) can be determined uniquely only if boundary conditions are specified (*e.g.* by prescribing the motion of a piston that drives the burnt gas). The question of whether a detonation wave may or may not propagate through a given mixture of fuel and oxidizer can not therefore be settled without specifying some kind of boundary condition.

If the boundary conditions are such that there is at least one intersection of the Rayleigh line with the Hugoniot curve, then the values of ρ_2 and p_2 at the intersection collectively define the thermodynamic state of the burnt gas. The *overpressure* associated with the detonation wave is defined to be $p_2 - p_0$.

The earliest attempt to calculate the speed of a detonation wave relative to the unburned gas by rational methods was apparently that of D.L. Chapman in England [*cf.* Chapman (1899) [10]]. Chapman's results were independently rederived by E. Jouget in France [Jouget (1905,1906) [11]]. Neither of these authors seemed to have fully appreciated the role of boundary conditions in determining the value of M in the system (19) and (20). Both authors instead proposed the *ad hoc* condition that the Rayleigh line intersect the Hugoniot curve at a single point of tangency. This condition is now called *Chapman-Jouget condition*, or C-J condition. Determination of M by the C-J condition fixes the values of p_2, ρ_2, u_2, *etc.* which are then called the *Chapman-Jouget values* of these quantities. Now the C-J value of the speed of a detonation wave relative to the unburned gas is determined by the chemical and thermodynamic properties of the gases undergoing reaction. It thus furnishes a convenient reference scale in the presentation of experimental results.

The first authors to substitute a proper treatment of boundary conditions for the C-J condition worked independently in three countries [Y.B. Zeldovich (1940)[12] in the USSR, J. von Neumann (1943)[13] in the U.S., and W. Döring

(1943)[14] in Germany]. These authors also took the opportunity to incorporate finite reaction rate chemistry in modeling the structure of the reaction zone. The contributions of these authors embody what is now called *the Zeldovich-von Neumann-Döring model* of a unidirectional detonation wave.

3.1.3 EXTERNAL WORK AND DETONABILITY LIMITS. A chemical reaction involving oxidation may be slow or rapid. The prototype of a slow oxidation reaction is corrosion (*e.g.* rusting of a sample of bare iron when exposed to air, moisture, and salt). Any common flame such as a candle flame may be taken as the prototype of a rapid oxidation reaction. The terms *combustion* and *burning* are synonyms that refer to any such rapid oxidation. All such rapid oxidation reactions are *exothermic, i.e.* they are accompanied by a release of thermal energy.

A homogeneous mixture of pure substances in thermodynamic equilibruim is called *flammable* if it will burn in response to some change in thermodynamic state (such as a rise in temperature). The flammability or nonflammability of a mixture of substances is, of course, dependent upon its chemical composition, *i.e.* the relative concentrations of the various substances in the mixture. If a certain list of substances is specified and if one considers all the mixtures that may be formed from them, then some mixtures may be flammable and others may not. Any boundary that separates those mixtures that are flammable from those that are not is called a *flammability limit.*

Flammability limits, as defined above, are chemical in nature and do not depend upon the boundary conditions to which a sample of material is subject. Some authors have proposed that the set of equilibrium mixtures that can be formed from a given list of substances can be divided unambiguously into two parts, namely 'detonable' and 'non-detonable'. If such a proposal were a good representation of nature, one could tabulate detonability limits from numerous detonation test results in the same manner as is done in the tabulation of flammability limits [*cf.* Lewis & von Elbe (1961)[15], table 10, p 535]. The main difficulty with this proposal is that the changes in the fluid properties across a detonation wave are *not* uniquiely determined by the chemical composition and thermodynamic state of the fluid approaching it. Indeed, the strength of an ordinary (inert) shock wave, as may be characterized by the parameter $M = u_0/a_0$ or the strength of the lead shock in a detonation wave is *not* determined entirely by the basic laws of mechanics, thermodynamics, or chemistry. The parameter M can, in fact, only be fixed by specifying boundary conditions, such as the motion of a hypothetical piston that abuts the fluid on the downstream side of the shock or detonation wave (as the case may be).

Suppose that a flammable mixture of gases will ignite if its temperature is raised above some threshold value T_{ai} (*i.e.* the *autoignition temperature*). By sending a piston-driven shock wave through it and by prescribing a piston speed sufficient to raise the ratio T_1/T_0 [*cf.* equation (10) above] above the level T_{ai}/T_0, one may ensure that the gas will ignite and that the resulting reaction zone will follow the shock. Such a procedure amounts to producing a detonation wave and the above argument suggests that all flammable mixtures are detonable.

The argument given above hinges on the idea that a piston can do work on a body of fluid in contact with it. If one allows the piston to do an arbitrarily large amount of such work in a given time interval, then one can always send a detonation wave through any flammable mixture of gases. This argument implies that 'detonability limits' are as broad as 'flammability limits'.

If, however, one incorporates restrictions on boundary conditions into one's definition of detonability limits, then one may well arrive at detonability limits that are narrower than flammability limits. One such restriction might assert that the piston is *at rest* relative to the unburned gas far ahead of it.

3.2 MULTIDIRECTIONAL PROBLEMS

3.2.1 INERT SHOCK WAVES

3.2.1.1 Taylor's expanding sphere problem. As was pointed out in section 3.1.1, the one-parameter family of solutions of the equations for steady non-reacting unidirectional flow with a shock wave can be generated by the solution of a 'piston problem'. Specifically, if gas in a tube is initially at rest and if the gas is set in motion at $t = 0$ by a piston whose velocity rises abruptly in the manner of a step function, then a shock wave propagates ahead of the piston into the region of undisturbed gas. The strength of this shock can be represented by the Mach number $M = u_0/a_0$ (see section 3.1.1 for definitions of the symbols). This shock strength, in turn, can have any positive value. Its value is determined by the speed of the piston. The values of all of the flow quantities behind the shock are then determined by equations (8), (9), and (10).

In the late nineteen thirties, G.I. Taylor in England addressed the question of whether one can formulate a problem in spherical geometry that is analogous to the piston problem described above. Taylor's efforts resulted in a manuscript titled 'The air wave surrounding an expanding sphere' which was submitted for publication to the Royal Society of London in 1939. It was not published until 1946 [Taylor (1946)[16]], owing, apparently, to security classification during World War Two.

Taylor's results show that if the radius R of the expanding sphere increases in time at a constant rate U_2, then a shock wave propagates into the surrounding fluid. The radius r_1 of this spherical shock also increases with time at a constant rate. Taylor's results include tabulations of the distributions of u/a and p/p_0 versus $r/(at)$ and $\beta \equiv U_2/a$, in which a and p_0 are the speed of sound and the fluid pressure, respectivley, in the remote undisturbed air, u is the local instantaneous fluid speed in the region between the expanding sphere and the shock, r is the distance from the center of the expanding sphere to any place where values of the flow quantities are sought, t is the time (relative to a hypothetical reference time when the expanding sphere had zero radius), and U_2 (as stated earlier) is the velocity of expansion dR/dt of the expanding sphere. As before, let the subscript '1' denote conditions immediately downstream of the shock. The ratios ρ_1/ρ_0 and T_1/T_0 may be expressed in terms of the ratio p_1/p_0 by means of the formulas

$$\frac{\rho_1}{\rho_0} = \frac{(\gamma-1) + (\gamma+1)(p_1/p_0)}{(\gamma+1) + (\gamma-1)(p_1/p_0)} \qquad \text{and} \qquad \frac{T_1}{T_0} = \frac{p_1}{p_0}\frac{\rho_0}{\rho_1} \quad ,$$

the first of which is deduced from the system (1), (2), and (5) [*ibid.*, equation (24)] and the second of which follows from the equation of state of an ideal gas. Table 1 and Figures 3 and 4 illustrate some of Taylor's results. In each of the smaller tables in Table 1, the value of p/p_0 corresponding to the largest value of $r/(at)$ is equal to p_1/p_0. Thus, Taylor's tables permit determination of p_1, ρ_1, and T_1 in terms of the driving parameter β and the thermodynamic state of the undisturbed gas. The distributions of ρ/ρ_1 and T/T_1 between the shock and the expanding sphere then follow from the tabulated values of p/p_0 and the adiabatic relations

$$\rho/\rho_1 = (p/p_1)^{1/\gamma} \qquad \text{and} \qquad T/T_1 = (p/p_1)^{(\gamma-1)/\gamma} \quad .$$

These results of Taylor would seem to offer promise in modeling the *initiation* of detonations in spherical geometry. Consider, for example, a localized region of burning gas in which the flame surface (or surfaces) are deflagrations. The instantaneous rate at which thermal energy is released by the burning is influenced by many variables, one of which is the instantaneous *area* of the flame front. For the purpose of comparison, suppose that the flame front at some instant is a closed surface that encloses a given volume. A flame front in the shape of a smooth sphere would have a smaller area (and would, therefore, yield a smaller rate of energy release by burning) than would a flame front with any other shape. At the opposite extreme, one can imagine a flame front with a highly convoluted shape (perhaps as a result of turbulent mixing) whose rate of energy release is, say, two orders of magnitude higher than is that of the spherical flame. Such a region of burning gas would, of course, expand and the flow about Taylor's expanding sphere might be a suitable model to describe the action of a localized region of burning gas on the unburned gas surrounding it. If one supposes that such a model is appropriate, then a scenario for the initiation of detonation might run as follows. The flame front in a localized region of burning gas becomes highly convoluted as a result of turbulent mixing. This convoluted flame front results in a release of thermal energy that is much larger than what would be released if the flame front were smooth and spherical. This rapid release of thermal energy causes the ball of burning gas to expand. This expanding ball exerts an action on the unburned gas surrounding it in the manner of Taylor's expanding sphere including, in particular, the production of a spherical shock wave. The temperature and velocity of the unburned gas both suffer abrupt rises as the spherical shock

$\alpha = 0{\cdot}2,\ \beta = 0{\cdot}203$

r/at	u/a	p/p_0
0·203	0·203	1·0752
0·214	0·182	1·0745
0·228	0·159	1·0727
0·253	0·127	1·0671
0·300	0·090	1·0571
0·374	0·056	1·0431
0·425	0·042	1·0362
0·594	0·018	1·0196
0·766	0·008	1·0087
1·000	0·000	1·0000

$\alpha = 0{\cdot}4,\ \beta = 0{\cdot}410$

r/at	u/a	p/p_0
0·410	0·410	1·295
0·430	0·369	1·293
0·451	0·334	1·286
0·471	0·303	1·280
0·512	0·211	1·263
0·614	0·162	1·213
0·697	0·113	1·173
0·799	0·069	1·122
0·901	0·035	1·068
0·984	—	1·015
1·000	—	1·003

$\alpha = 0{\cdot}5,\ \beta = 0{\cdot}523$

r/at	u/a	p/p_0
0·523	0·523	1·400
0·544	0·481	1·397
0·564	0·444	1·391
0·586	0·411	1·386
0·627	0·353	1·363
0·669	0·304	1·338
0·711	0·262	1·310
0·774	0·209	1·265
0·836	0·162	1·219
0·900	0·120	1·171
0·940	0·093	1·137
0·083	0·065	1·100
1·017	0·031	1·050

$\alpha = 0{\cdot}6,\ \beta = 0{\cdot}638$

r/at	u/a	p/p_0
0·638	0·638	1·569
0·660	0·597	1·566
0·723	0·489	1·539
0·787	0·405	1·494
0·850	0·332	1·437
0·936	0·249	1·349
0·978	0·209	1·300
1·020	0·167	1·245
1·042	0·145	1·186
1·067	0·114	1·169

$\alpha = 0{\cdot}7,\ \beta = 0{\cdot}761$

r/at	u/a	p/p_0
0·761	0·761	1·808
0·782	0·717	—
0·826	0·640	1·786
0·890	0·541	1·736
0·934	0·484	1·692
1·000	0·404	1·612
1·043	0·353	1·550
1·087	0·302	1·480
1·109	0·275	1·442
1·130	0·240	1·399
1·145	0·225	1·365

$\alpha = 0{\cdot}8,\ \beta = 0{\cdot}891$

r/at	u/a	p/p_0
0·891	0·891	2·105
0·935	0·805	2·096
0·980	0·729	2·067
1·025	0·662	2·022
1·068	0·598	1·965
1·114	0·537	1·898
1·158	0·478	1·820
1·203	0·417	1·733
1·225	0·384	1·677
1·242	0·357	1·630

$\alpha = 1{\cdot}0,\ \beta = 1{\cdot}180$

r/at	u/a	p/p_0
1·180	1·180	2·959
1·227	1·088	2·939
1·274	1·004	2·889
1·321	0·927	2·822
1·368	0·853	2·731
1·415	0·779	2·621
1·463	0·704	2·485
1·482	0·670	2·413

$\alpha = 1{\cdot}2,\ \beta = 1{\cdot}520$

r/at	u/a	p/p_0
1·520	1·520	4·250
1·570	1·421	4·231
1·620	1·330	4·169
1·671	1·233	4·067
1·722	1·157	3·927
1·772	1·071	3·747
1·800	1·029	3·636

$\alpha = 1{\cdot}4,\ \beta = 3{\cdot}953$

r/at	u/a	p/p_0
1·953	1·953	6·317
2·010	1·843	6·286
2·065	1·742	6·191
2·120	1·643	6·033
2·175	1·544	5·811
2·215	1·470	5·607

$\alpha = 1{\cdot}6,\ \beta = 2{\cdot}560$

r/at	u/a	p/p_0
2·560	2·560	9·89
2·603	2·474	9·87
2·649	2·385	9·82
2·696	2·291	9·72
2·750	2·198	9·50
2·824	2·050	9·07

$\alpha = 1{\cdot}8,\ \beta = 3{\cdot}60$

r/at	u/a	p/p_0
3·60	3·60	19·7
3·66	3·47	19·7
3·73	3·35	19·5
3·79	3·22	19·0
3·86	3·09	18·3
3·90	3·03	17·9

Table 1. Results from Taylor (1946)[16] on the air-wave surrounding an expanding sphere. Here $\alpha = U_2/c_2$, in which c_2 is the speed of sound in the air at the surface of the sphere. See text for definitions of the remaining symbols. Note that $\beta = U_2/a$, in which a is the speed of sound in the remote undisturbed air. Thus, α and β are two alternative parameters for representing the *rate of driving* of the air by the expanding sphere.

ORIGINAL PAGE IS
OF POOR QUALITY

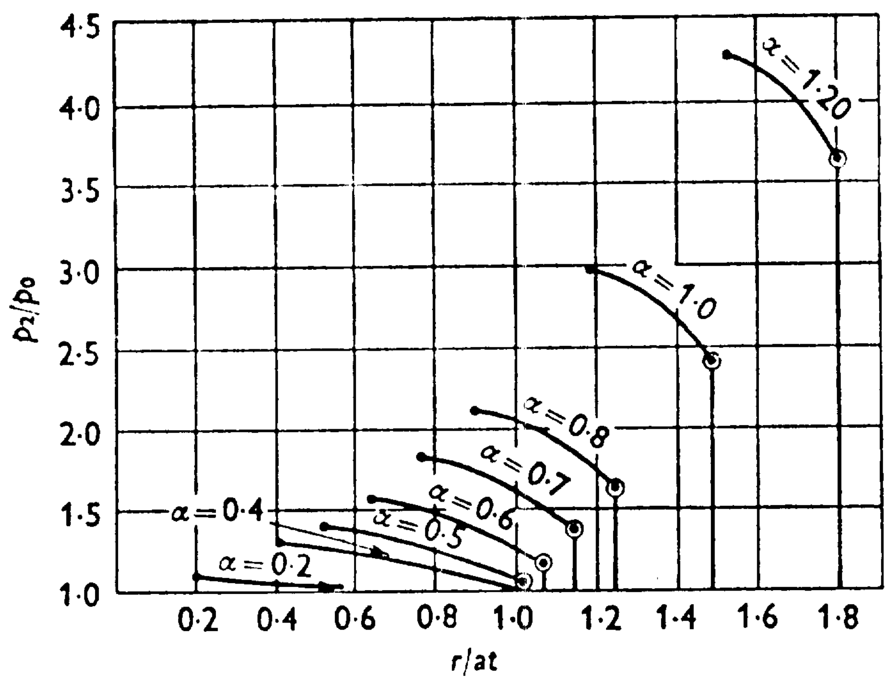

Figure 3. Plots of the pressure distributions in Table 1 [Taylor (1946)[16]]. Each curve corresponds to a particular rate of expansion of the sphere. The leftmost point on each curve corresponds to the surface of the sphere; the discontinuity at the right of each curve corresponds to the shock wave.

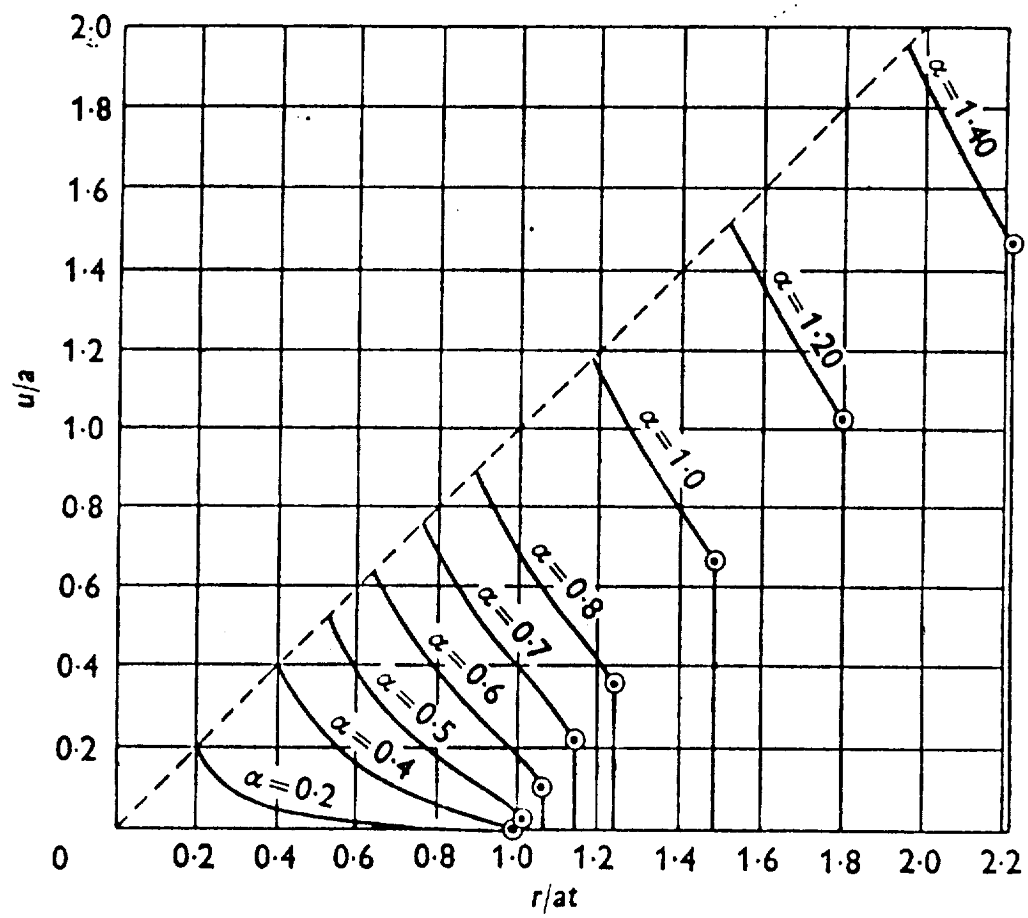

Figure 4. Plots of the radial velocity distributions in Table 1 [Taylor (1946)[16]]. As in Figure 3, the step discontinuities represent the shock wave for each rate of driving. The dashed line represents the trajectory of the surface of the expanding sphere.

passes by. If the latter is of sufficient strength to satisfy the conditions for ignition of the shocked gas, then the shocked gas will begin to react. If, moreover, those conditions are sustained for a sufficient duration of time, then the reaction will proceed to completion. Such a shock followed by a reaction zone is, of course, a detonation wave. The foregoing scenario thus constitutes a mechanism for initiation of a spherical detonation, as asserted.

3.2.1.2 Taylor's fixed-total-energy blast wave problem. In a review article published in *Annual Reviews of Physical Chemistry*, J.H.S. Lee of McGill University [Lee (1977)[17]] discussed efforts to model the intiation of spherical detonations. One such effort (*cf.* p 91 of that paper) employed another of G.I. Taylor's contributions to the theory of explosions [Taylor (1950)[18]]. This paper was written in 1941 in support of the early work on the atomic bomb and remained classified for nine years. Taylor formulated the problem by supposing that a spherical blast wave is generated by the sudden release of a fixed total energy E, which then represents the sum of the thermal and kinetic energies of the blast. In contrast to the action of conventional high explosives, this release of energy was not accompanied by a release of gas through the vaporization of condensed matter. As in the expanding sphere problem, Taylor sought a solution of the equations of motion of compressible (inviscid nonheatconducting) flow in which the distributions of the flow quantities, expressed in terms of appropriate nondimensional variables, are self-similar at all times. Taylor showed that such self-similar solutions exist only in the case when the strength of the shock wave is asymptotically large, thus permitting one to replace the rightmost member of (9), for example, by its asymptotic limit as $M \to \infty$.

Taylor's results include formulas relating the radial velocity dR/dt of the shock to the time t for a given blast energy E. In the model discussed by Lee, a critical value of E was proposed by equating the Chapman-Jouget velocity of a detonation wave [*cf.* section 3.1.2 above] with dR/dt and equating the time t to the time τ for completion of the chemical reaction (the so-called *induction time*). Lee remarks that the values of E so computed are about three orders of magnitude less than are the energies of blasting devices needed to produce spherical detonations in experiments. Lee offers some *ad hoc* explanations for the discrepancy. Curiously, Lee does not impute significance to the discrepancy between the necessarily moderate shock strength in the shock waves produced by blasting caps and the infinite shock strength assumed in Taylor's fixed-E blast wave model. As Taylor points out in his paper, his fixed-E blast wave solution is comparable to blasts produced by conventional condensed matter explosives only if the mass of the air enclosed by the shock is much greater than the mass of the explosive. I do not believe that the conditions of the blasting cap experiments cited by Lee fulfill this condition within the time interval of interest any better than they fulfill the condition of asymptotically large strength.

Lee (1977) does not mention any of Taylor's papers other than the one containing Taylor's theoretical model of the atomic bomb blast. He may be aware of Taylor's work on the air wave surrounding an expanding sphere and have good reasons for rejecting it as a model for initiating spherical detonations. I have not seen any such reasons, however, and lacking them, I am inclined to regard the mechanism for initiating spherical detonations described in the preceeding section as more believable than the one described by Lee (1977).

3.2.2 PROPAGATION OF A SPHERICAL DETONATION WAVE. In his many studies of spherical explosions during World War Two, Taylor also addressed the problem of how to model the *propagation* of a spherical detonation wave. Taylor's theory of the spherical detonation was formulated in the same year as and prior to his work on the fixed total energy blast wave. At that time (January 1941), the standard model for the propagation of detonation waves was the Chapman-Jouget model discussed in section 1.2 above. As I stated there, the important role of boundary conditions in determining the shock strength is not incorporated in the C-J model. Taylor's spherical detonation wave is predicated on the assumption that the C-J condition is satisfied and the applicability of Taylor's spherical detonation model is limited accordingly. In their book *Detonation*, Fickett and Davis (1979)[20] remark that the problem of spherical detonations has still not been properly treated. It is possible, therefore, that Taylor's World War Two contribution, limited as it is, had not been superceded as of 1979. At this point, however, one should call attention to the important book *Similarity and Dimensional Methods in Mechanics* by L.I. Sedov [Sedov (1959)[21]]. In chapter four of that work, Sedov formulates a general analytical framework for generating self-similar solutions of the equations of gas dynamics in one, two and three dimensions. Sedov not only recovers all of the results of Taylor that I have cited so far, but is also able to replace some of Taylor's numerical solutions with closed-form analytical ones. Sedov's contribution goes beyond Taylor's in that Sedov is able to delineate the complete set of circumstances under which self-similar solutions of the equations of reactive gas dynamics with one space coordinate (as occur, for example, in the problem of spherical detonations) are possible. Fickett and Davis do not cite Sedov's book, so it may be that their characterization of post war work on spherical detonations is overly harsh.

Taylor's model of the spherical detonation wave is consistent with the view that a spherical detonation, once initiated, can propagate through the whole region occupied by explosive, *i.e.* there is no *a-priori* reason to suppose that a spherical detonation will extinguish itself after it reaches a certain radius.

As in problems discussed earlier, Taylor sought and found a solution of the equations of motion of a gas in which the distributions of the flow quantities expressed in terms of appropriate nondimensional variables, were self-similar for all times. Since the details of these distributions are less germane to the purposes of this report than is the fact that the whole cloud of gas detonates, I will set aside further discussion of Taylor's theory of spherical detonations.

3.3 REMARKS ON CONFINEMENT

The possibility that a detonation wave will ultimately result from ignition of a given sample of flammable gas is strongly dependent upon boundary conditions. Thus, if the gas is in a tube closed at one end and if the gas is ignited at the closed end, then the likelihood that the resulting flame front will evolve into a detonation is much greater that if the gas were in a spherical balloon high above the ground and the gas were ignited at the center. These two geometries typify 'confined' flows and 'unconfined' flows, respectively.

The notion of confinement is hard to quantify directly, at least if one tries to tie it to geometries of particular solid boundaries in contact with an explosive gas. What really seems to matter is the *dimension* of the *space* in which the gas is allowed to move. Thus, if a gas is constrained to move along parallel streamlines, it is more confined that if it is allowed to move radially along rays perpendicular to an axis (*i.e.* in two dimensional *cylindrically* symmetric motion). This motion, in turn, is more confined than is motion along rays emanating from a point (*i.e.* in three dimensional *spherically* symmetric motion).

The idea that one can better gauge confinement by counting space dimensions in which gas may move than by looking at the detailed geometries of confining walls becomes clear when one contrasts the case when gas is ignited in a tube closed at one end with the case when gas is ignited in a tube closed at *both* ends. If confinement is to be implicated as a factor that always increases the likelyhood of detonation and if wall geometry were the essence of confinement, then gas in a tube closed at both ends should be more prone to detonation than is gas in a tube closed at only one end. I do not believe that such a prediction would be borne out be experiment. Venting of the tube at one end allows the burning gas at the other end to expand and act like a piston that sends a shock wave ahead of it. The formation of this shock wave is a basic step in the evolution of a detonation wave. Sealing a tube at both ends could inhibit turbulent mixing of a initial subsonic flame front, thereby preventing it from accelerating to supersonic velocity and thus inhibiting one mechanism for shock formation.

4. BACKGROUND ON DETONATION OBSERVATIONS

The preceeding section was devoted to descriptions of basic physical phenomena, definitions of terms, and attempts to isolate the basic cause and effect relationships in such phenomena as the initiation of unidirectional and spherical detonation. Thus, while the last section was devoted primarily to theory, the present one is devoted to observations. The number of new papers appearing each year in which results of experiments on detonation are reported is quite large. I have found the review articles by J.H.S. Lee (1977) [17] and Marshall Berman (1985) [22] to be especially useful as introductions to this vast literature. The book by Strehlow (1968) [9] is also an excellent introduction to the general subject of combustion theory and observation. The experimental studies discussed in this section are restricted to those I have read that seem to me to be most informative in regard to the hazard of hydrogen explosions at KSC shuttle launch pads.

4.1 PROPAGATION OF DETONATION WAVES DOWN TUBES AND CHANNELS

4.1.1 LOCAL EXPLOSIONS. Consider a tube filled with an explosive mixture of gases and closed at one end. It may happen that if the gas in the tube is ignited at the closed end, a flame propagates toward the open end, acelerates and eventually evolves into a detonation wave that propagates all the way to the open end of the tube. A beautiful set of photographs, which record many of the physical processes that take place in such an experiment was published by Urtiew and Oppenheim (1966)[23]. One curious feature of detonation waves captured by these photographs is the repeated occurence of localized spherical explosions (which Urtiew & Oppenheim called 'the explosion within the explosion'). Thus, even though the lead shock in a detonation wave may be very nearly planar, the flow behind it is, by no means unidirectional. The intermittent generation of three dimensional local explosions seems to accompany all observations of detonation initiation and propagation.

4.1.2 DETONATION CELL WIDTH AND THE EMPIRICAL FORECASTING OF DEFLAGRATION-TO-DETONATION TRANSITION. If the inside surface of a tube is covered with a smoked foil and if a detonation wave is then sent down the tube in the manner described above, then the detonation wave will scour the foil selectively leaving a cell-like pattern on it [*cf.* Figure 5, taken from Strehlow (1968)[9]]. The task of determining the precise mechanism to account for this wall scouring is a challenge for theoreticians that need not concern us here. Whatever their cause, however, the detonation cells furnish an experimentally observable length scale that typifies the thickness of a detonation wave.

The detonation cell width depends upon the mole fractions of the fuel, the oxidizer, and of any diluting substance that may be present in the mixture of gases upstream of the detonation wave. Given a particular chemical reaction involving combination of a fuel with an oxidizer, one may define a special ratio of the molar concentration of fuel to the molar concentration of the oxidizer which corresponds to the ratio of the same constituents in the reaction product. Such a ratio is called *stochiometric*. Thus, in the reaction $2H_2 + O_2 \rightarrow 2H_2$, a stochiometric mixture of H_2 to O_2 would contain two moles of H_2 for each mole of O_2 . A parameter that represents the closeness of a given mixture to a stochiometric one is the *equivalence ratio* ϕ defined as follows:

$$\begin{pmatrix}\text{equivalence}\\ \text{ratio}\end{pmatrix} \equiv \phi \equiv \frac{\begin{pmatrix}\text{mole fraction of fuel to oxidizer in a}\\ \text{given mixture of substances}\end{pmatrix}}{\begin{pmatrix}\text{mole fraction of fuel to oxidizer in a stochimetric}\\ \text{mixture formed from the same substances}\end{pmatrix}}$$

ORIGINAL PAGE IS
OF POOR QUALITY

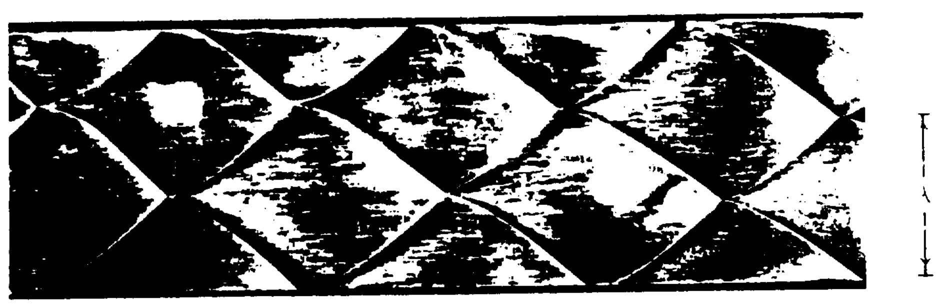

Figure 5. Photograph of the pattern produced on a smoked foil on the wall of a tube down which a nominally planar detonation wave propagates [from Strehlow (1968) [9]]. The wave propagated from left to right. The symbol λ denotes the *detonation cell width*.

Thus, a mixture is fuel-rich or fuel-lean according to whether ϕ is greater than one or less than one, respectively. The value $\phi = 1$ corresponds, of course, to a stochiometric mixture.

By plotting detonation cell width *versus* equivalence ratio, one has a basis for comparing results involving different chemical reactions. An example of such a plot is given in Figure 6 from Berman (1985)[22], which illustrates the dependence of detonation cell width (measured parallel to the plane of the detonation wave) upon equivalence ratio ϕ for hydrogen-air detonations with varying degrees of steam dilution. There does not appear to be any simple accurate fundamental method for the direct analytical calculation of the detonation cell width. By allowing for finite reaction rates in a one dimensional model of the reaction zone behind the lead shock, however, one can define a length scale (the *induction length*) that scales with the thickness of this zone. This induction length may be correlated with the detonation cell width and the curves in Figure 6 illustrate such a correlation.

Many empirical correlations may be expressed in terms of the detonation cell size. Thus, for example, if the plotted detonation cell size for a given mixture of gases is larger than the bore of a tube in which one wishes to detonate that gas, then there is reason to believe that in that tube the gas (in the absence of piston driving) will seem less detonable. Several authors have proposed such ideas and have reported evidence in support of them. One remark made by many such authors is that detonability limits are scale-dependent and that larger-scale boundaries are more conducive to detonation than are boundaries of smaller scale [*cf.* Berman (1985)[22]].

A second kind of empirical correlation involving the detonation cell width is a correlation between the size of the smallest obstacle capable of influencing deflagration-to-detonation transition (DDT) for a given mixture of gases and the standard width of the detonation cells for that mixture. Sherman, Tiezen, and Benedick (1986)[24], for example, have found experimental evidence that a deflagration front propagating down a channel across a regular array of fence-like obstacles may undergo transition to detonation and that this transition to detonation will be influenced by the fences if the spacing between them is of the order of two to three times the detonation cell width. The validity of such a correlation would indicate that small detonation cell sizes correspond to more explosive gases, *i.e.* gases in which DDT may be triggered by smaller obstacles. For stochiometric mixtures of hydrogen and air (with no steam dilution) the detonation cell width λ is between four and six millimeters [*cf.* Figure 6]. If, however, the H_2-O_2 ratio in the mixture is kept the same but steam is added to bring the total steam fraction to twenty percent, then the detonation cell width rises to a value between ten and twelve centimeters. Raising the steam fraction to thirty percent raises the detonation cell size to about thirty centimeters. Hydrogen-air-steam mixtures with steam fractions above fourty-five percent are so inert that no attempts to produce detonation waves in them have yet succeeded.

The observations on detonation described above suggest that the addition

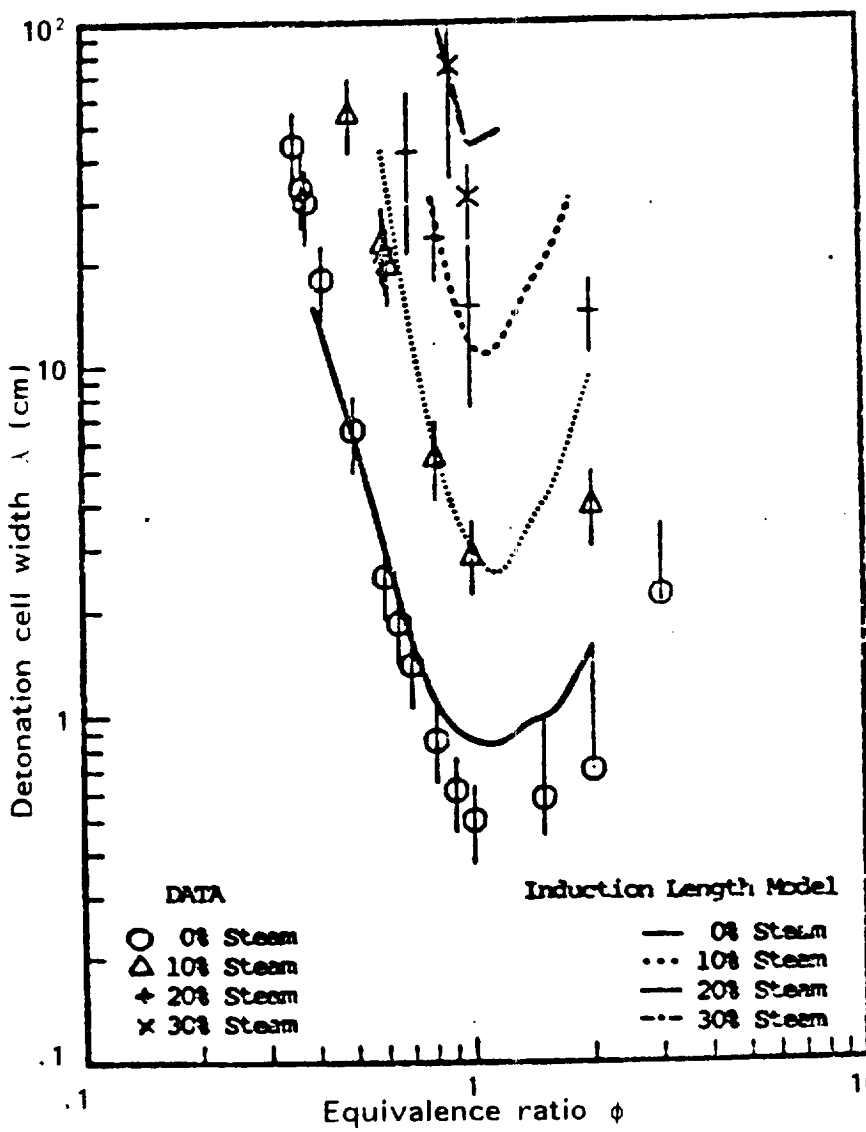

Figure 6. Detonation cell width λ versus equivalence ratio ϕ for hydrogen-air-steam mixtures and correlation with calculated 'induction lentgh' (*i.e.* a typical streamwise thickness of a planar detonation wave, as may be calculated in the Zeldovich-von Neumann-Döring model)[from Berman (1985)[22]].

of steam to the exhaust plume of the space shuttle main engines exerts a powerful effect in reducing the detonability of the gases in it. Such considerations undoubtably played a role in the design of the steam inerting system for the exhaust duct at the Vandenburg launch site. In this context, the effect of the sound supression water spray (SSWS) on the main engine exhaust plume is obviously favorable.

4.2 EXPERIMENTS ON UNCONFINED DETONATIONS. An older study by the Arthur D. Little Company [Anonymous (1960)[25], hereinafter referred to as ADL] contains an impressive compendium of engineering work done in support of the Atlas Centaur program. The report contains results of experiments on detonation of hydrogen-oxygen-air mixtures in spherical balloons situated at a remote distance [*i.e.* many balloon diameters] away from the ground or any other walls. In these experiments, detonations were produced by placing some flame source at the center of the balloon and causing it to ignite. The flame sources ranged from 'weak' sources, represented by sparks, to 'intermediate' sources, represented by squib flames, and 'strong' sources represented by blasting caps and other condensed matter detonators.

Some of the results reported in ADL seem reassuring in the context of this report. Thus, the authors of ADL report (p 18) that 'detonation will not occur when hydrogen is vented to the atmosphere as long as the hydrogen-air mixtures are unconfined and are initiated by ignitors of the non-explosive type'. This conclusion was based upon observations of spherical flames produced at the centers of balloons by weak sources. In these experments, no direct means were provided to produce convolutions of the flame fronts and it may well be that the flames remained nearly spherical. As was remarked in section 3.2.1.1 above, a spherical flame front has the smallest surface area and concomitant rate of energy release of all possible flames that enclose a given volume. Thus, the relatively benign characteristics of the spherical flame produced in the ADL experiments on hydrogen-air mixtures may not be representative of what could happen if the flame front were allowed to be wound up in turbulent eddies (as might be produced, for example, by passage of the flame front across an array of turbulence-producing obstacles). The authors of the ADL report were aware of the importance of turbulence in the flame front. Indeed, they cited such turbulence as their reason for abandoning an attempt to determine the minimum spark energy necessary to trigger a detonation [*cf.* ADL, pp 57-58]. One may surmise from the discussion in ADL that the direct effects of the spark were overwhelmed by the effects of turbulence produced by the instrument supports.

4.3 FURTHER OBSERVATIONS ON DEFLAGRATION-TO-DETONATION TRANSITION. The article by Berman (1985)[22] reviews several experiments on the propagation of flames through bags filled with flammable gases. In one example [*cf.* Moen, Bjerkvedt, Jenssen, and Thibault (1985)[26]], a flame front propagates down the bag, undergoes distortion, and forms a 'tongue of flame' that advances ahead of the main flame front (*cf* Figure 7). When

ORIGINAL PAGE IS
OF POOR QUALITY

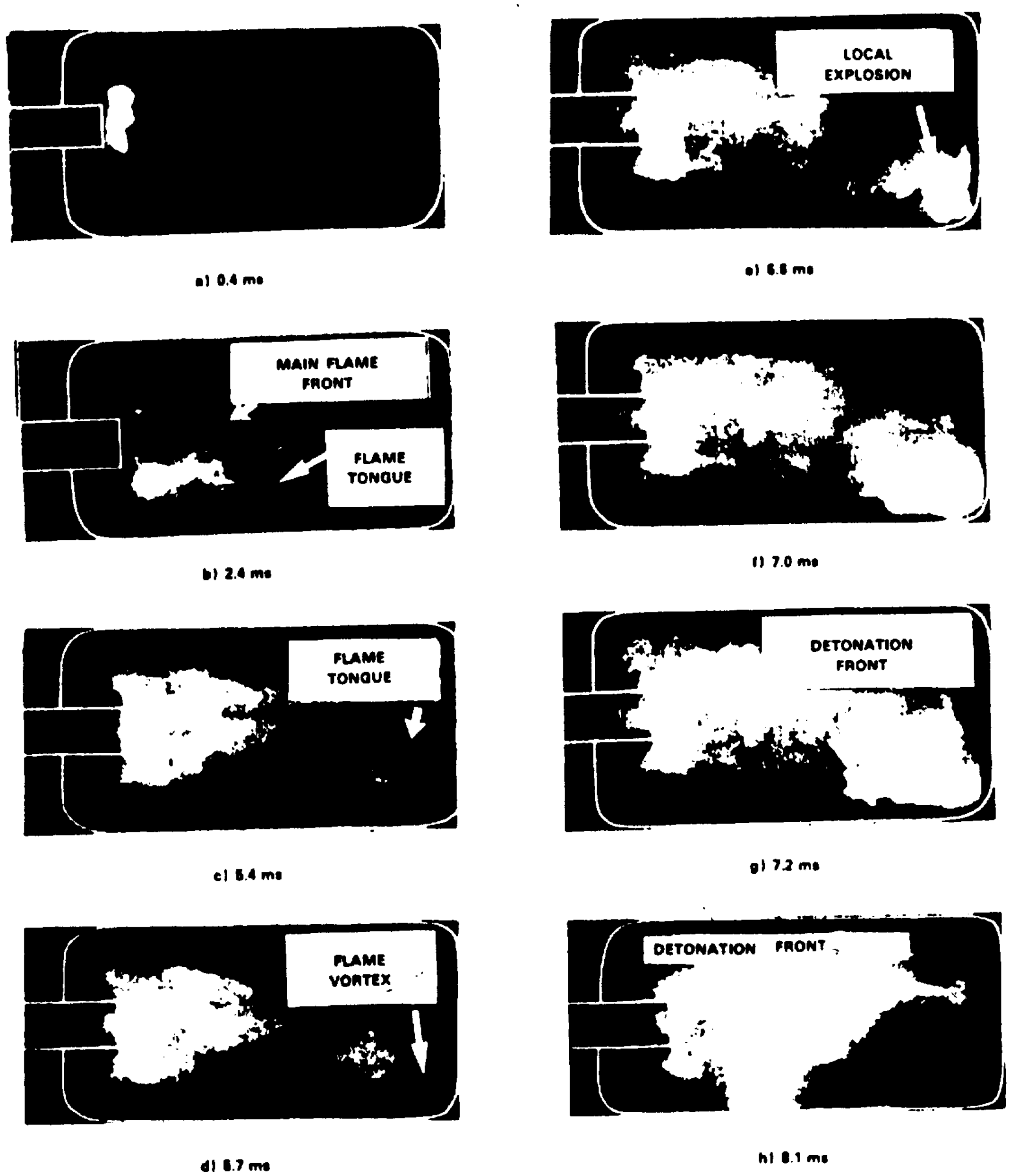

Figure 7. Sequence of still photographs illustrating a case of turbulence-induced deflagration-to-detonation transition in a large gas bag bounded only by one flat floor [from Moen, *et al.* (1985)[26]].

this tongue of flame reaches the far end of the bag, it is wrapped up in a corner eddy. A detonation then originates within this corner eddy and the resulting shock wave propagates through the rest of the facility. In this experiment, the gas bag abutted a solid floor, but was otherwise unconfined. Although the mixture of gases was acetylene and air, Berman (1985)[22] points out that the mixture has the same equivalence ratio and is thus comparable to a hydrogen-air mixture with 19% hydrogen. For comparison, a stochiometric mixture of hydrogen and air has 30% hydrogen. The detonation observed by Moen, *et al.* was not planned as part of their experiment. The reassuring conclusion from the ADL report cited earlier loses some of its force when compared with these results of Moen *et al.*

Results analogous to those of Moen *et al.* have been obtained by German investigators [see Berman (1985) for the original sources] in a large gas bag supported by a metal frame. It appears that passage of a deflagration over one of these supports resulted in the shedding of an eddy which then became the center of a spherical detonation.

In assessing the relevence of these experiments to the conditions at KSC shuttle launch pads, it is important to realize that the gases in the gas-bag experiments were well-mixed, the bags prevented the gases from dispersing, and the gas was initially at rest. All subsequent motion was due to non-uniform energy release by burning. At the KSC shuttle launch pads, the gases are not well-mixed, they are free to disperse, and there is considerable motion in the flame trench, owing to the momentum of the gas in the deflected SSME exhaust plume. The flow inside a jet engine combustor might, in fact, represent the conditions in the flame trench more accurately that does the flow in the gas-bag experiments, owing to the nonuniformity of the fuel-oxidizer mixture, the presence of an overall through flow, and the presence of turbulent mixing.

5. SCENARIO FOR A CATASTROPHIC EXPLOSION

5.1 A SEQUENCE OF ESSENTIAL EVENTS

In section 1.2 above, I listed two questions that guided my work this summer, the first of which was 'Is there a *set of events* common to all credible scenarios leading to a catastrophic explosion near the orbiter?' For the purpose of discussion, I will postuate that the answer is 'yes' and propose the following sequence of essential events.

E1 One or more of the space shuttle main engines discharges unburned hydrogen.

E2 The usual flame in the exhaust plume is extinguished (at least locally).

E3 Some of the hydrogen in the exhaust plume (perhaps the gas below the water curtain) collects in an unreacted cloud rather than burning in the usual blow-torch fashion.

E4 At some later time, the gas in the unreacted cloud is *ignited*.

E5 The flame front is subjected to rapid distortion by turbulent mixing, thus causing a disproportionately large rate of release of thermal energy compared to that released by a laminar flame.

E6 Thermal expansion of the rapidly burning gas forces the unburned gas in its neighborhood out of its way, thereby sending a compression wave into it.

E7 The compression wave generated in E6 steepens to become a shock wave in the usual way.

E8 Passage of the shock wave initiates combustion of the shocked gas.

E9 The combustion initiated by passage of the shock produces rapid thermal expansion which then drives the shock in a self-reinforcing manner (*i.e.* the shock wave becomes a detonation wave).

E10 The detonation wave propagates to the boundary of the cloud of explosive gas, after which it degenerates to a (nonreacting) blast wave. *

E11 The blast wave propagates until it strikes the shuttle orbiter.

5.2 NECESSARY CONTRIBUTING CONDITIONS

Several of the above events can take place only if certain conditions are satisfied. Let t denote the time variable and let t_{E1}, t_{E2}, t_{E3}, ... denote the times corresponding to events E1, E2, E3, ... , respectively. I propose that the necessary contributing conditions corresponding to events E1-E11 listed above are:

NCC1 ($t \leq t_{E2}$) A physical mechanism is avaliable to extinguish the usual flame in the exhaust plume.

NCC2 ($t \geq t_{E3}$) The *amount* of explosive gas and its *placement* relative to the orbiter are such that complete detonation of the material in the cloud could produce a damaging overpressure on the orbiter.

NCC3 ($t \geq t_{E3}$) Dilution of unburned hydrogen with water (from all sources) does not make the mole fraction of H_2 to H_2O so high or low as to exceed the flammability limits for all ternary mixtures of H_2, H_2O, and air.

*It is, of course, conceivable that the shuttle orbiter may abut the cloud of explosive gas, in which case the detonation wave may strike the orbiter directly.

NCC4 ($t \geq t_{E3}$) A mechanism is available to ignite the unburned gas in the cloud.

NCC5 ($t > t_{E4}$) A mechanism is available to induce turbulent mixing in the fluid containing the flame front.

NCC6 ($t > t_{E7}$) The shock wave generated in E7 is of sufficient strength to initiate combustion of the shocked gas.

NCC7 ($t > t_{E7}$) The state of the shocked gas remains conducive to combustion during a long enough time interval for fairly complete combustion to take place.

NCC8 ($t > t_{E10}$) The speed (if any) with which which the center of the explosive cloud moves relative to the orbiter is less than the speed of the blast wave produced in E10 relative to the cloud.

NCC9 ($t > t_{E10}$) The influence of the boundaries is such that the shock wave or detonation wave strength does not diminish to safe levels before the orbiter is struck.

Conditions NCC1-NCC9 are 'necessary' in the sense that if any one of them is blocked, the sequence of events E1-E11 would be interrupted and a catastrophe avoided. The study by Howard (1987)[2] cited in the Introduction may be interpreted as an effort to evaluate the credibility of NCC2. His results indicate that NCC2 is quite credible, *i.e.* it is likely to be satisfied in a typical flight readiness firing or launch abort. The study by Bransford & Voth (1987)[4], which was also cited in the Introduction, may be interpreted as an effort to evaluate the credibility of NCC2 and NCC3. Their results indicate that neither of these results is easy to discredit, owing primarily to the great practical difficulty of estimating the time-dependent spatial distributions of the relative concentrations of H_2, H_2O, and air in the flame trench under realistic conditions.

The description given in section 3.2.1.1 above of how a spherical detonation may be initiated suggests that there may be some necessary contributing conditions in the above list that are easier to discredit than are the conditions examined by Howard (1987)[2] and Bransford & Voth (1987)[4]. Thus, for example, the residual jet momentum of the exhaust plume in the flame trench may cause enough distortion of the fluid to affect conditions NCC6, NCC7, or NCC8. It may well be that the (benign) statistically stationary flow in the combustor of a jet engine may be a more realistic model of flow in the flame trench than is the model of a transient explosion in a quasi-steady body of fluid.

6. JUXTAPOSITION OF REASSURING AND DISQUIETING FACTS

6.1 REASSURING FACTS

In assessing the hazard of hydrogen explosions at space shuttle launch pads one may identify some facts as reassuring. The followinng list is representative.

- If one accepts the idea that the explosivity of a gaseous mixture can be quantified (perhaps by the detonation cell size), then by any such characterization the sound supression water spray acts to make the gases in the exhaust plume of the SSME less explosive.

- The most sobering experimental observations on deflagration-to-detonation transition discussed in section 4.3 above were under conditions that differ substantially from those that prevail in the flame trench at space shuttle launch pads under real operating conditions. In particular, flow due to passage of a deflagration through an initially stationary well-mixed cloud of explosive gas (as in the most sobering experiments) is not the same as flow in the flame trench (which may more nearly resemble the flow in a jet engine combustor).

- The lower density of hydrogen and water vapor compared to air at the same temperature and pressure provides a mechanism for dispersal of explosive gases, namely bouyant convection.

- Residual jet momentum in the deflected exhaust plume acts to transport the explosive gas away from the orbiter.

- Accidental detonations of gases from H_2-O_2 rocket engines are rather rare events. Thus, Littlefield (1987)[3] was able to document only six confirmed detonations out of over 16,000 test firings.

- No explosions have been observed in two aborts and six flight readiness firings at KSC space shuttle launch pads.

6.2 DISQUIETING FACTS

Alongside the above list of reassuring facts, one may list some that are disquieting. Thus,

- The amount of unburned hydrogen discharged by the SSMEs after the hydrogen burn off ignitors are spent (say 400 pounds) is very much greater than the amount needed to produce a blast wave capable of damaging the orbiter (say 6 pounds if detonated at a distance 200 feet from the base of the orbiter) [Howard (1987)[2]].

- Several experimental studies have led to the conclusion that deflagration-to-detonation transition is scale-dependent and that larger scales are more conducive to it [Berman (1985)[22]].

- Several experimental studies have led to the conclusion that deflagration to detonation transition can be triggered by passage of a deflagration across an obstacle and that the threshold size of such an obstacle (as a multiple of the detonation cell width λ) can be quite small [*cf.* Sherman, *et al.* (1986) and section 4.1.2 above].

- Older experimental studies like the one conducted by the Arthur D. Little Company [Anonymous (1960)[25]] which led to the conclusion that unconfined detonations in spherical balloons containing mixtures of hydrogen and air could not be produced by weak ignition sources (like sparks or squibs) were predicated on the assumption that the rate of energy release by the resulting spherical flame is not accelerated by turbulent mixing. Such an experimental test might be quite unrepresentative of the situation in a real flame trench, where the flow is likely to be turbulent. This admonition holds *a-fortiori* if the trench is loaded with instrument holders and other turbulence-producing obstacles.

- Finally, although accidental detonations of gases discharged by H_2-O_2 rocket engines are indeed rare events, they do nevertheless occur.

7. RECOMMENDATIONS

The work that led to this report was guided by the two questions listed in section 1.2 above. I propose that the answer to the first question 'Is there a set of events common to all credible scenarios leading to a catastrophic explosion near the orbiter?' is 'yes'. I have thus proposed a list of such a set of events (*cf.* section 5) and have arranged these events into chronological order. To address the second question, '[Are any] of the above events precluded by present hardware and operating procedures at KSC?' I have proposed a list of 'necessary contributing conditions' all of which must be met if the catastrophe scenario cited above is to be credible. The idea is that *if* any one of these necessary conditions is blocked, *then* the catastrophe is prevented. After reflecting on the credibility of the nine necessary conditions listed in section 5, I have not identified a single one which is easy to discredit, though some might be less difficult to discredit than others.

In an ideal world, one might aspire to achieve a quantitative scientific understanding of the complete three-dimensional unsteady flow in the flame trench under all anticipated operating conditions. The combination of complicated boundary geometry, and the multiplicity of physical processes (*e.g.* phase changes, chemical reactions, heat transfer, *etc.*) operating at once in the flow, however, easily exceeds the capabilities of all methods for achieving such an understanding (computation, analysis, and experiment) with which I am familiar, nor do I believe that such capabilities could be developed in the forseeable future, even with the expenditure of copius resources. In formulating recommendations for further work, therefore, one should take care to recommend tasks which at least *appear* to be tractable. For this purpose, I propose a third guiding question (which augments the two questions given in section 1.2 above), namely

Q3 What conditions would have to be met before one could, in good conscience, abandon further work on the unburned hydrogen problem?

Such a list of conditions might include the following ones.

C1 One must accept the proposition that there is a set of events common to all credible scenarios for a catastrophe and be confident that one has identified all of the events in that set.

C2 One must be confident that one has identified a set of necessary contributing conditions to a catastrophe, any one of which, if blocked, would forestall the catastrophe.

C3 One must be confident that there is at least one necessary condition that is absolutely precluded by present hardware and operating procedures. Here, of course, redundancy is preferable.

The foregoing discussion leads to the following recommendations.

- Devote some future effort on the unburned hydrogen problem to further consideration of the list of necessary contributing conditions for a catastrophe.

- After adopting a list of necessary contributing conditions for a catastrophe, devote some future effort to finding and interpreting simple ideal models of selected flow details. Such details might include: (i) 'flame holding' by stationary obstacles in the flame trench (in the manner of 'flame holders' in the combustor of a jet engine); (ii) distortion of an initially spherical flame front by turbulent mixing and its possible effect on the initiation of spherical detonations; (iii) the action of the sound supression water spray on the SSME exhaust plume, particularly the manner in which drops of liquid water disintegrate and ultimately affect the concentrations of gaseous H_2O in the region below the spray; (iv) the action of bouyancy and residual momentum in the deflected exhaust plume on dispersal of the unburned hydrogen.

Interpretation of simple models of flow details such as those listed above might permit one to dismiss one or more of the necessary contributing conditions for a catastrophe as incredible. Alternatively, if such future studies indicate that certain catastrophe scenarios are indeed credible, then changes in hardware and operating procedures inspired by such studies could produce a real improvement in the safety of shuttle operations.

8. CONCLUSIONS

- A local fireball whose flame front propagates only subsonically (*i.e.* a deflagration) may evolve into one whose flame front propagates supersonically (*i.e.* a detonation) if the rate of release of thermal energy is accelerated by turbulent mixing or by any other mechanism that rapidly increases the flame area. Such deflagration-to-detonation transition is possible even in completely unconfined flow. Thus, the absence of blasting caps or other high energy sources in the KSC flame trench does not, by itself, justify the belief that a hydrogen-air mixture in it could not be detonated by other ignition sources. This conclusion follows from the experimental studies cited in section 4.3, the theoretical considerations reviewed in chapter 3 [see especially section 3.2.1.1] and it is consistent with the conclusions of a study by the Arthur D. Little Company on spark ignition of hydrogen-air mixtures in spherical balloons [see the penultimate 'disquieting fact' cited in section 6.2].

- Any flammable mixture of gases is detonable in the sense that it is possible to produce a one-dimensional detonation wave that propagates through it. Indeed, such a detonation wave may always be produced by placing the gas in a long tube and driving it with a piston. Specifically, if the gas is initially at rest and if the piston undergoes a step change in speed from zero to some constant speed U, then a detonation wave will always result if U is above a certain threshold (whose value depends upon the chemistry of the gas and its initial thermodynamic state). In such an experiment, the boundary does work on the fluid. 'Detonability limits' can therefore be distinct from and narrower than 'flammability limits' only of one adopts a definition of detonability limits that rules out such working on the fluid by the boundaries (at least beyond a certain limited time interval). This conclusion follows from the discussion in section 3.1.3 above.

- Accurate modeling of all the phenomena in the flame trench is not possible at present nor is it likely to become possible any time in the forseeable future. Even without such accurate modeling, however, there are realistic prospects for ruling out accidental hydrogen detonations at space shuttle launch pads. By identifying a list of necessary contributing conditions for a catastrophe and by formulating simple ideal models of selected flow details, there is reason to believe that, in time, one may either discredit one or more of the necessary contributing conditions (thus certifying the safety of the present shuttle system) or identify a change in hardware or operating procedures (which would permit such a certification of the modified system). Such eforts would seem to be worthwhile.

REFERENCES

1. Breit, T.J. & Elliott, G. 'Hydrogen disposal investigation for the space shuttle launch complex at Vandenburg Air Force Base.' *Proceedings, Institute of Environmental Sciences,* 10th Aerospace Testing Seminar, Los Angeles, March 1987.

2. Howard, F.S. 'Hydrogen detonation: quantity versus distance for 1.32 psig pressure.' Technical Report TR-87-2, NASA Kennedy Space Center DM-MED-11, September 1987.

3. Littlefield, M.D. 'Historical data/statistical analysis for LH_2-*LOX* engine testing.' Report KSC-DM-3141, NASA Kennedy Space Center, DM-MED-11, September 4, 1987.

4. Bransford, J.W. & Voth, R.O. 'Assessment of unburned hydrogen hazards associated with launch pad operation of the space shuttle orbiter main engines.' National Bureau of Standards, Center for Chemical Engineering, Boulder, Colorado, October, 1987.

5. Stokes, G.G. 'On a difficulty in the theory of sound.' *Philosophical Magazine,* Series 3, Vol. 23, pp 349-356. Also *Mathematical and Physical Papers of George Gabriel Stokes,* Johnson Reprints Corporation, 1966, Vol 2, pp 51-58.

6. Rankine, W.J.M. 'On the thermodynamic theory of waves of finite longitudinal disturbance.' *Phil. Trans. Roy. Soc.* Vol. 160, pp 277-288, 1870.

7. Hugoniot, H. 'Memoire sur la propagation du movement dans le corps et spécialement dans les gas parfait.' Première partie, *Jour. de L'Ecole Polytechnique,* Cahier VII 1887 pp 3-97; Deuxieme partie, Cahier LVIII, 1888, pp 1-125.

8. Liepmann, H. & Rosko, A. *Elements of Gasdynamics.* Wiley, 1957.

9. Strehlow, R.A. *Fundamentals of Combustion.* International Textbook Co., 1968; Reprinted by Krieger Pub. Co., Melbourne, FL, 1979.

10. Chapman, D.L. 'On the rate of explosion in gases.' *Philosophical Magazine,* Series 5, Vol 47, pp 90-104, 1899.

11. Jouget, E. *Journal of Pure and Applied Mathematics* Series 6, Vol. 1 p 347, 1905 and Vol. 2, p1, 1906.

12. Zeldovich, Ya. B. 'On the theory of propagation of detonation in gaseous systems.' NACA TM 1261, 1950. Translation of 'Teoriya Goreniya i Detonatsii i Gasov.', *J. Exp. Theoret. Phys.* USSR Vol. 10, p 542, 1940.

13. von Neumann, J. 'Theory detonation waves.' O.S.R.D. Report no. 549 Ballistic Research Lab, File no. X-122, 1942. Also in *John von Neumann, Collected Works*, edited by A.J. Taub, Macmillan Company, N.Y., Vol. 6, pp 203-218.

14. Döring, W. 'Über den Detonationsvorgang in Gasen.' *Annalen der Physik*, Vol. 43, pp 421-436, 1943.

15. Lewis, B. & von Elbe, G. *Combustion, Flames, and Explosions in Gases.* Second edition, Academic Press, N.Y. 1961.

16. Taylor, G.I. 'The air wave surrounding an expanding sphere.' *Proc. Roy. Soc. (Lond.)* A Vol. 186, pp 273-292, 1946; Also *Scientific Papers of G.I. Taylor*, Cambridge U. Press, Vol. 3, pp 412-428, 1963.

17. Lee, J.H.S. 'Initiation of gaseous detonation.' *Annual Reviews of Physical Chemistry*, Vol. 28, pp 75-104, 1977

18. Taylor, G.I. 'The formation of a blast wave by a very intense explosion.' *Proc. Roy. Soc. (Lond.)* A pp 159-174, 1950; Also *Scientific Papers of G.I. Taylor*. Cambridge U. Press Vol. 3, pp 493-509, 1963.

19. Taylor, G.I. 'The dynamics of combustion products behind plane and spherical detonation fronts in explosives.' *Proc. Roy. Soc. (Lond.)* A Vol. 200, pp 235-247; Also *Scientific Papers of G.I. Taylor*, Cambridge U. Press, Vol 3, pp 465-478, 1963.

20. Fickett, W. & Davis, W.C. *Detonation*. University of California Press, Berkeley, 1979.

21. Sedov, L.I. *Similarity and Dimensional Methods in Mechanics*. Academic Press, N.Y., 1959.

22. Berman, M. 'The effects of scale and geometry on hydrogen-air detonations.' Paper presented at the 23rd ASME/AIChE/ANS Conference, Denver, August 6-9, 1985. Department of Energy report number DE 85-006762 [Available NTIS].

23. Urtiew, P.A. & Oppenheim, A.K. 'Experimental observations of the transition to detonation in an explosive gas.' *Proc. Roy. Soc. (Lond.)* A, Vol. 295, pp 13-28, 1966.

24. Sherman, M.P., Tiezen, S.R., & Benedick, W.B. 'The effect of obstacles on flame acceleration and transition to detonation in a large channel.' Paper presented at the 21st International Symposium on Combustion, Munich, August 3-8, 1986.

25. Anonymous, 'Final report on an investigation of the hazards associated with the storage and handling of liquid hydrogen.' Arthur D. Little Company, Report no. ADL C-61092, USAF Headquarters, Air Research and Development Command, Air Force Ballistic Missle Division, Los Angeles, July 15, 1960.

26. Moen, I.O., Bjerketvedt, D., Jenssen, A., & Thibault, P.A. 'Transition to detonation in a large fuel-air cloud.' *Combustion and Flame*, Vol. 61, pp 285-291, 1985.

INDEX OF TERMS