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13. ABSTRACT (Maximum 200 words)

A pilot-scale supersonic combustion tunnel was designed and constructed to operate with initial stagnation temperatures up to 900 K and static pressure and stagnation temperature ranges of 0.01-0.1 atm. and 290-900 K, respectively, in the test chamber without vitiation of the nitrogen/oxygen gas supply. Through the addition of hydrogen in the upstream settling chamber, the effective operating stagnation temperature in the test section was extended to 1100 K. The tunnel facility was instrumented with a Schlieren/shadowgraph system and charge-coupled device (CCD) intensified imaging of chemiluminescence from excited state hydroxyl radicals to study the initiation and combustion properties of nitrogen-diluted hydrogen/oxygen mixtures under Mach 3.0 flow conditions over both flat plate and wedge-shaped center bodies. Reaction initiation by recovery effects on noncatalytic and catalytic surfaces, as well as through seeding of the flow with radicals, was investigated.

14. SUBJECT TERMS

Mixing, Ignition, Supersonic Flow, Scramjet

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Objectives:

Supersonic combustion has received considerable attention in recent years for application to air-breathing propulsion systems at hypersonic flight speeds. The increased intake air recovery temperatures associated with flight in the hypersonic range (beyond Mach 6) point to utilizing thermal self-ignition of fuels in supersonic ramjet combustors. Improved understanding of chemical kinetics, heat transfer, and mixing processes in high speed flows is critical to successful implementation and optimization of the engine design. These issues form the basic building blocks necessary to develop computational models of sufficient robustness to project scaling effects as different engine designs are studied. Computational fluid dynamics (CFD) has seen major breakthroughs thanks to ever-increasing computing power, speed, storage, and improved algorithms. But the simplified and/or empirical nature of the engineering submodels makes it imperative that benchmark experiments are available for investigating various aspects of these high speed flows and to provide a primary database with which to validate the numerical modeling efforts. It is important to initially examine situations in which the flow conditions are simplified (laminar) in order to decrease the overall modeling complexity of the system. A two-dimensional, reacting, supersonic laminar flow is one such system which can be realistically studied in an experimental setting.

The objectives of the work under this AASERT Grant (Grant No. F49620-93-1-0478) were to augment efforts performed under the ongoing AFOSR URI Program "Turbulent Reacting Flows at High Speed" (Grant No. F49620-93-1-0427). Specifically, this work pursued the development and application of techniques for achieving localized, controlled ignition and heat release in supersonic, reacting flows. To accomplish these tasks, a pilot Mach 3 Combustion Tunnel facility capable of accommodating various ignition sources and characterization diagnostics was developed. Ignition processes of nitrogen diluted hydrogen/oxygen mixtures were studied near and over the surfaces of two types of center-body models (flat plate and wedge) utilizing Schlieren/shadowgraph as well as chemiluminescence imaging. Results from studies performed in the pilot scale facility provided fundamental insight into the governing physical processes of high speed reacting flows, as well as design information for the construction of a full scale combustion facility at the Forrestal campus.

In addition to providing general design background for the full scale facility, the present work was directed toward developing and analyzing methods for achieving localized, controlled ignition and heat release within a supersonic reacting flow. Specifically, the issue of ignition of hydrogen-oxygen-nitrogen mixtures in a laminar boundary layer over a flat plate or wedge in supersonic flow was addressed. Boundary layers in high speed flows can generate heat through viscous dissipation providing a mechanism for stimulating ignition. If the boundary layers are laminar rather than turbulent, the modeling complexity of the problem is substantially simplified.

Hydrogen was chosen as the test fuel because the H_2-O_2 chemistry has been extensively studied in a variety of experimental systems over a wide range of conditions, and chemical kinetic modeling efforts here at Princeton have been extensive (Yetter, et al., 1991; Kim, 1994). Under the parent grant, these kinetics have recently been studied and

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validated experimentally at sub-atmospheric pressures, and perturbations of the kinetics by possible contaminants such as NO_x continue to be under investigation.

The unique explosion limit behavior of the hydrogen-oxygen system provides an innovative means of potentially igniting reactive pre-mixed H_2 - O_2 - N_2 mixtures in a supersonic stream. Explosion limits of combustible mixtures are essentially mappings of the pressure and temperature conditions that separate regions of slow and explosively fast reaction for a particular equivalence ratio. The "classical" explosion limits for a stoichiometric H_2 - O_2 mixture are shown in Fig. 1. Above the limits, the reaction chemistry is very fast from thermal self-heating, but more importantly from chemical chain branching. A point between the second and third limits in the non-explosive regime is used to represent initial conditions in the settling chamber of a supersonic wind tunnel. Isentropic expansion to Mach 3, and subsequent recovery in a boundary layer at near-constant pressure assuming an adiabatic wall thermal recovery factor of about 0.85 puts the system inside the second explosion limit. This diagram supports the possibility of mixing the reactants at conditions where the reaction chemistry is slow (and therefore not likely to proceed to ignition in the residence times available), and then creating through recovery downstream conditions in the supersonic stream where the chemistry is chain-branched and very rapid in comparison to the available residence times.

Maintaining laminar flow conditions in such experiments is desirable for several reasons. Numerical modeling for laminar flows is less computationally intensive because it eliminates the fluctuation of velocities, concentrations, and other variables. Turbulent transport and its interaction with a chemically reacting system often makes modeling problems intractable. Maintenance of laminar conditions requires that test section static pressures be very low (0.01-0.07 atm). Most combustion studies in supersonic wind tunnels to date have employed static pressures on the order of one atmosphere.

Research Activities:

Figure 2 shows the arrangement of the pilot scale supersonic facility constructed to perform this work. The test section itself was manufactured of 304 stainless steel with quartz windows on the nozzle/test section. An electrically heated packed bed, followed by heated and insulated transfer lines was utilized as the primary means of increasing the stagnation enthalpy of the nitrogen/oxygen flows to the settling chamber upstream of the nozzle/test section. For extended operation at higher stagnation temperatures, controlled quantities of hydrogen were injected at the entrance to the settling chamber and oxygen flows were supplemented to further increase the enthalpy of the stream by vitiation. Successful operation with runs as long as seven minutes or more have been achieved with flow rates around 15 g/s. An ejector was used to achieve the desired pressure ratio P_0/P_{exit} (7:1) for tunnel startup. The nitrogen motive flow was utilized to dilute the tunnel gases, resulting in reasonable exhaust temperatures and quenching any reactions downstream of the ejector. A silencer was also installed downstream of the ejector to reduce ambient operational noise.

Figure 3 is a photograph of the settling chamber, nozzle and test section, with a thermocouple and pitot probe in place where the center-body models were placed in this work. The settling chamber has a 7.62 cm diameter circular cross-section, with a smooth

transition to two-dimensional conditions in the nozzle section (rectangular cross-section 7.62 cm by 2.54 cm at the inlet, 12 cm long). The nozzle contour was designed to provide a smooth and ideally isentropic transition from subsonic speeds ($M_0 << 1$) to a supersonic design Mach number (M_{test}) of 3. Test section dimensions are 2.54 cm by 2.54 cm over a 15 cm length. The parallel walls of the tunnel consist of removable plates with two polished optical-grade fused quartz windows 27.84 cm long and 5.00 cm high. The windows provided universal access for optical diagnostics, including ultraviolet (UV) imaging of spontaneous emission from electronically excited hydroxyl radicals (see below). A diffuser was incorporated downstream of the test section to decelerate the flow with minimal loss in total pressure. Finally, addition of trip wires to the nozzle walls was used to prevent laminar separation of the flow during startup and operation, as well as eliminate shock-induced boundary layer transition which inevitably results in an increased boundary layer thickness. Further design details are available in the M.S.E. thesis of Mr. Fielding. Table 1 summarizes the operational characteristics of the facility.

Table 1: Summary of the Operating Characteristics

Design Mach number:	3	
Settling Chamber		
Stagnation Temperatures:	300 - 1100	K
Stagnation Pressure:	0.46 - 1.5	atm
Test Section		
Static Temperatures:	110 - 400	K
Static Pressures:	0.01 - 0.1	atm
Reynolds number:	20000 - 175000	per inch
Mass flow rates:	10 - 30	gm/sec

Because run times were short, a microcomputer-based system was developed to acquire, display, and save important variables during operation of the wind tunnel. Data were logged on an IBM PC equipped with an Analog Devices A/D board (16 analog channels with 0-10 volt input signals at a 31.2 kHz sampling rate and ± 0.02% full-scale accuracy). Pressures were measured using variable capacitance absolute pressure gauges (0.5% of reading with a temperature coefficient of 0.04% reading/°C). Flow rates of the fuel and oxidizer were measured (±0.5%) using mass flowmeters. Choked orifice calculations were used to define the primary nitrogen flow (+5%/-2%) from stagnation parameter measurements.

Static conditions inside the test section were calculated using isentropic flow relationships, the conditions upstream of the nozzle inside the settling chamber, and the test section Mach number. Total temperature (± 3 K) was measured with a type K exposed junction thermocouple located at the centerline of the settling chamber. Total pressure measurements were obtained at a static tap in the settling chamber wall at the same axial location as the total temperature thermocouple.

Nitrogen was used as the main tunnel flow (Liquid Carbonic, >99.998%). Oxygen (Airco, >99.993%) was mixed several meters upstream of the stagnation chamber and

hydrogen (Matheson >99.99%) was injected into the tunnel flow at points in the settling chamber section.

Flow visualization inside the supersonic test section was achieved through the use of Schlieren or shadowgraph techniques. An electronic stroboscope followed by an adjustable iris was used as a point light source for a typical two-mirror Schlieren system. A high resolution video camera and video cassette recorder were used to obtain real-time and recorded Schlieren images. Spontaneous emission from electronically excited hydroxyl radicals (OH*) within the nozzle and test section was also imaged using a UV-sensitive video camera. The OH* radicals which are produced in a reaction zone are de-excited by

$$OH^* + M = OH + M \qquad \text{(quenching)}$$

$$OH^* = OH + h\nu \qquad \text{(emission)}$$

producing chemiluminescence from the electronic transition $^2\Sigma^+$-$^2\Pi$ in the ultraviolet OH band at 306.4 nm. A glass UV filter assembly was used to reduce visible and infrared emission records (generated from hot metal surfaces). An analytical line filter (10 nm band width, centered at 307.1 nm), was also used in selected cases to verify that chemiluminescence arising from the (0,0) transition of the electronically excited hydroxyl radicals was indeed the source of uv emission. However, the low peak transmittance required increased gain, reducing the resolution of the video image, and thus, the glass filter assembly was utilized in a majority of the work.

Experimental Results

Numerous experiments were conducted to investigate chemical reaction of the hydrogen-oxygen system in a laminar boundary layer formed over two different test model geometries including:

- Flat plates, with and without catalytic platinum coating
- 12.7 degree (total angle) wedge

Supports for the models were typically streamlined wedge shapes positioned such that the surface of the model was at the centerline of the flow stream, and the supports were fastened to the lower wall of the test section. Disturbances to the flow stream in the form of oblique shocks and the reflected shock train remained below the model surface, leaving the boundary layer on the top surface of the model undisturbed.

In addition to implementing different test section models, increases in stagnation temperature and variation of radical concentrations in the entering flow were studied by varying the location and magnitude of hydrogen injection upstream of the nozzle throat. Operating pressures could not be varied significantly, however, due to ejector operating constraints. As the location of the hydrogen injector exit plane was moved closer to the nozzle throat, less time was provided for fuel mixing with the nitrogen and oxygen. With the injector further upstream, turbulent Reynolds numbers inside the settling chamber, combined with longer residence times due to low subsonic convective velocities provided effective mixing for the gas stream prior to entering the two-dimensional transition. For injector locations nearest the nozzle throat, the fuel was poorly mixed within the flow. Exemplar observations over the two center-body types are presented in Figs. 4, 6-9, with conditions for Figs. 6, 7 and 9 summarized below in Table 2.

Table 2: Summary of Experimental Conditions for Figs. 6, 7, and 9

Test Section Geometry	Injector Pos. (cm)	T_0 (K)	P_0 (atm)	Mole Fraction (%)		Figure	Notes
				$H_{2,\,inj}$	O_2		
Flate Plate	-29.8	920	0.65	5%	10%	6	a
Flate Plate	-14	930	0.66	3%	10%	7	b
Wedge	-2.54	1070	0.53	1%	20%	9	c

[a] Chemiluminescence in boundary layer and wake
[b] Emission outlines shock structure
[c] Chemiluminescence surrounds wedge

For the flat plate experiments a 0.16 cm thick stainless steel flat plate of length 5.4 cm was inserted at the centerline of the wind tunnel. In some of the experiments, the top surface of the plate was coated with a thin catalytic film of platinum, approximately 0.1 mm thick. The flow was turned along the bottom of the plate by a 14° angle, in order that the boundary layer formation along the top of the plate remain undisturbed by the

presence of an oblique shock. The tip of the flat plate was positioned 8.9 cm from the nozzle throat, at the beginning of the constant area test section.

A typical shock formation over a flat plate similar to that used in the reacting flow experiments is shown in Figure 4 for a non-reacting flow with a stagnation pressure of 0.6 atm and stagnation temperature of 420 K. Clearly visible are the oblique shock created from turning the flow beneath the plate, and the subsequent expansion fan. The shock structure seen above the plate is the weak shock created from initial formation of the boundary layer along the top surface of the plate. Measurements of the shock angles give a value for the free stream Mach number of 2.8. This is lower than the design value of Mach 3 because boundary layer growth along the contoured nozzle and windows of the test section effectively decreases the area ratio. When this effect on the area ratio is taken into account, the computed Mach number for these conditions is 2.85, in good agreement with the experimental measurement. The boundary layers are visible over both the plate and at the walls of the test section, and the shear layer formed in the wake of the test geometry is also apparent. Measurement of the boundary layer thickness over the plate gives a value of 0.6 mm, in excellent agreement with a calculated value of 0.56 mm at the end of the flat plate assuming a laminar boundary layer. The flat plate used in reacting flow experiments described below differed from that in Fig. 4 in that the rear portion of the plates was flat instead of tapered.

Several positions of hydrogen injection were investigated in both the flat plate and wedge model testing (Figure 5). A typical result for fuel injection at position #1 is documented in Fig. 6. Combustion heating was used with a hydrogen flow rate of 1% by volume to obtain the noted stagnation conditions. Chemiluminescence was observed to fill the entire converging portion of the nozzle, clearly indicating that the reaction was initiated at a location upstream of the throat. The flow was quenched in the nozzle, and gray scale images of OH chemilumenscence along with other noted flow characteristics are shown in the figure. Chemiluminescence was visible in the boundary layer on the top and bottom of the plate, as well as in the subsonic wake at the rear of the plate.

The qualitative nature of the diagnostic made it difficult to quantify how much of the fuel was consumed prior to entering the test section. However, one-dimensional calculations indicated that reaction was probably completed upstream of the nozzle. Consistent with complete mixing of the injected hydrogen, chemiluminescence did not appear preferentially over the top or bottom surface of the plate, and absolute intensities varied slightly for different trial runs. Typical boundary layer thickness over the top of the plate was measured to be 1 mm, and the luminous region within the boundary layer appeared to vary in thickness over its length.

When settling chamber total temperatures were lowered such that ignition of the hydrogen did not occur upstream of the throat, no chemiluminescence was observed in the test section. The absence of pre-reaction inside the settling chamber was identified by a decrease in total temperature during fuel injection rather than a temperature rise, and the lack of chemiluminescence in the contraction of the nozzle. Thus, high radical concentrations frozen in the flow after the expansion appear to lead principally to recombination effects inside the boundary layer.

With the injector positioned closer to the nozzle throat and at the entrance to the two-dimensional transition, ignition occurred upstream of the contraction, and test section

chemiluminescence was no longer confined to the boundary layer and the wake region of the flat plate. The emission, shown in gray scale in Fig. 7, filled the test section for hydrogen mass flow rates of 3% by volume of the total flow. Beneath the plate, the oblique shock and expansion fan are clearly outlined as a result of the chemiluminescence. The intensity of the chemiluminescence clearly increased behind the oblique shock, and then decreased in intensity as the pressure drops through the Prandtl-Meyer expansion.

Some luminosity was again present in the boundary layer on the plate surface, increasing in intensity at a distance of 1.5 cm from the plate tip. The thickness of the luminous layer was around 0.4 mm (± 0.15 mm) compared with a non-reacting laminar calculated value of 0.9 mm. Chemiluminescence did not always appear in the boundary layer, and in instances where occurred, it appeared at the start of hydrogen injection and then tended to disappear as the tip of the plate began to heat.

As with the previous injector position, unless reaction was initiated upstream of the nozzle, no chemiluminescence was observed in the test section. Test section temperatures in the wake of the flat plate were measured in excess of 1000 K for the maximum injected hydrogen flow fraction. Finally, for a fuel injection location of 2.54 cm from the throat of the nozzle, no chemiluminescence was observed anywhere in the nozzle or in the tunnel. Test section temperatures measured in the wake of the flat plate showed significant temperature drops during hydrogen injection.

A 12.7 degree (total angle) wedge geometry was designed such that oblique shocks formed over both sides of the wedge, with consequent increase in static pressure and temperature. The rear of the wedge was truncated to create a large re-circulation zone in the wake and the model thickness was increased to 3.18 mm. It was anticipated that the longer residence times associated with local subsonic velocities in the wake would make conditions more favorable for reaction. Overall length of the model is 2.7 cm.

Schlieren images of the wedge in supersonic flow is presented in Fig. 8. From the angle β of the shock emanating from the tip of the wedge and the flow deflection θ, the Mach number was determined to be 2.6. The structure of the wake was visible including the corner expansion, wake shock, and re-compression shock in the downstream region. Slight asymmetry in the flow downstream of the wedge resulted from the model support (swept-back shape silhouetted in the figure) oblique shocks from the side and lower wall, and the interaction with the two-dimensional wake.

With 1% hydrogen injection located at location #3, chemiluminescence surrounded the wedge as shown in gray scale in Figure 9. The pattern clearly outlined the fluid mechanical structures such as the oblique shocks emanating from the wedge tip. The luminosity appeared to extend over the length of the nozzle expansion from the injector to the wedge location and throughout the remainder of the test section. However, luminous intensity in the wake was virtually nonexistent. Attempts to ignite the mixture in the wake using a 0.25 mm tungsten wire as a thermal source were unsuccessful.

Accomplishments/Findings:

Chemiluminescence has been observed inside the test section using the ignition techniques described above and with two different plate geometries. For the flat plate geometry with catalytic surface, reaction was observed in the boundary layer and wake

region of the plate for stagnation temperatures of 920 K and pressures of 0.6 atm. However, no differences were apparent with or without platinum coating. Thus no conclusive experimental evidence was found to support the effectiveness of the platinum surface in enhancing the reaction. Zero dimensional modeling calculations suggest that the observed chemiluminescence was primarily a result of radical recombination reactions. With a wedge geometry and increased stagnation temperatures up to 1070 K, reaction was observed in a region behind the oblique shocks generated from the leading edge of the model. In this case, reaction was stimulated through a combination of the higher free stream temperatures and radical concentrations.

Zero and one dimensional modeling calculations were utilized to assist in qualitatively interpreting observations. These calculations suggest that the noted emissions were due primarily to radical recombination conditions, with much of the radicals generated in the pre-reaction phase rather than from locally enhanced reaction of hydrogen and oxygen near the plate surface. However, the modeling work brought to light new insights both to the experimental observations and to the proposed mechanism for achieving pre-mixing and ignition discussed depicted in Fig. 1.

Using a hydrogen-oxygen kinetic mechanism experimentally validated under the parent grant to this work, zero-dimensional calculations can be performed to determine under what environmental parameters reaction will be initiated and proceed in the available observation times. The analyses are best represented in terms of a Damköhler number, Da , where

$$\mathrm{Da} = \frac{\tau_f}{\tau_c}$$

A characteristic time, τ_c, for the overall reaction can be expressed by examining the ratio

$$\tau_c = \frac{[H_2]_{in}}{\left.\frac{d[H_2]}{dt}\right|_{max}}$$

where $[H_2]_{in}$ is the concentration of hydrogen injected into the system, and $d[H_2]/dt_{max}$ is the maximum rate of change in hydrogen concentration. This time includes both the time for the reaction initiation and a measure of the time necessary to consume the initial reactants.

Characteristic observation time is defined using a characteristic length divided by the velocity of the stream.

$$\tau_f = \frac{L_c}{U_0}$$

In the experimental system, obvious choices for these values would be the desired characteristic reaction length scale and the free stream velocity,

$$U_0 = M_\infty \sqrt{\gamma RT}$$

where γ is the specific heat of the mixture, R the gas constant, and T the local absolute temperature. Convective times within a boundary layer formed in supersonic flow are considerably longer than those of the free stream, approaching infinity at the surface.

However, to spread the reaction into the flow above a surface, Da>1 must exist in the flow.

The effect of varying the pressure on Damköhler number is shown in Figure 10 for an equivalence ratio of 0.5. As pressure is increased from 0.01 to 3 atm, Da becomes a linear function of initial temperature). The sudden drop in Da at the low temperature limit of each curve corresponds to the explosion limit condition.

From this information, contours of Da = 1 can be constructed in the pressure-temperature plane for a Mach 3, ϕ = 0.5, H_2 - air system, with varying characteristic lengths, as represented in Figure 11. These characteristic lengths estimate the distance over which the fuel would be consumed a supersonic free stream. Two calculations are represented corresponding to isobaric and isothermal conditions. It is significant to notice the convergence of the isobaric Da=1 contours above approximately 0.7 atm, as a result of chemical branching, delineated by the extended second limit. When the release from the reaction is included in the analysis, the pressures at which reaction can be obtained in a given characteristic length become lower. However, for a given characteristic length, the isobaric and isothermal results converge as operating pressure is reduced. At these conditions, the disappearance of initial reactants does not yield large exothermicity, but large quantities of radicals (with high heats of formation). The overall reaction rate of fuel becomes the limiting reaction time rather than the time required for reaction initiation. In the experiments presented above, the conditions were such that reaction times could not be obtained in the length scale of the models unless recovery temperatures were of the order of 1800 K (which could not be achieved within experimental constraints). These results suggested that successful operations of the pilot tunnel can be obtained with different ejector designs and operating pressures in the test section higher than about 0.5 atm. The important new finding, is that there is a limiting pressure below which exothermicity is not achieved from the reaction, and reaction rates of the fuel, not chemical initiation become the limiting kinetics. The operating principles depicted in Fig. 1 appear to be achievable in a range of operating parameters where the third limit explosive condition is avoided in the mixing time, and the after initiation by recovery remains substantially exothermic. Continuing work will look at these conditions using more variable ejector/supply conditions available in the gas dynamics laboratory at the Forrestal campus.

Personnel Supported

Drs. Dryer, Smits and Yetter have been associated with the present work. A second-year graduate student (academically advised by Dr. Dryer), Mr. Joseph Fielding, has performed the research and was supported by these resources. Mr. Fielding has submitted an M.S.E. thesis which describes the work in greater detail and will be approved by the University in January, 1997.

Publications: "An Experimental Study of Supersonic Laminar Reacting Boundary Layers", J. Fielding, M.S.E. Thesis, Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, January, 1997. MAE Report No. 2090-T.

Interactions/Transitions

a) Participation: none
b) Consultative/Advisory Functions: none
c) Transitions: none

Discoveries, Inventions or Patent Disclosures: none

Honors/Awards: none

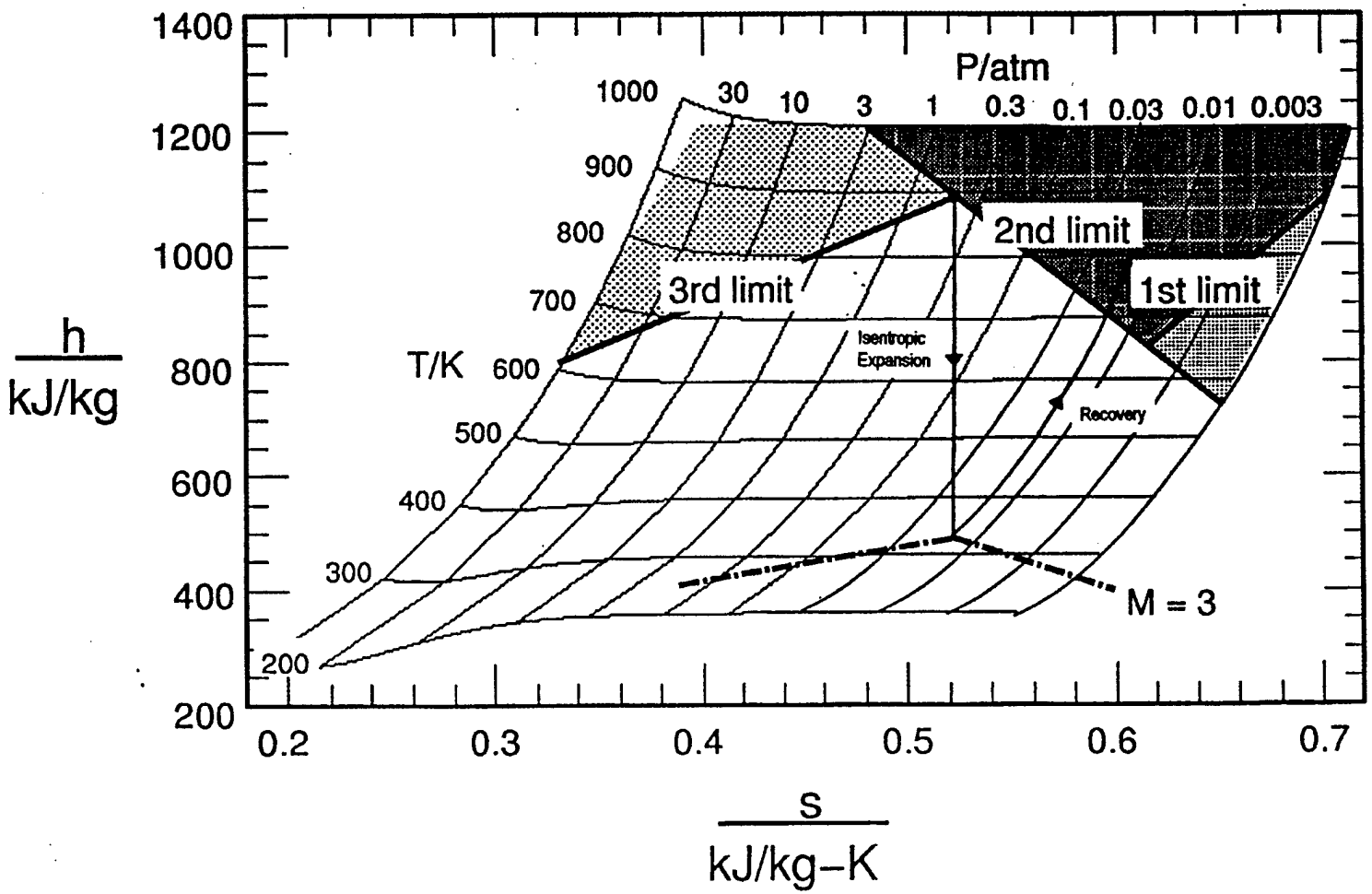

Figure 1: Mollier diagram (enthalpy-entropy) of the operating concept for the Supersonic Combustion Facility. The hydrogen-oxygen explosion limits are sketched, along with a line showing static conditions at Mach 3 using these limits as stagnation conditions (courtesy Yetter).

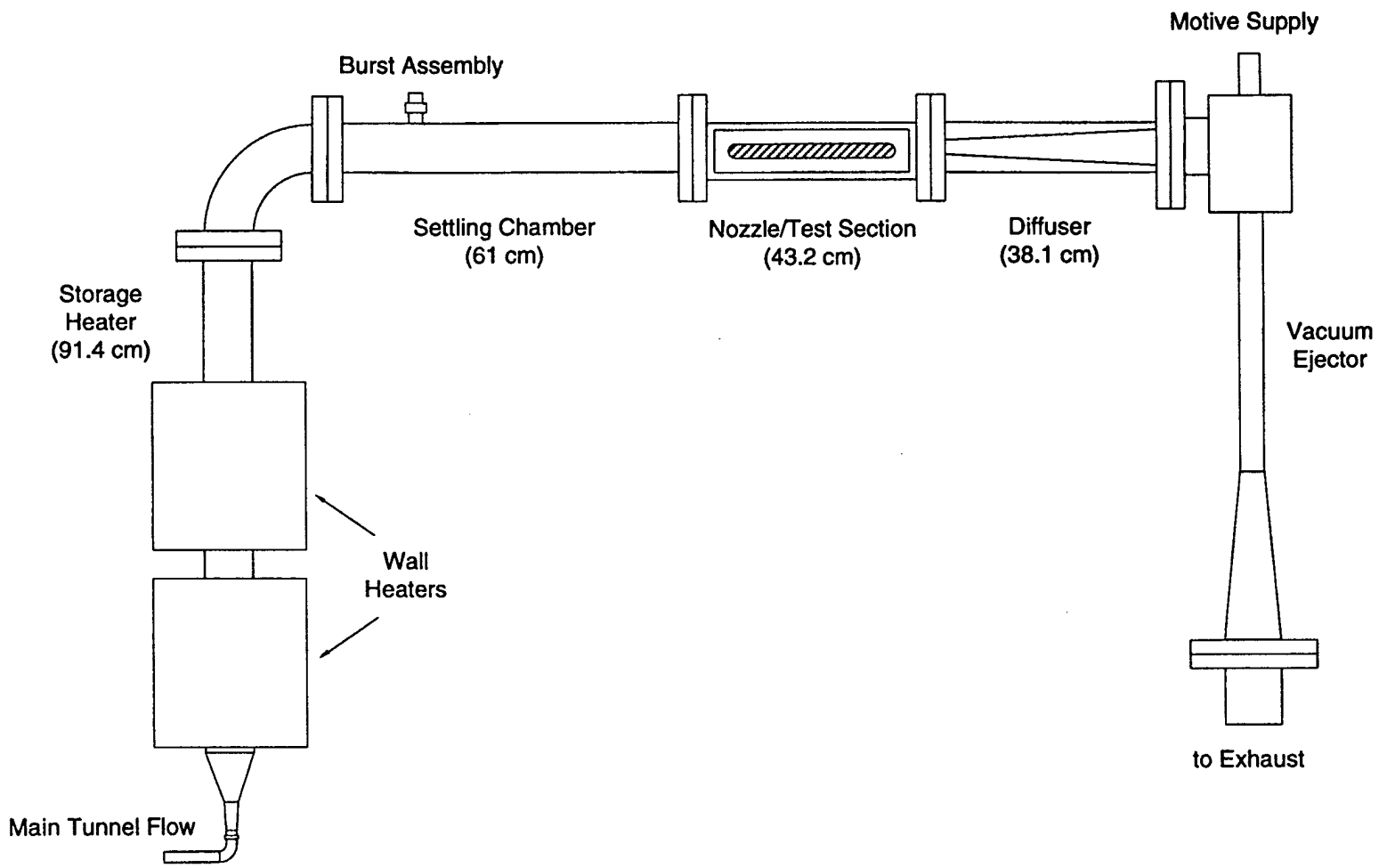

Figure 2: Schematic of the supersonic combustion facility (to scale).

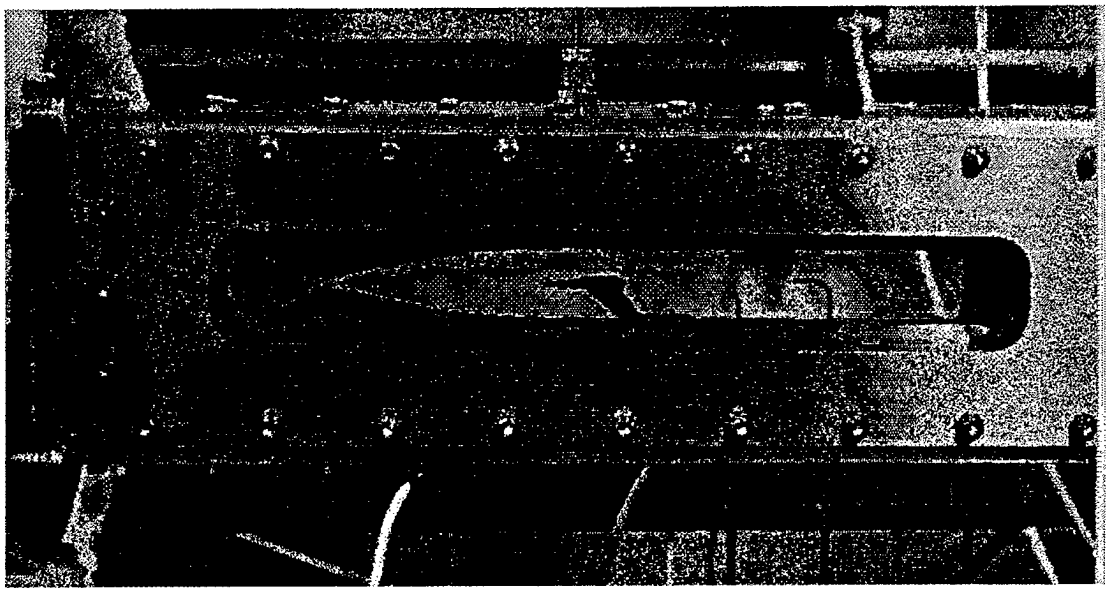

Figure 3: Photograph of the test section showing test model in place with pitot and temperature probes inserted into the test section. Ruler is 10.2 cm long.

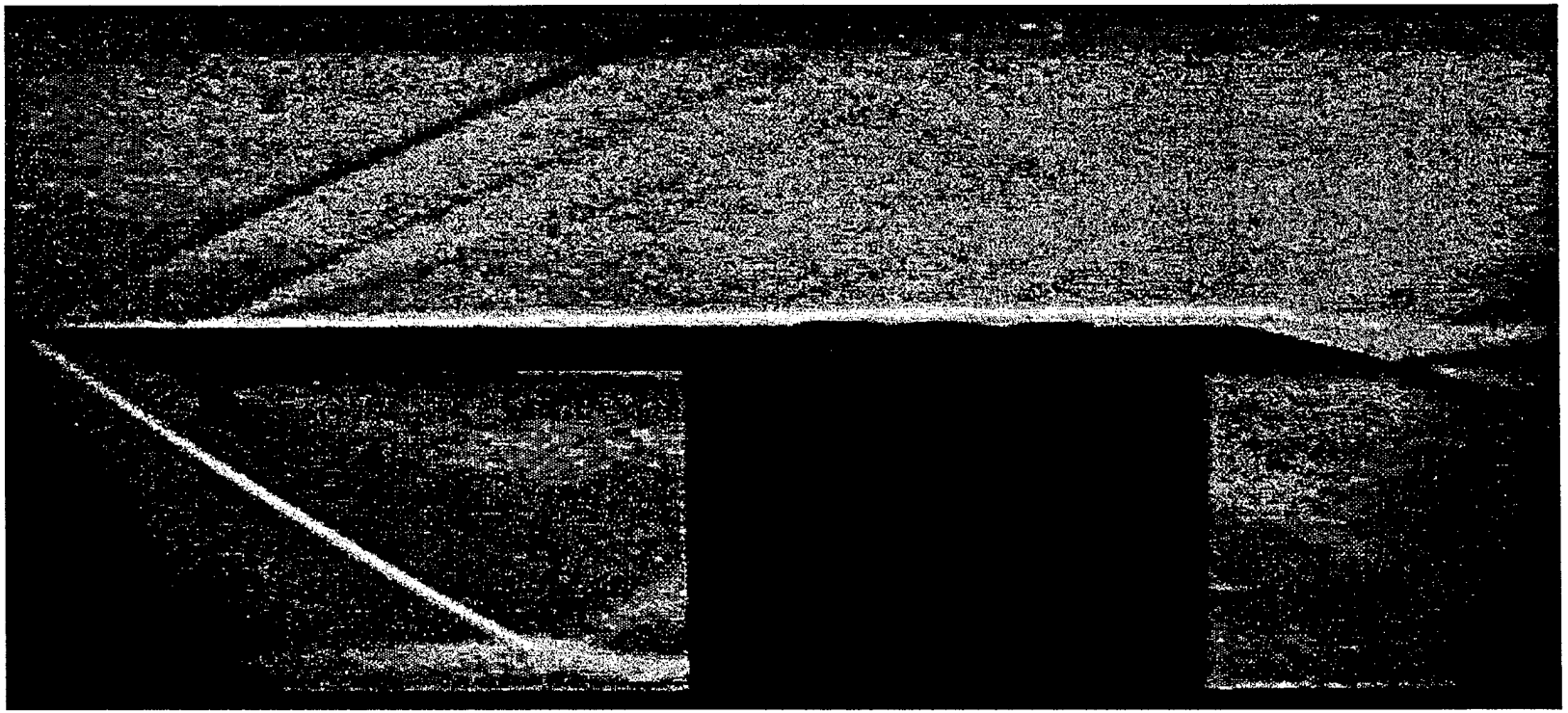

Figure 4: Schlieren frame of flow over a flat plate at Mach 2.8 in the Supersonic Combustion Facility.

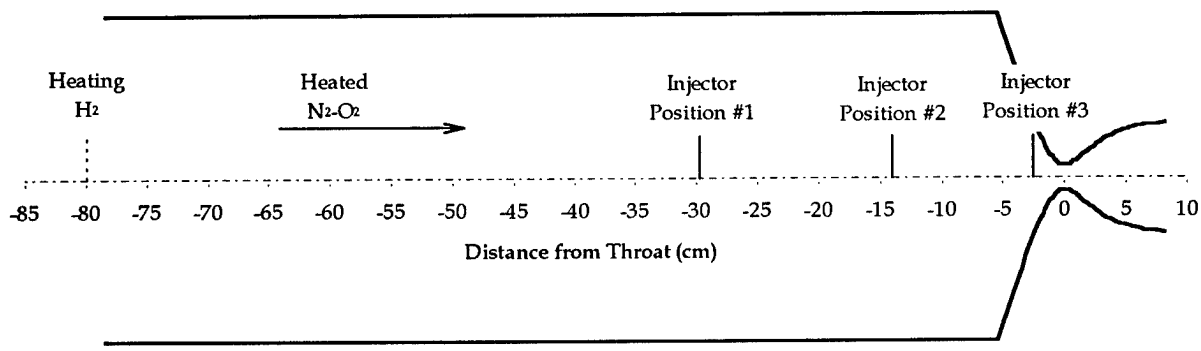

Figure 5: Schematic of the injector positions used in this study relative to the throat and nozzle. The start of the settling chamber occurs at x = -80 cm, and the test section begins at x = +9 cm.

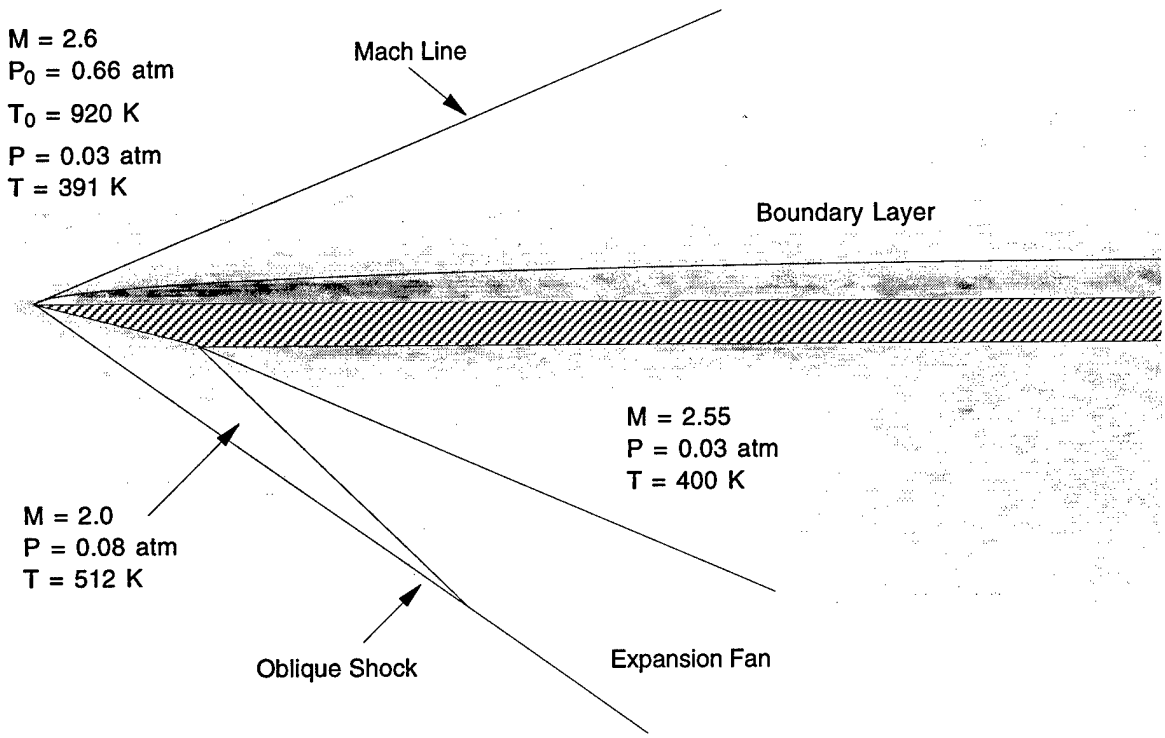

Figure 6: Chemiluminescence over the flat plate with fuel injection at position #1. The thickness of the plate (visibly outlined by the emission) is 0.16 cm.

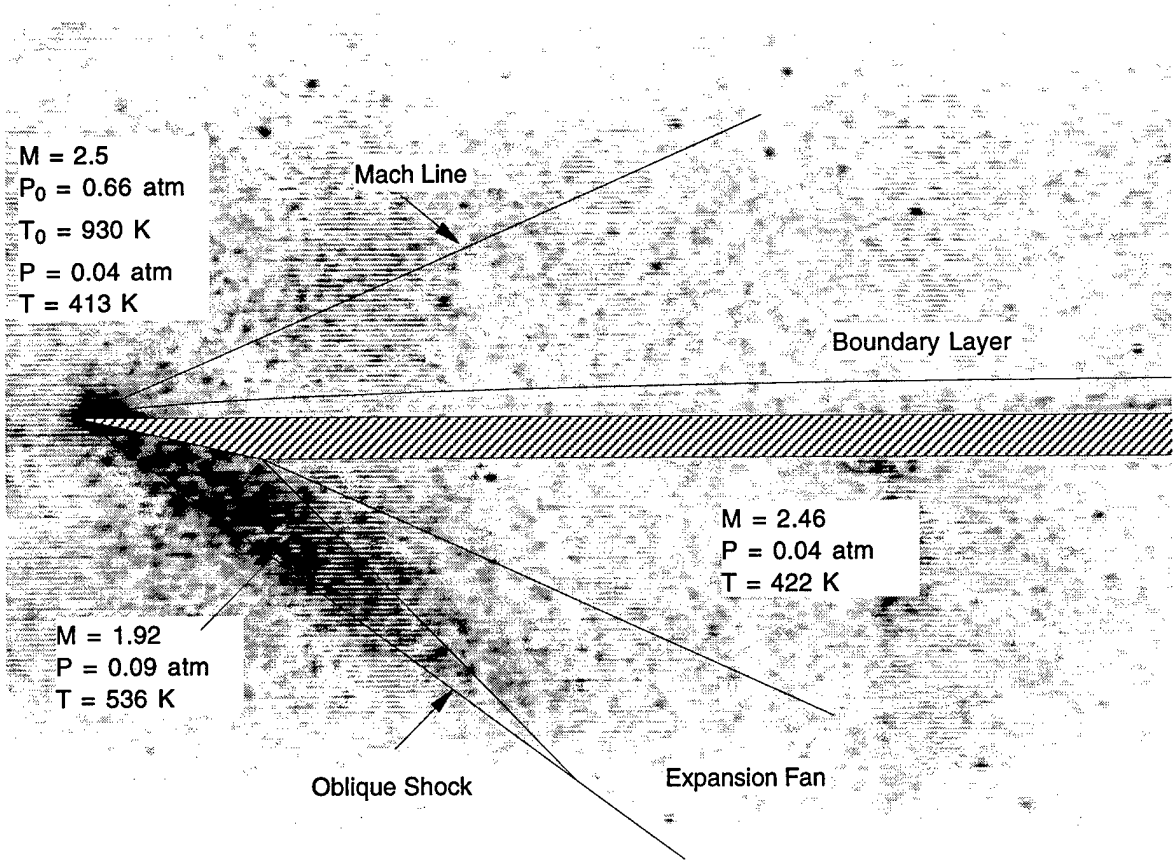

Figure 7: Chemiluminescence over the flat plate for injector position #2. Emission is now most intense in the region behind the oblique shock, and the boundary layer emission appears less intense than in the previous figure.

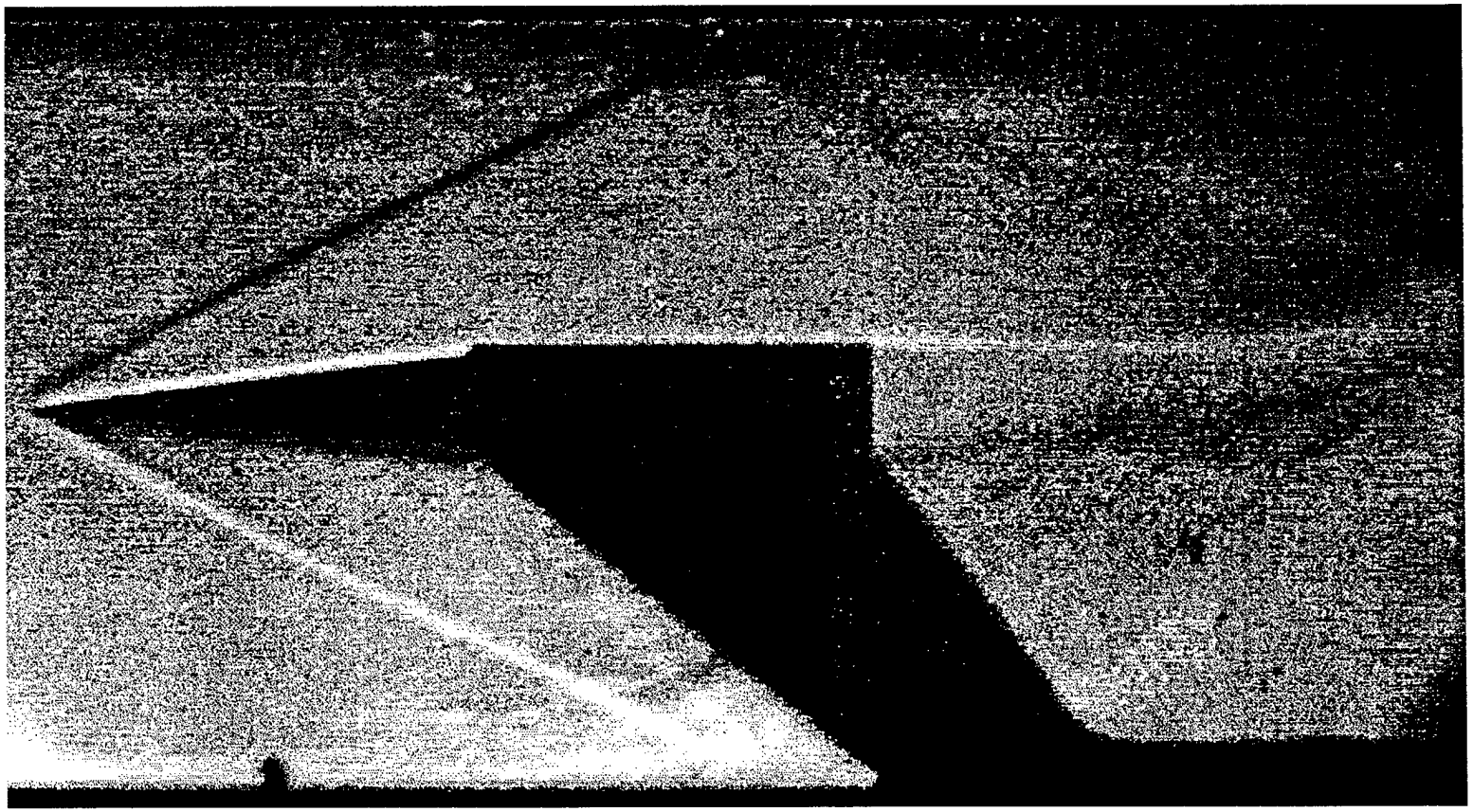

Figure 8: Schlieren frame of the wedge test model at Mach 2.6 in the SCF.

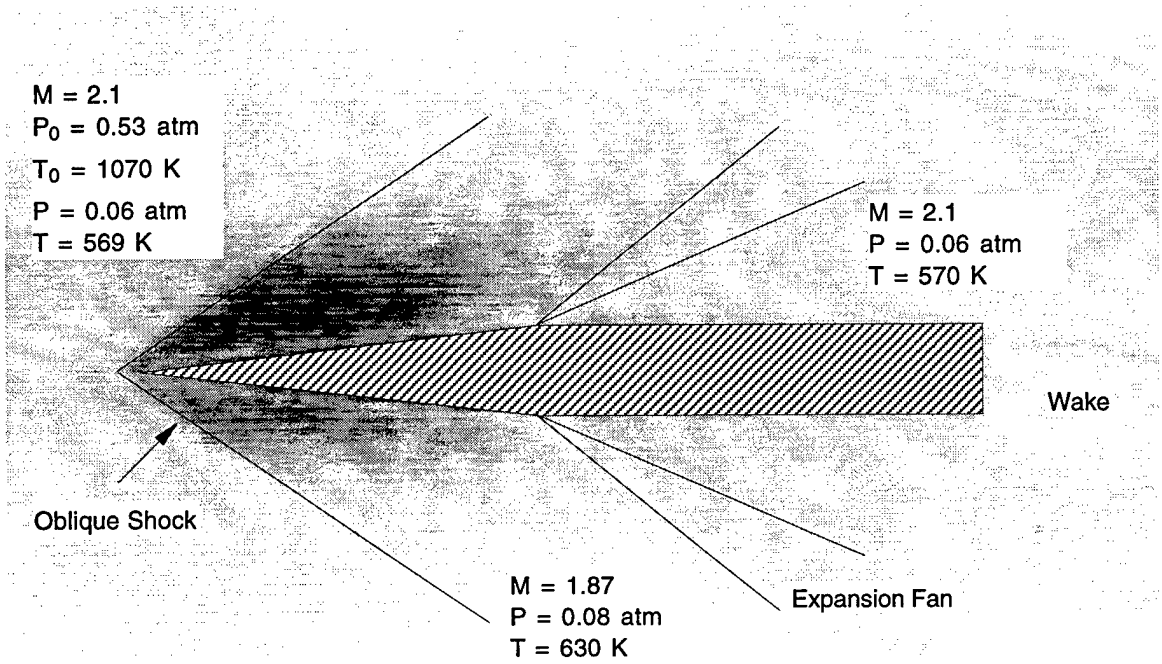

Figure 9: Chemiluminescence surrounds the wedge with the injector at position #3. The most intense region of emission occurs behind the oblique shock near the front of the wedge.

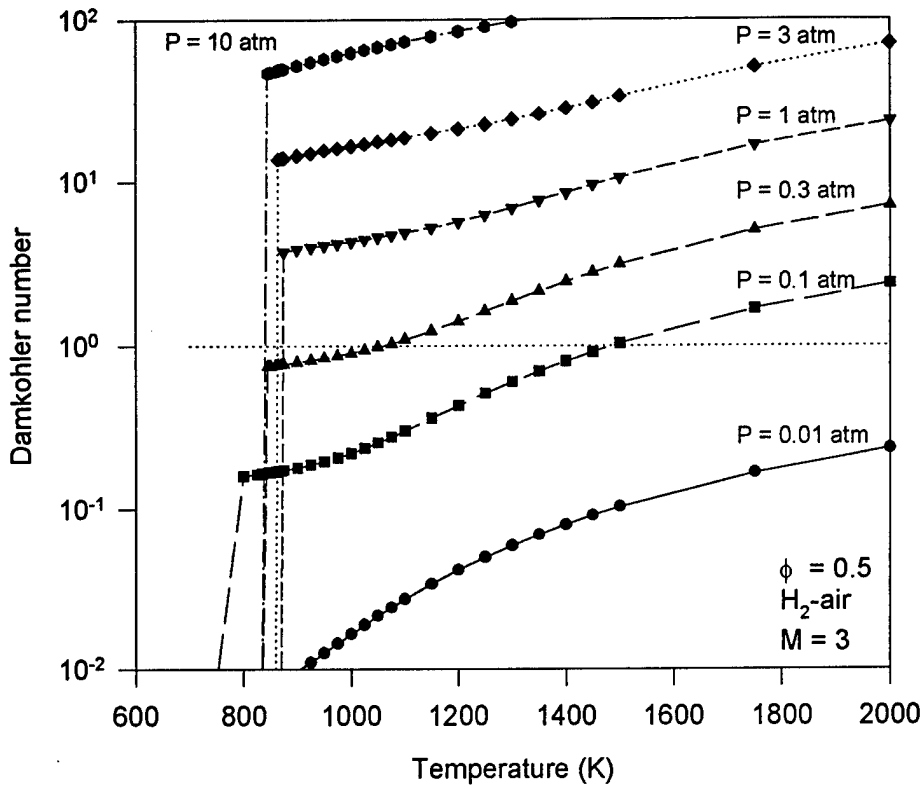

Figure 10: Effect of varying pressure on Damköhler number as a function of initial temperature. Conditions correspond to $M_\infty = 3$, and an equivalence ratio of 0.5.

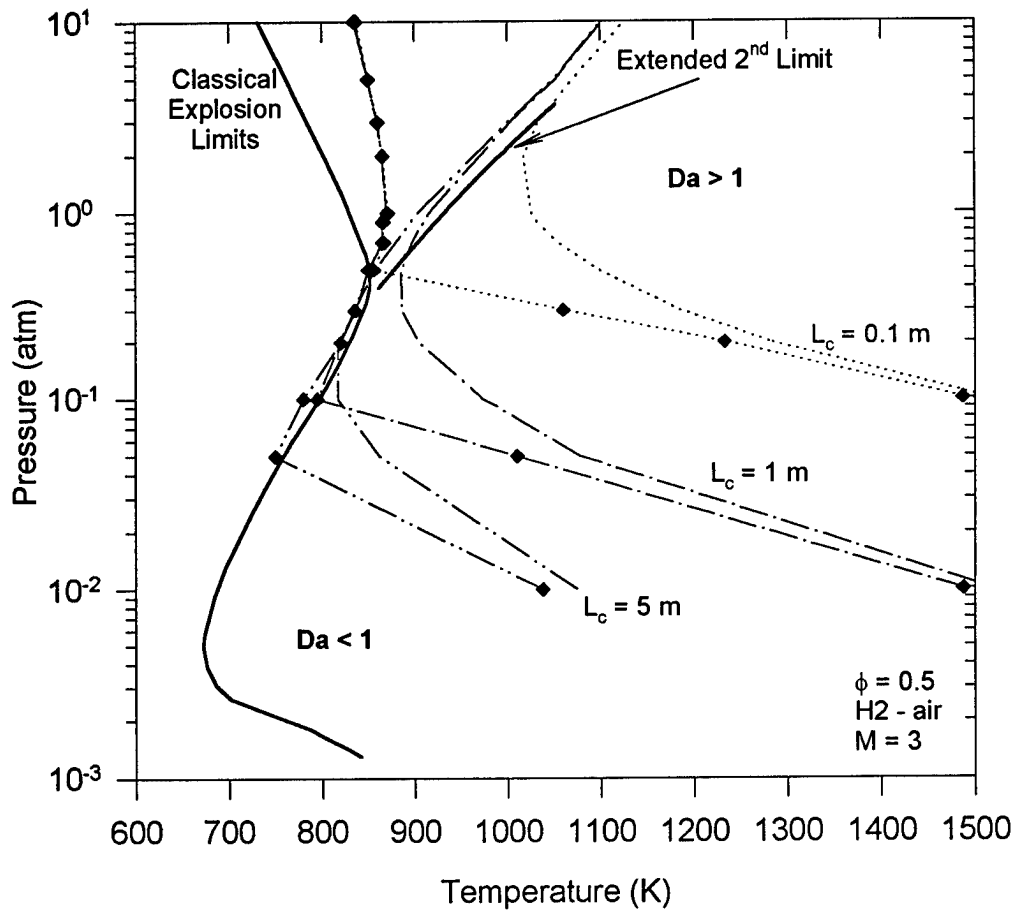

Figure 11: Contours of Da=1 in the pressure-temperature plane for different characteristic lengths. Lines with symbols are isobaric calculations and those without symbols are isothermal.