CHEMICAL REACTING FLOWS

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SUMMARY

Future aerospace propulsion concepts involve the combustion of liquid or gaseous fuels in a highly turbulent internal airstream. Accurate predictive computer codes which can simulate the fluid mechanics, chemistry, and turbulence-combustion interaction of these chemical reacting flows will be a new tool that is needed in the design of these future propulsion concepts. Experimental and code development research is being performed at Lewis to better understand chemical reacting flows with the long-term goal of establishing these reliable computer codes.

Our approach to understanding chemical reacting flows is to look at separate, more simple parts of this complex phenomenon as well as to study the full turbulent reacting flow process. As a result we are engaged in research on the fluid mechanics associated with chemical reacting flows. We are also studying the chemistry of fuel-air combustion. Finally, we are investigating the phenomenon of turbulence-combustion interaction. This presentation will highlight research, both experimental and analytical, in each of these three major areas.

INTRODUCTION

Chemical reacting flows of aerospace propulsion systems have features similar to internal flows in ducts, nozzles, and turbomachinery. The flows are typically highly turbulent, with large secondary flows and three-dimensional flow characteristics. Flow oscillations and unsteadiness are usually prevalent in these flows. However, there are additional features unique to flows with combustion that add a great deal of complexity to the process. This includes a substantial increase in temperature as the flow moves downstream, and a significant change in fluid properties due to fluid species changes. In addition, the time scale for combustion is often orders of magnitude different from the fluid flow time, and there is often a strong interaction between the turbulent flow and the combustion process. These complex features not only make experimental studies difficult but also significantly affect the methods for simulating these flows on the computer.

The research activities in chemical reacting flows are divided into three areas, as shown in figure 1:
Fluid mechanics, which looks at the fluid flow phenomena associated with combustion without the added complexity of including heat release. Research includes studying the multiphase processes of fuel sprays, and the highly three-dimensional and time varying flows that typically exist in real propulsion systems.

Combustion chemistry, which concentrates on the combustion of fuel and oxidizer without including the fluid mechanics. Research is seeking to understand the ignition process of fuel and oxidizer and to probe the detailed chemistry to obtain an accurate combustion model for future fluid codes. Catalytic combustion is also being studied as a fuel processor for high-speed propulsion.

Turbulence-combustion interaction, which looks at both the fluid mechanics and the chemistry of combustion and their effects on each other. Work is being done to understand the dominant physics of turbulent reacting flow and to construct accurate computer codes to simulate this flow. Also, as a useful "numerical experiment," the technique of direct numerical simulation is being used to better understand chemical reacting flows.

These three major areas of activities are all being performed to achieve the long-term goal of obtaining an accurate predictive code with coupled fluid mechanics and chemistry which will be needed in the design of future aerospace propulsion systems. This paper will look at an example of the research in each of these three areas.

FLUID MECHANICS

In this area, an important research activity is the study of the multiphase flows of liquid fuel sprays in air. The fuel-spray process is extremely important in terms of engine efficiency, durability, and operability. The ultimate objective of the research is to develop a computer code that can accurately model the fuel and air mixing with subsequent combustion. Since these processes are very complicated, the model is being approached in a series of steps of increasing complexity. Particle-laden jets were initially studied in order to assess the capability of current two-phase flow models (refs. 1 to 4). Evaporating liquid sprays and combusting sprays are now being studied.

Figure 2 shows the arrangement of the particle-laden jet experimental study. An air jet containing solid glass beads (39 µm, Sauter mean diameter) discharged downward into a still environment. Particle-laden jets with three swirl numbers were studied. Nonintrusive measurements of velocity were obtained with a two-channel laser velocimeter. Particle size and velocity were measured with a phase/doppler particle anemometer. The gas phase was seeded with nominal 1-µm-diameter aluminum oxide power to measure gas-phase velocities.

Figures 3 and 4 present typical results from the particle-laden jet study. A contour plot of experimentally measured axial velocity of the gas phase (left side) and particle phase (right side) is illustrated in figure 3. It is evident that, initially, the gas phase has a higher velocity than the particle phase. The particles are initially accelerated by the gas phase, and then their velocity begins to decay. Because of their inertia, the rate of decay of axial velocity is slower for the particles than the gas. Shown in figure 4 are predictions from the SSF model at 10 diameters downstream of the tube exit.
This model tracks particle trajectories in the computed gas-phase flowfield and allows momentum exchange between phases. The model also considers effects of gas-phase turbulence on particle trajectories. Predictions from the model show reasonable agreement with the data. More details on these experiments and a full description of the computer code and model can be found in references 1 to 4.

Future directions for multiphase flow research include evaporating liquid sprays and combusting liquid sprays. Evaporating sprays are currently being studied under contract at the University of California, Irvine, and Allison Gas Turbine as part of the HOST Program. Results have been reported in references 5 to 9. The test cell where the particle-laden jets were studied is currently being modified to study liquid fuel sprays with combustion.

COMBUSTION CHEMISTRY

An example of the research in the area of combustion chemistry is the study of the chemical kinetics of hydrogen-air combustion.

In a supersonic ramjet (scramjet) propulsion system, the time required between the injection of fuel into the airstream and its combustion point is very important with regards to the length of the engine and its weight. These high-speed propulsion concepts will be tested in wind tunnels where the air has been heated to simulate the temperatures and velocities of the air that would be ingested into the engine as the vehicle flies at high Mach numbers in the atmosphere. Research is underway to determine the combustion delay time of hydrogen fuel and air and to determine the effects of air contaminants in the wind tunnel on this combustion delay time.

Shown in figure 5 is a schematic of a scramjet engine. Air at supersonic velocity enters the engine where fuel is injected. At a position downstream from this injection point, the fuel will burn with the air. The information which we are seeking is to determine how far from the fuel injection point will a stable flame exist in a supersonic airstream of various Mach numbers. Also, since heated wind tunnels have small amounts of contaminants or additives in the air, we are studying the effects of these contaminants on this combustion delay time.

Shown in table I are the levels of four major air contaminants which exist in the two U.S. hypersonic wind tunnels when they are simulating a Mach 7 flight speed. Carbon dioxide and water vapor are known to lengthen the combustion delay time. Nitric oxide and nitrogen dioxide, although orders of magnitude smaller in concentrations, would tend to shorten the combustion delay time.

Stoichiometric H₂-O₂ ignition delay times were measured behind reflected shock waves at 1.1 atm pressure over the temperature range 1300 to 950 K by using a chemical shock tube. A picture of the facility is shown in figure 6. A chemical kinetic model was then constructed, and the data from the shock tube experiments were compared with model predictions. The proposed chemical
kinetic model predicted ignition delay times in excellent agreement with the experimental data, as shown in figure 7.

Applying the chemical kinetic computer model to the prediction of combustion delay time for a scramjet flying at a Mach 7 flight condition yielded a 70-cm distance between the fuel injection point and the flame front, as shown in figure 8(a). When the wind tunnel contaminants were taken into account, this distance was significantly shorter: only 13 cm between the fuel injection point and the flame front (fig. 8(b)). Thus, the small concentration of contaminants (nitric oxide and nitrogen dioxide) resulted in over 80 percent reduction in combustion length. Not only is this effect important in evaluating wind tunnel experiments of propulsion concepts, but it also indicates that trace additives into the flow could significantly shorten the required engine length and thereby considerably reduce weight.

Preliminary results of this work have been reported in reference 10. This work is continuing to explore the effects of these trace contaminants or additives and to better quantify their potential benefit to future scramjet designs.

TURBULENCE-COMBUSTION INTERACTION

While it is important and quite useful to look at the fluid mechanics and the combustion chemistry aspects of chemical reacting flows independently, to get a full understanding of the dominant phenomena of these flows, we must examine the interaction of turbulent flow with combustion. Activities in this area include both numerical code development work and experimental research.

TURBULENT REACTING FLOW

The objective of this work is to understand the coupling between fluid dynamics and combustion and to establish an accurate computer code which simulates the dominant features of turbulent reacting flow. Existing combustion data sets are incomplete for validating computational computer codes. Especially lacking are the inlet and exit boundary conditions, as pointed out in a review report, reference 11. An experiment is being constructed which focuses on many of these features of turbulent reacting flow, both steady state and unsteady. This experiment is to examine a plane free shear layer with combustion. Turbulent reacting flow computer codes, both steady state and time accurate, are also being developed concurrently, and the database from the experiment will serve as a means to validate these new computer codes.

Excellent free shear layer experiments have been carried out, and are reported in the literature (e.g., ref. 12). The data are incomplete, however, for validation of advanced combustion models (ref. 13), and more experimental information is required.

The objectives of the planar reacting shear layer experiment, shown as a schematic in figure 9, are (1) to understand the coupling between fluid dynamics and combustion and (2) to establish a data set to validate computer codes which simulate the physics and chemistry of high-speed chemical reacting flow. A complete description of this experiment is presented in reference 14. Two
gas streams, one of hydrogen and nitrogen, the other of air, will mix downstream of a plane splitter plate. Combustion will occur where the fuel and air have properly mixed. Pressure oscillations in this closed duct will exist because of the dynamic features of the flow, and the interactions between these pressure oscillations and the combusting shear layer will be examined. The unique features of this experiment are (1) a continuous flow capability, (2) flow velocities of both the air and the hydrogen–nitrogen mixture which are in the high subsonic range, (3) the air will be heated ahead of the mixing shear layer without any contamination effects, and (4) the heat release in this experiment will be quite high, typical of propulsion systems. The experiment is in fabrication, and nonintrusive instrumentation is being purchased. Experiments are expected to begin in spring of 1989.

In the numerical code development area, two activities are highlighted. In the first code development effort, a time-accurate version of a two-dimensional finite volume code has been used to calculate forced shear flows (ref. 15). The code is fully second-order accurate in time and space. QUICK differencing is used for the convective terms, and block correction combined with Stone's strongly implicit algorithm is used to solve the pressure correction equation. A two-equation turbulence model is used to represent three-dimensional, small-scale turbulent motions. The large, two-dimensional scales of motion are calculated exactly.

Shown in figure 10 are vorticity contours for a two-dimensional, numerical calculation of a forced shear layer at a Reynolds number of about 100 000. The positive and negative vorticity contours originate at the boundary layers, specified at the inlet of the computational domain. Forcing is applied at a long wavelength, and smaller scale vorticities spontaneously develop as a result of the natural instability of the layer. These small-scale vorticities cluster on the scale of the longer, forced wavelength. Small pockets of positive vorticity persist as remnants of the low-speed boundary layer. The collective interaction of these small-scale vortices, merging into larger scale structures, largely controls the dynamics of the shear layer. These calculations were performed on the NAS Cray 2 computer.

In the second code development effort, a new computational fluid dynamics (CFD) code, the RPLUS code, has been developed for the study of mixing and chemical reactions in the flowfields of the ramjets and scramjets. The code employs an implicit finite-volume, lower-upper symmetric successive overrelaxation scheme (LU-SSOR) (refs. 16 and 17) for solving the complete two-dimensional Navier-Stokes and species transport equations. The RPLUS code is written in generalized curvilinear coordinates and therefore can handle any arbitrary two-dimensional geometry. The implicit LU-SSOR scheme requires only scalar diagonal inversions while most other implicit schemes require block matrix inversions. The use of scalar diagonal inversions offers order-of-magnitude efficiency improvement over conventional implicit schemes, which require the inversion of block matrices, when large systems of partial differential equations must be solved, such as the reacting flows in ramjets and scramjets.

The validity of the code has been demonstrated by comparing the numerical calculations with both experimental data and previous numerical results over a wide range of flow conditions (ref. 17). The code was then used to calculate the mixing and chemical reactions of a hydrogen jet transversely injected into a supersonic airstream. Figure 11 illustrates the inflow conditions and the
static pressure contours. The injected high-pressure hydrogen expands rapidly and yields large pressure gradients along the jet path. This figure indicates that the jet partially blocks the axial flow and yields a strong bow shock just ahead of the injector. The two bow shocks resulting from the two hydrogen jets at top and bottom walls intersect at the center plane and yield a large pressure rise. This code is continuing to be developed, including expanding to three dimensions, in order to be applied to practical complex problems of interest.

CONCLUDING REMARKS

Research in the area of chemical reacting flow will lead to an understanding of this complex flow and accurate predictive computer codes. Activity in this topic is focused on three areas: fluid mechanics, combustion chemistry, and turbulence-combustion interaction. Results from this research will provide important technical tools we need to develop new aerospace propulsion systems for the year 2000 and beyond.

REFERENCES


**TABLE I. - HEATED WIND TUNNEL AIR CONTAMINANTS**

<table>
<thead>
<tr>
<th>Contaminant</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide, percent</td>
<td>5 to 10</td>
</tr>
<tr>
<td>Water vapor, percent</td>
<td>13 to 17</td>
</tr>
<tr>
<td>Nitric oxide, percent</td>
<td>0.9</td>
</tr>
<tr>
<td>Nitrogen dioxide, percent</td>
<td>0.025</td>
</tr>
</tbody>
</table>
Figure 1. - Major areas of research for chemical reacting flows which focus on common long-term goal.

Figure 2. - Particle-laden swirling flow experiment.
Figure 3.- Measured gas and particle axial velocities of particle-laden swirling jet (nonswirling case).

Figure 4.- Radial profiles of axial velocity for particle-laden swirling jet at x/d = 10 (nonswirling case; particle diameter, 39 μm (SMD)).
* How far will stable flame be from fuel injection point?

* What is effect of air contaminants or additives on this combustion delay?

Figure 5. - Schematic of scramjet engine, used to define combustion delay time.

Figure 6. - NASA Lewis Chemical Shock Tube Facility.

Figure 7. - Comparison between predictions of combustion delay time using hydrogen-oxygen chemical kinetic model and measured combustion delay time from shock tube experiments.
CALCULATED COMBUSTION DELAY FOR MACH 7 SCRAMJET FLIGHT CONDITION:

(A) BASED ON PURE DRY AIR.

(B) BASED ON PURE AIR WITH CONTAMINANTS OR ADDITIVES.

Figure 8. - Calculated comparison between wind tunnel and pure dry air effects of combustion time delay in scramjet engine at Mach 7 flight condition.

FEATURES
• CONTINUOUS FLOW
• HIGH SUBSONIC VELOCITY
• NONVITIATED AIR PREHEAT
• HIGH HEAT RELEASE

Figure 9. - Schematic of planar reacting shear layer experiment.
Figure 10. - Spatially evolving shear layer: instantaneous vorticity against background of averaged Reynolds stresses.

**STEADY STATE FLUID MECHANICS COMPUTER CODE:**

**COMPUTER CODE RESULTS OF GASEOUS FUEL JET—AIR MIXING AND COMBUSTION IN INTERNAL DUCT FLOW, SHOWING STATIC PRESSURE CONTOURS**

![Static pressure contours](image)

Figure 11. - Static pressure contours for hydrogen injection into Mach 4 airflow calculated using RPLUS code.
CONCLUDING REMARKS TO THE INTERNAL FLUID MECHANICS RESEARCH SESSION

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and
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The internal fluid mechanics research program at NASA Lewis is a balanced effort between the conduct of experimental research and the development of computational tools. The program has been briefly described by highlighting research efforts in three areas: inlets, ducts, and nozzles; turbomachinery; and chemically reacting flows. Much of the computational focus of the inlets, ducts, and nozzles area has been on the development and validation of parabolized Navier-Stokes codes. In the future, more emphasis will be placed on three-dimensional Reynolds averaged Navier-Stokes methods. The experimental effort will continue to provide a fundamental understanding of the fluid flow physics to develop new and/or improved flow models, and to provide benchmark datasets for validation of both parabolized and Reynolds averaged Navier-Stokes methods.

In the turbomachinery area, the program encompasses a variety of computational and experimental approaches. Special emphasis is placed on the Reynolds averaged Navier-Stokes equations, the unsteady Euler equations, and the average passage equations. The experimental emphasis is on high response time--resolved measurements and on measurements within rotating machinery blade passages.

Activity in chemical reacting flow research is focused on fluid mechanics, combustion chemistry, and turbulence/combustion interaction. Emphasis is placed on Reynolds averaged Navier-Stokes solvers and direct numerical simulation. The experimental activity includes unsteady reacting flows, shock tube kinetics, and multiphase flow phenomena.

In conclusion, it is noted that as numerical methods are improved and the ability to compute complex fluid physics is enhanced, it is critical that the users be aware of the code validity and limitations. These limitations can only be established by a careful systematic evaluation of each numerical scheme. It is by this systematic approach and the involvement of the ultimate user community that internal computation fluid mechanics will grow in importance as a practical tool for the analysis and design of aerospace propulsion systems.
This paper presents an overview of current and recently completed aeropropulsion instrumentation and controls research at NASA Lewis Research Center. The focus of the aeropropulsion instrumentation research is on miniature sensors and optical measurement systems that are needed for aeropropulsion research. The controls research is focused on the development of fiber-optic-based hardware necessary to implement a "fly-by-light" control system as well as on the development of advanced control methods that are needed for propulsion systems of increasing complexity and highly coupled aircraft and propulsion systems. Also included in this paper is an overview of the Lewis high-temperature electronics program. This program is directed toward developing silicon carbide solid-state electronic technology in order to produce electronic devices with a temperature capability of 400 °C and higher.
I - INTRODUCTION
Norman C. Wenger

NASA Lewis has a long history of research and technology programs in instrumentation and controls for propulsion. These programs are motivated by the many specialized needs for instrumentation in propulsion research that could not be met by standard commercially available instrumentation, and in the case of controls, by the need to develop techniques and hardware for maximizing the performance of increasingly more complex propulsion systems. This paper will present a few of the recent highlights from the Lewis program as well as provide insight on future program directions.

The Lewis instrumentation and controls program has been focused on satisfying the needs of the aeropropulsion industry and on taking maximum advantage of newly emerging technological opportunities. There are numerous drivers that impact the Lewis program. The major program drivers for aeropropulsion research instrumentation are as follows:

- Experimental research
- Performance validation
- Reduced cost of testing
- Computer code validation
- More hostile measurement environments
- New materials (e.g., ceramics, composites)

Experimental research, namely the exploration of fundamental phenomena and development of a basic understanding of propulsion system performance, and performance validation of both components and entire systems have always been the traditional roles for instrumentation.

The reduction of propulsion system testing costs, while always an important factor, grew extremely important in the early 1970's when both utility and labor costs began to escalate rapidly. Considerable effort was initiated back then and continues to the present to design and operate experiments, facilities, and instrumentation to acquire the required information at minimum cost.

Computer code validation is probably today's major instrumentation program driver because of the strong emphasis being placed on computational efforts. Code validation typically requires large amounts of data with not only high accuracy but with a high degree of spatial resolution and with minimal disturbance of the measurand by the instrument. These requirements have provided a great impetus in the development of today's nonintrusive-laser-based instrumentation.
The need for instrumentation to operate in more hostile measurement environments has always been a strong program driver, but the need has increased in recent years because of strong emphasis on hot section durability enhancement. Improving the ability to predict the life of turbine engine hot section components was the primary goal of the recently completed Lewis-managed program in turbine engine hot section technology, which was also known as the HOST Program. Many of the instrumentation highlights in the following sections are a result of the HOST Program.

Today's instrumentation research program is being strongly driven by the needs to make measurements on and around propulsion system components made from ceramics and ceramic-composite materials. These new materials not only allow the propulsion system environments to become even more hostile, but they present difficulties and limitations in our ability to install sensors on these materials. Sensors and lead wires can no longer be installed into grooves cut into the component surfaces. With ceramic components, all measurements must be made either with miniature surface-mounted sensors or via remote sensing techniques.

The Lewis instrumentation research program has always been geared to readily adapt opportunities and techniques from other research activities in order to continue the advancement in measurement capability. Some of the major technologies that have impacted instrumentation are listed as follows:

- Computers (minicomputers, microcomputers)
- Lasers
- Electro-optical devices/fiber optics
- Thin-film technology
- Solid-state electronics (e.g., sensor/electronics integration)

As expected, computers head this list. Computer technology is the basic enabling technology that has permitted the automation of instrument systems and the development of "smart" instruments. Modern instrument systems normally include a high degree of automation not only with respect to data acquisition, but also with respect to calibration, instrument health monitoring, and aids to servicing and maintenance.

Lasers, electro-optic devices, and fiber optics have opened up the field of nonintrusive measurements. The laser anemometer is perhaps the best example of where these impacting technologies have permitted a major new measurement capability to emerge.

Thin-film technology has opened up the field of minimally intrusive surface sensors. It is now possible, in some cases, to sputter-deposit, through a series of masks, a complete sensor directly on the surface of a component. Much work must be done in this area before thin-film sensors are widely used on aeropropulsion system components.

Solid-state electronics has made a significant impact on instrumentation in many areas. However, since virtually all solid-state electronic devices available today are silicon based and since silicon devices are temperature limited, most solid-state electronic devices associated with instrumentation are found on the control room end of the measurement systems and not on the
sensor end. There are many advantages to integrating the electronics with the
sensor, and indeed much research is underway nationally to develop a variety of
these integrated sensors. However, since the basis for this work is silicon
technology, there is going to be a definite upper limit on the temperature
capabilities for these devices. The upper limit for silicon-based devices is
about 300 °C (575 °F). Thus, there is a need to investigate semiconductor
materials that have higher temperature capabilities than that of silicon if the
needs for integrated sensors in advanced propulsion systems are to be met. A
subsequent section of this paper, High-Temperature Electronics, describes the
Lewis program to develop high-temperature solid-state devices.

Some of the major drivers in the Lewis controls research and technology
program are listed as follows:

- Propulsion system performance
- Integration of engine, inlet, nozzle, and aircraft control systems
- Durability/maintainability of propulsion system (condition monitoring/
diagnostics)

First and foremost on the list is propulsion system performance. Propulsion
system complexity is increasing at a rapid rate and presents a major challenge
to the controls engineer. The number of measured parameters and controlled
variables has been increasing almost linearly with time since the 1950's for
both military and commercial engines. The controls engineer has been forced
to deal not only with this increasing system complexity but also with greatly
expanded mission requirements which require operation over increasingly larger
flight envelopes.

One approach toward increased aircraft capability is through greater
integration of the various propulsion and flight control systems. This inte-
gration of controls can give worthwhile benefits in conventional takeoff and
landing aircraft, and is virtually mandatory in STOVL aircraft if the pilot is
to perform any other functions than operating the aircraft. The control is the
critical link between the propulsion and flight systems and the pilot. The
controls engineer is faced with the task of designing a system that can meet
all of the technical requirements mandated by flight and propulsion systems
and, at the same time, providing a manageable interface for the pilot.

As control system functionality continues to increase, greater demands
can and will be placed on the control system. One of these is the issue of
durability and maintainability of the propulsion system. Information being
acquired by today's aircraft control system is sufficient, with proper inter-
pretation, to tell a great deal about the current health and condition of the
propulsion system. Such monitoring systems are, of course, in current use.
As knowledge increases as to the relationship between component life and the
operating environmental history of that component, a significant future capa-
bility will be the prediction of remaining component life. The role of the
propulsion control system, in the future, will change from its current reactive
role, where it strives to maintain the engine at some prescribed operating
point in the face of random disturbances, to where with its greater system
intelligence it will operate the engine on the basis of more global considera-
tions such as overall mission requirements, current system health, and remain-
ing component life.
The opportunities and technologies that have made a major impact in aero-propulsion controls are as follows:

- Computers
- Solid-state electronics (e.g., sensor/electronics integration)
- Fiber optics
- Expert systems

Here also, computers head the list. The development of lightweight, high-speed, reliable digital computers has greatly enhanced control system capability compared to the previous hydromechanical technology.

Solid-state electronics, embodied in many forms, has made and continues to make significant impacts in the control sensor area. One dramatic improvement, discussed previously in this section, will come with the availability of solid-state devices that are capable of operating at high temperatures, so that the sensor and electronics can be integrated.

Fiber optics holds the promise of lighter weight control systems with greater immunity to electromagnetic interference. With today's rapid increase in avionic systems on board all types of aircraft, it is extremely important that these systems do not interfere with each other nor exhibit susceptibility to external interference. In stealth applications it is also important that these systems not radiate. Fiber-optic-based control systems hold the promise of meeting these requirements.

Expert systems are beginning to make inroads into many areas, including aero-propulsion controls. The final section of this paper will present insight to how Lewis envisions the use of expert systems as essential building blocks in an intelligent control system.