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Rate-dependent energetic processes in hypersonic flows

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ABSTRACT

In celebration of the first 60 years of the Air Force Office of Scientific Research, several studies of hypersonic flows dominated by rate-dependent energetic processes are revisited. The work presented shows the evolution and advancement of computational capabilities in this area, and illustrates some key lessons learned over the previous decade or so. Early work with Leyva and Hornung in the California Institute of Technology T5 Free-Piston Shock Tunnel had the goal of validating thermochemical models for high-enthalpy flows. Several of these flows are re-analyzed with more advanced numerical methods, resulting in improved comparisons with the experimental measurements. This work was followed by a series of experiments in the Calspan-University at Buffalo Research Center (now CUBRC Inc.) facilities at lower enthalpy conditions. Initial comparisons were poor, but with a better understanding of the facility behavior and the inclusion of key finite-rate processes, excellent agreement was obtained for nitrogen flows. An interesting study related to plasmadynamics and finite-rate processes in a different type of flow is discussed. Finally, it is shown that recent advances in numerical methods that are beginning to enable the direct numerical simulation of key rate-dependent energetic processes in hypersonic flows.

1. Introduction

Over the past decade or so, the AFOSR has been the primary U.S. funding agency for the basic study of hypersonic and high-energy flows. For a brief period, NASA also funded this area through its Fundamental Aeronautics program. However, recent shifts in priority eliminated this support, and now the AFOSR is once again the sole source of fundamental research support in this area. The support provided by the AFOSR has led to huge improvements in the ability to predict the behavior of hypersonic flows, and many outstanding problems have been solved. In this article, a few of these success stories are revisited, and with this retrospective, it is shown that significant improvements in the understanding of these flows has been made.

Hypersonic and high-enthalpy flows are different than most types of aerodynamic flows because they are highly energetic. For example, a low-earth re-entry capsule travels at approximately 7.5 km/s relative to the atmosphere, resulting in a flow with a total enthalpy of 28 MJ/kg, about six times the energy density of high explosive. When this flow passes through the bow shock, its temperature increases to extreme levels, causing many non-ideal processes to occur – these include vibrational energy excitation, gas-phase chemical reactions, ionization, electronic energy excitation, and thermal radiation. When the high-energy gas interacts with the vehicle surface, additional processes may occur, including gas-surface reactions, catalysis of reactions by the surface, and ablation and removal of the thermal protection system (through oxidation, nitridation, sublimation, and pyrolysis of the surface material). These processes may absorb or release energy as they take place.

All of these processes occur at finite-rates, and these rates are often comparable to the rate of fluid motion. For example, a reaction can be initiated at one location, but not be completed until the gas has moved a significant distance down stream. Fig. 1 illustrates an extreme example of competing time scales – here the flow field over a 10 cm sphere is plotted, along with a streamline through the flow. The numbers indicate the cumulative number of collisions that a notional gas particle would experience as it travels through the flow field. For this high-altitude case (80 km), the gas particle experiences only about 130 collisions. If an internal energy relaxation process takes on the order of 1000 collisions to reach equilibrium (typical of vibrational relaxation in air), then clearly this relaxation process does not reach completion and the vibrational energy state is far from equilibrated. This is an example of a nonequilibrium flow, in which the finite-rate thermo-chemical processes (internal energy relaxation and chemical reactions) are not in a state of local thermodynamic equilibrium.

Therefore, even in a steady-state hypersonic flow there is a competition between rate-dependent energy relaxation processes and the dynamics of gas motion. If the flow is unsteady, then there is the potential for more complex rate-dependent processes to occur as the flow exchanges energy between its kinetic, thermal, internal, and chemical modes. The magnitude and rate of energy

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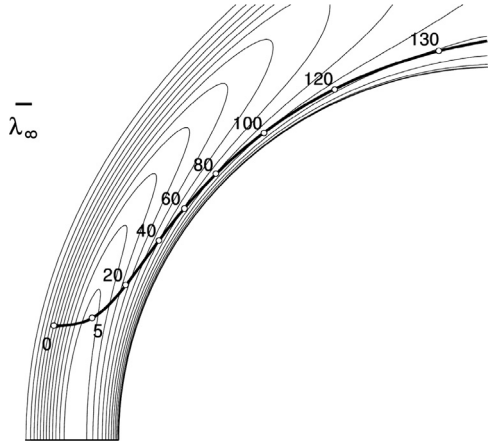

Fig. 1. Mach 17 flow over a 10 cm sphere at 80 km altitude; density contours and a streamline showing the cumulative number of collisions along the streamline.

transfer between modes are important factors for flow control and manipulation. Recent research is starting to show how the flow unsteadiness can be tuned to the specific energy transfer processes to control the flow dynamics. Much more work is needed to understand these processes and to develop effective control strategies.

The intent of this article is not to survey the literature in the simulation of energetic flows with rate-dependent processes, but to give some examples of this class of flow. The literature has many additional examples, and it is not possible to provide a complete review of this large body of work. Thus, the work discussed is representative of the progress made by the field in the simulation of high-speed energetic flows.

AFOSR's sustained support of basic hypersonic flow physics is deeply appreciated, and the support of talented AFOSR program managers (Drs. Len Sakell, John Schmisseur, and Steven Walker) over the past fifteen years is gratefully acknowledged; without their guidance and financial support the research findings discussed in this paper would not have been possible. Recent support from the Department of Defense National Security Science and Engineering Faculty Fellowship (NSSEFF) is also greatly appreciated.

2. Progress in the simulation of energetic flows

The simulation of high-enthalpy, high-speed flows started in the late 1980's with work mostly at NASA Langley Research Center, led by Dr. Peter Gnoffo. Concurrent work at Stanford University and NASA Ames Research Center was conducted with guidance from Profs. Robert MacCormack and Dean Chapman and Drs. Steven Deiwert and Chul Park. I was fortunate to work in this latter group, and my doctoral thesis work was focused on this topic. From the initial stages of the work, the emphasis was on understanding the interaction between finite-rate energetic processes and gas motion. There was a great deal of skepticism that CFD methods could be successfully applied to these complex flows.

In the early stages of the work, the field was concerned with the derivation of the conservation equations and developing rudimentary methods for their solution. Then, as methods were developed and codes written to obtain initial nonequilibrium flow simulations, the primary emphasis became trying to prove that the solutions were representative of reality, which required the validation of the finite-rate thermo-chemical models used in the codes. There was also the ongoing task of improving the robustness of the implicit algorithms required for these flows. Following the code validation studies on basic shapes, the field began to focus on parallelization and scaling to enable the solution of much larger problems with more sophisticated physical models. In the last several years, there has been greater emphasis on improving the accuracy and efficiency of the numerical methods to enable the simulation of ever more difficult unsteady flow simulations. The following discusses some of the highlights of this research.

3. Summary of governing equations

In order to provide some context for the following discussion, this section briefly discusses the governing equations for high-enthalpy hypersonic flows. Emphasis is given to the key processes that contribute to the energy transfer processes; further details are available in the literature [1–3]. It is beyond the scope of this article to discuss the numerical solution of the governing equations, and the reader is referred to the many papers in the field. Recent publications summarize some of this work [4,5].

When the flow is not in a state of local thermodynamic equilibrium, it is necessary to solve a conservation equation for each chemical species and for all relevant internal energy modes. The statement of mass conservation of species s is given by

$$\frac{\partial \rho_s}{\partial t}+\frac{\partial}{\partial x_j}(\rho_s u_j+\rho_s v_{sj})=w_s \tag{1}$$

where ρ_s is the mass density of species s, x_j are the coordinate directions, u_j is the bulk gas velocity, v_{sj} is the species s mass diffusion velocity, and w_s is the chemical source term. Here, the rate of gas motion is primarily determined by the magnitude of the velocity, and the rate of chemical reactions is given by the source term. Thus, it is possible to construct a relative reaction rate by forming the non-dimensional ratio of w_s to the fluid motion rate – this is commonly known as the Damköhler number.

The momentum conservation equation is identical to that of a non-reacting compressible flow, and as such it will not be reproduced here. The key difference is that the pressure is constructed as the sum of the species partial pressures.

The conservation equation of internal energy depends on the form of internal energy being tracked. Here, consider a generic internal energy per unit volume, E_i, which could represent the total gas rotational or vibrational energy, the vibrational energy of a particular species, or the electronic energy of a particular mode, for example. For complex flows, it may be necessary to track more than one internal energy mode to correctly model the behavior of the internal energy state. The relevant conservation equation is

$$\frac{\partial E_i}{\partial t}+\frac{\partial}{\partial x_j}\left(E_i u_j+q_{ij}+\sum_s E_{is} v_{sj}\right)=Q_i \tag{2}$$

Here, q_{ij} represents the diffusive transport of internal energy due to gradients of internal energy, and the sum over species is the transport of the internal energy due to mass diffusion. The source term, Q_i, represents the rate of energy transfer to the internal energy mode due to relaxation of that mode. Importantly, Q_i must also include terms to represent the rate of energy removal and addition to the internal energy due to chemical reactions. For example, consider a diatomic gas and assume that the vibrational energy needs to be tracked to quantify the relaxation of the internal energy modes; if some fraction of that gas dissociates, the vibrational energy associated with the molecules that dissociate must be removed from the vibrational energy pool. Similarly, if the gas recombines, the vibrational energy state of the newly-formed molecules must be modeled. Clearly, the relative magnitude of the source term and internal energy flux forms another non-dimensional time scale for internal energy relaxation.