3.3 Fluid Dynamics

Group Leaders: Robert Moser and Michael Norman

Faculty: Ronald Adrian, Hassan Aref, S. Balachandar, Robert Moser, Michael Norman, Rizwan-uddin, and Surya (Pratap) Vanka

Research Scientists: Prasad Alavilli, Dinshaw Balsara, John Hayes, Fady Najjar, and Danesh Tafti

Postdoctoral Research Associates: James Ferry, Kiseok Lee, and Biing-Horng Liou

Graduate Research Assistants: Prosenjit Bagchi, Louis Demers, Zhiqun Deng, Jacob Langford, Dmitri Pouchkin, Sarma Rani, Christopher Tomkins, Stefan Volker, and Bradley Wescott

Overview

The Fluid Dynamics group works on system-scale solid rocket motor core flow model development as well as subscale model development relevant to the turbulent dynamics of the combustion interface, dispersion and combustion of Al particulates in the core flow, and crack flow. A major focus is the development of appropriate large eddy simulation (LES) models for the core flow using insights gained from direct numerical simulation (DNS) and particle imaging velocimetry (PIV) laboratory experiments.

Code Development

We have made great advances in the simulation of the rocket core flow during this program year. The fully integrated, GEN1 code is well underway and is expected to be completed in Y3.

Core Flow Solver — ROCFLO

Alavilli, Najjar, and Tafti have significantly enhanced the GEN1 core flow solver, *ROCFLO*. The flow solver has been adapted for parallel computation on distributed memory machines using MPI for interprocess message communication. The implementation is very general and portable across as wide range of supercomputers. Each computational block is updated independently, after which data are exchanged in a communication phase. Good load balance may be achieved by assigning to each processor one or more computational blocks. Thus efficiency is retained even in the presence of disparate computational block sizes.

Another refinement is latency hiding. Moving boundary computations entail a 20-30% overhead associated with generation of the dynamic meshes for the evolving computation. By overlapping the grid regeneration phase with the communications, some of this overhead is hidden and scalability is improved. The parallel performance of *ROCFLO* has been tested on a number of platforms including ASCI Red (2048 processors), ASCI Blue Mountain (1024 processors), ASCI Blue Pacific (512 processors), NCSA Origin2000 (128 processors), PSC Cray T3E (512 processors), and a heterogeneous Intel Pentium II/III cluster (80 processors). Selected performance data are presented in Fig. 3.3.1.

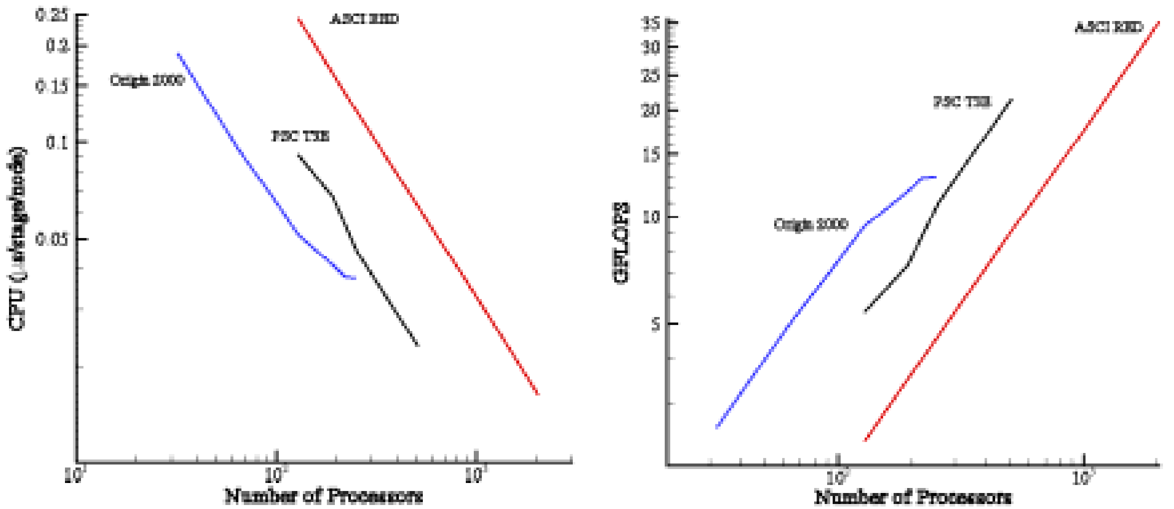

Fig. 3.3.1: *ROCFLO* total elapsed time and performance on fixed problem (36 million nodes per test).

Several initial validation tests of *ROCFLO* have been carried out. An inviscid flow about a NACA 0012 airfoil was computed and results compared very well to results from the *ARC2D* code from NASA-Ames. Alavilli and Tafti have simulated the core flow in the Space Shuttle Reusable Solid Rocket Motor (RSRM) using *ROCFLO*. A detailed model of the RSRM has been created that included details of the 11-point star grain at the head end and the nozzle downstream. The multi-block computational meshes, comprising about 3.5 million nodes, are shown in Fig. 3.3.2. Steady and unsteady computations are performed on this full configuration, but on the first coarse level of the mesh with about 400,000 nodes. The steady state results are compared to Space Shuttle data. The axial variation of pressure, temperature and Mach number along the centerline of the rocket is compared to available shuttle data in Fig. 3.3.3.

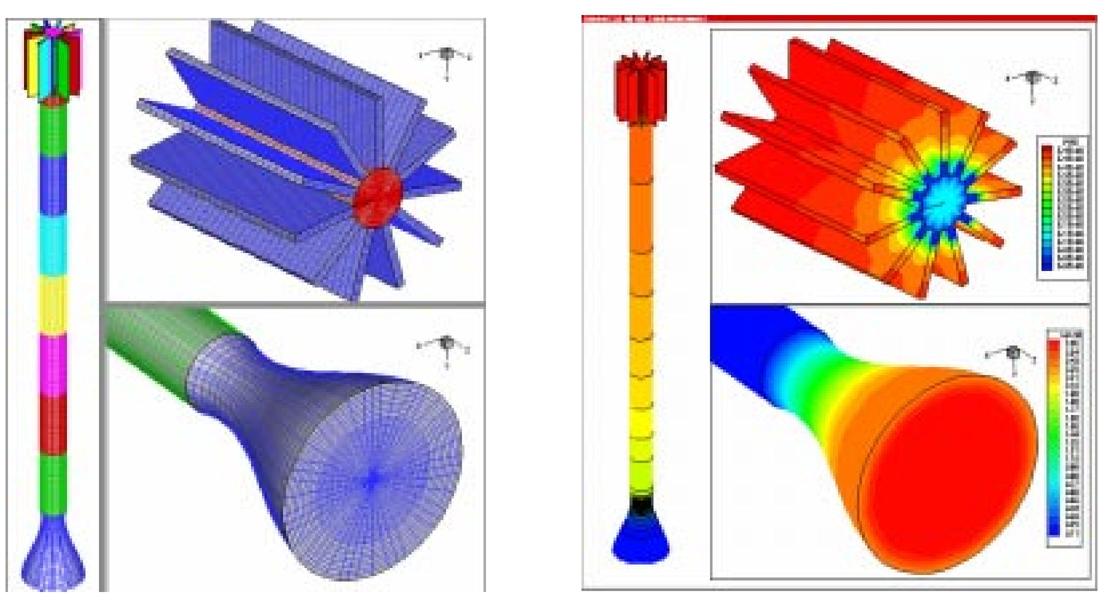

Fig. 3.3.2: RSRM mesh including 11-point star grain and computed steady state solutions.

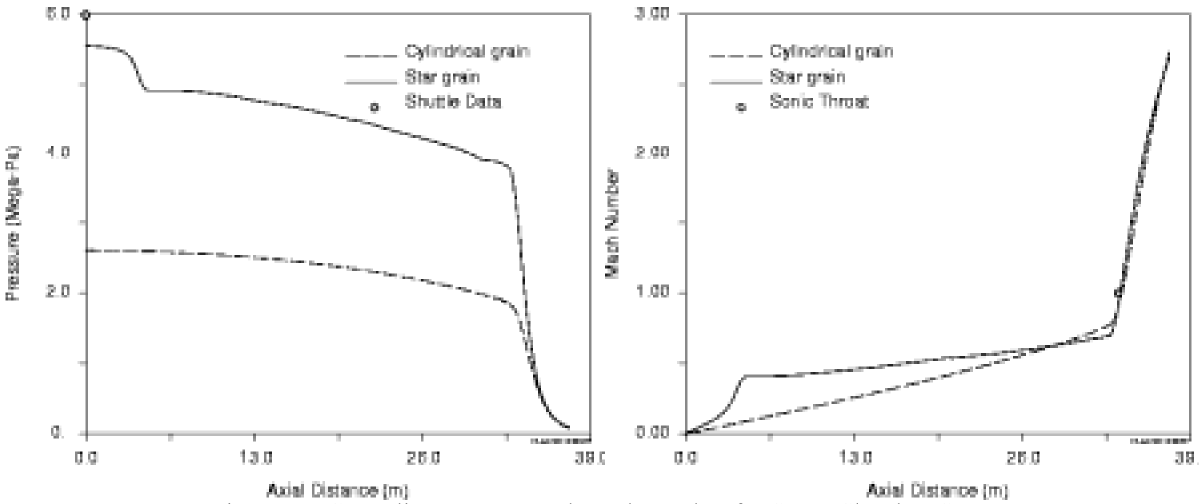

Fig. 3.3.3: Centerline pressure and Mach number for Space Shuttle RSRM.

Propellant Surface Regression

In order to simulate long duration burns of the solid propellant rocket, a critical ingredient is a mathematical model to represent the surface regression induced by burning. Alavilli has developed and implemented a simple geometrical algorithm in *ROCFLO* to model surface regression. A propagation law, which enforces the instantaneous volumetric burn rate on surface elements, is posed as a system of hyperbolic partial differential equations and solved numerically. The hyperbolic system is marched in time and the successive solutions yield the profiles of the grain as it burns back. This method leads naturally to the rounding-off of sharp protrusions (convex corners) into the flow and an opening-up of concave cusps, which qualitatively mimicks physical nature. Figure 3.3.4 shows a sample computation showing the burn profiles for a star grain section.

Unstructured Mesh Code for Crack Failure

Liou and Balsara, in collaboration with Geubelle, Hwang and Acharya in the Structures and Materials Group, have developed a compressible fluid dynamics code for simulating crack failure of the propellant grain. A 2-D unstructured, self-adaptive, flow solver based on higher order Godunov methodology was developed. The flow solver can accommodate moving boundaries, thus making it very adept at tracking the evolution of the propagating crack tip/s even in complicated situations where cracks branch out. In a major effort, the fluid code was integrated with the solids code. Additional details regarding the preliminary results of this collaborative project can be found in the Structures and Materials section of this report.

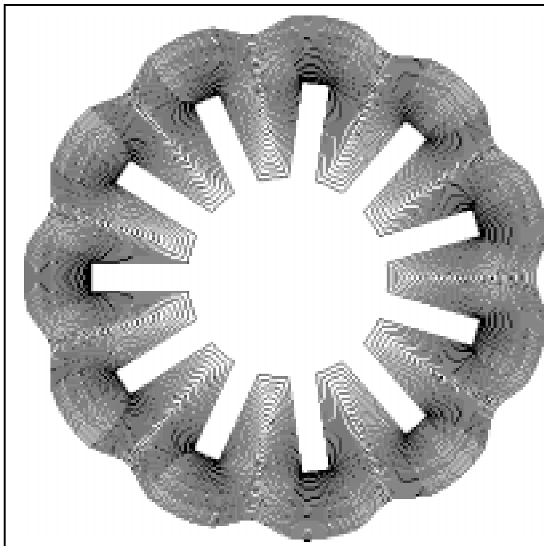
Fig. 3.3.4: Burn profiles for star grain computed using surface regression formulation

Turbulence Modeling

Efforts in turbulence modeling are in three related areas: classical Large Eddy Simulation (LES) model implementation and validation within the GEN1 code; Direct Numerical Simulation (DNS) and Particle Imaging Velocimetry (PIV) data acquisition for wall driven flows; and new LES model development for core flow applications.

Moser, Volker, and Langford are applying the formalism of optimal Large Eddy Simulation to develop LES models that will be applicable to the solid rocket problem. This is being pursued in three important directions. First, the optimal LES formalism is being used to investigate the properties of LES evolutions when defined relative to finite volume filters. This is the discretization underlying practical codes such as *ROCFLO*, so this investigation will allow us to create LES models that account for the numerical discretization in such simulations. By using the statistical information from a turbulent DNS, we are able to determine optimal computational operators appearing in the LES evolution equations. Second, the occurrence of strong inhomogeneities in a flow, such as those occurring near a wall or the propellant surface, cause considerable difficulty in LES because the assumptions underlying most models are violated in such strong inhomogeneities. However, the optimal LES formalism is valid in this situation, so we are using it to develop models that are valid near a solid wall. An optimal model for the near-wall region in a channel flow has been determined and its error properties measured. It is currently being analyzed to obtain a simplified characterization that will be useful in actual simulations (such as in *ROCFLO*). Third, the flow in a solid rocket is driven by strong transpiration, which makes the character of the turbulence to be modeled in this flow fundamentally different from that in the standard turbulence model problems. To account for this, the optimal LES formulation must be applied to a transpiration-driven flow. The planar periodic rocket direct numerical simulation (described below) was performed to provide such a model problem.

Lee and Moser are conducting a Direct Numerical Simulation (DNS) study of fully developed injection driven turbulent flows inside a circular pipe and Large Eddy Simulation (LES) modeling for strongly inhomogeneous flows. Numerical experiments on flows in a circular pipe with uniform side wall mass flow injection are performing by solving modified Navier-Stokes equations in a cylindrical coordinate system. Injection driven pipe flow undergoes axial acceleration, which in our simulations is treated using a multi-scale asymptotic formulation, leading to a modified Navier-Stokes equation. In deriving this formulation, it is assumed that the magnitude of the turbulence fluctuations is scaled with the mean velocity. The resulting equations are solved using a newly developed spectral method with stiffly stable time-splitting algorithm. The program is fully parallelized using OpenMP on the SGI Origin2000.

Najjar and Moser are developing a model problem representing the internal flow dynamics in the combustion chamber of a solid propellant rocket employing Direct Numerical Simulations (DNS). The flow is an injection-driven planar channel and is referred to as “a planar periodic rocket” (PPR). To account for the streamwise acceleration caused by the injection, while preserving the streamwise homogeneity, a multi-scale asymptotic representation is invoked. DNS computations have been performed for a wall injection Reynolds number of 400 and a non-dimensional axial location of 50. A numerical representation consisting of 512x193x384 Fourier-Chebychev modes was found to capture all the turbulent scales adequately. Parallel code portability was achieved with MPI and an efficient implementation of the kernels for Fast Fourier Transforms, FFT, was supplied by Wray at the Stanford ASCI Center. Large-scale computations have a sustained performance of 0.95μs/Δt per gridpoint on 128-processors of the ASCI Red system, resulting in 40Mflop/s per processor. It is observed that the near-wall turbulence of this strongly transpired flow does not resemble that in a non-transpired wall-bounded turbulence, either structurally or statistically. One of the primary accomplishments for the year in this project is the conduct and completion of production runs to create a database of 100 instantaneous turbulent fields separated by one eddy turnover time, for use in turbulence model development.

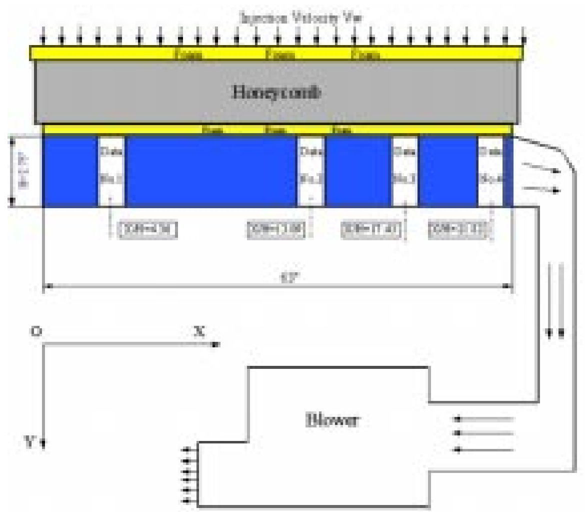

Fig. 3.3.5. Schematic of planar rocket chamber simulation experiment

An apparatus to produce a canonical, non-reacting turbulent flow that simulates many aspects of the turbulence produced in a solid rocket chamber has been constructed, Fig. 3.3.5. It utilizes wall injection of air to mimic the release of gas from a plane, burning solid propellant surface. The core flow of cylindrical chambers with wall injection is predicted by Culick's (AIAA J. 4, 1462-64,1966) inviscid, laminar, self-similar solution and used as a model of rocket core flow comparison of mean velocity profiles measured in the experiment to the planar equivalent of Culick's solution reveal substantial differences, the flow being retarded much more by the injecting wall. The instantaneous flow field in Fig. 3.3.6 shows that there are large levels of turbulence created in the model rocket chamber that could explain the large drag at the injecting wall. However, direct numerical simulations indicate that the injection suppresses turbulence, and they are consistent with the laminar solution. It is conjectured that the observed differences may be due to the boundary conditions in the experiment, which allow fluctuations that do not exist in the the-

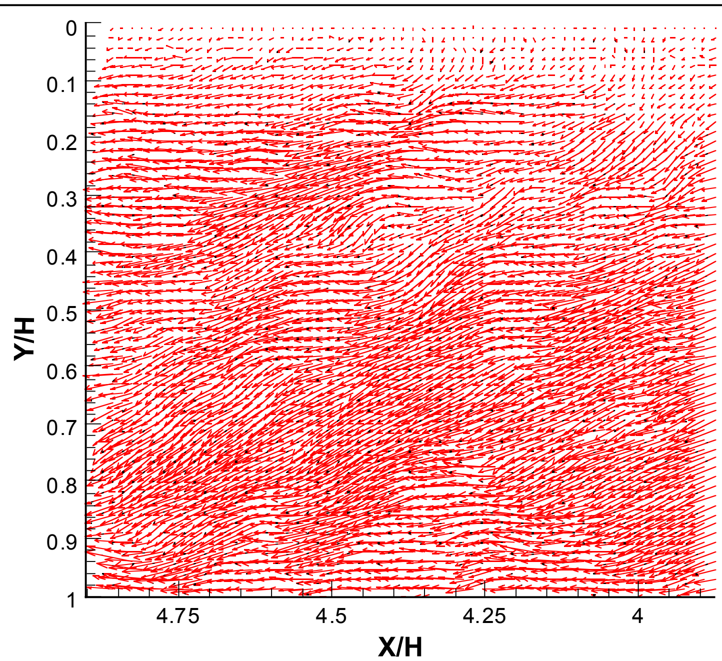

Fig. 3.3.6. Instantaneous velocity field measured in the x-y plane of core flow. Note large level of turbulent fluctuations

ory or in the ideal boundary of the numerical simulations.

Aluminum Particles

Ferry and Balachandar have been numerically investigating the behavior of particles in channel flow. We have identified a range of particle diameters for which particles tend to congregate, and statistics that predict where congregations will occur (Fig. 3.3.7). This yields critical information for the sub-grid scale modeling of particle distribution, which in turn affects, e.g., radiative heat transfer. We have investigated the nature of the velocity gradients that a particle experiences in a turbulent flow. Using state-of-the- art force law models, we are able to estimate the magnitude of flow-gradient effects on particles and thereby determine the region of parameter space for which better force laws are needed (cf. the microsimulations of Balachandar and Bagchi). Such a law will be necessary to evolve the larger particles in an SRM. To evolve the smaller particles, we have developed a method that is similar to, but much more efficient than, traditional Eulerian techniques. Tests of its range of applicability are underway, and preliminary results are promising.

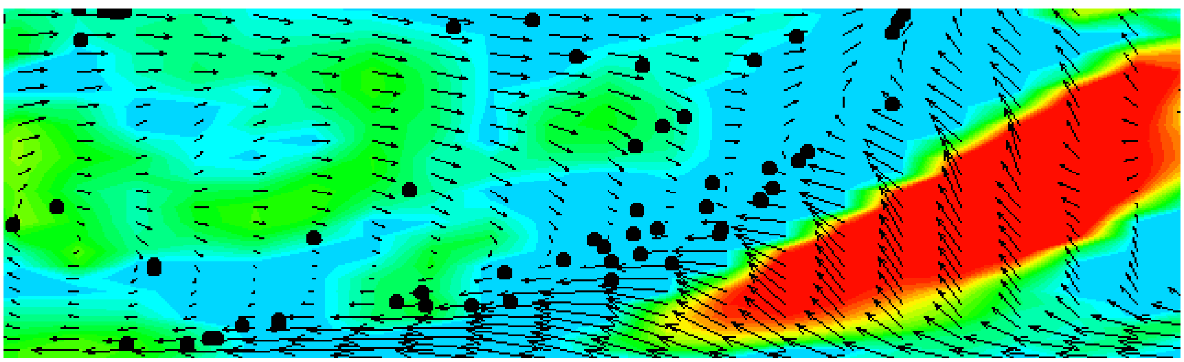

Fig. 3.3.7: Close-up of particles in channel flow. Particles congregate in inclined shear layer (where left-going and right-going fluid collide) and avoid regions of large swirling strength (red)

Alavilli, Balachandar, Najjar and Ferry have begun to implement particles in *ROCFLO*. Efficient communication techniques developed in the channel flow code are being used here to move particles between processors. To contend with the time-varying particle workload, we are investigating methods of dynamic load balancing.

Rani and Vanka have performed an LES study of the modification of turbulence in a fully-developed turbulent pipe flow due to dispersed heavy particles using a 64 (r) × 64 (θ) × 128 (z) grid. An Eulerian-Lagrangian approach has been used for treating the continuous and the dispersed phases, respectively. The particle equation of motion included only the drag force, which is the predominant force for heavy particles ($\rho_p/\rho_f >> 1$). Three different LES models are being used in the continuous fluid simulation: “No-Model” LES (coarse-grid DNS), Smagorinsky’s model, and Schumann’s model.

The effect of particles on fluid turbulence is investigated by tracking 100,000 particles of 20 μm diameter. Our studies confirm the preferential concentration of particles in the near wall region. It is observed that the inclusion of two-way coupling reduces the preferential concentration of particles. In addition, it was found that two-way coupling attenuates fluid turbulence. The effect of 100,000 particles on fluid turbulence was not significant. Hence

100,000 computational particles each consisting of ten individual particles are being tracked. However, we expect the above trends to differ depending upon the particle diameter and volumetric and mass fractions. The effect of SGS fluctuations on particle dispersion and turbulence modulation is yet to be investigated. Other relevant statistics for the continuous and the dispersed phases are collected for the cases of one-way and two-way coupling. These statistics are compared to study the modulation of turbulence by the particles.

Aref and Pushkin are studying particle coagulation and fragmentation kinetics relevant to the process of rocket propellant combustion. This is a complicated process of melting and coalescence of Al particles embedded in the propellant itself, and the distribution of ash particles carried by the hot gases in the rocket and ultimately deposited inside the nozzle or expelled with the flow. The issue of how to model the various populations of solid particles resident in the flow is our current focus. We have been studying a set of models due originally to Smoluchowski (1916) and established in the literature for the kinetics of coagulation and fragmentation. Instances of particle coagulation from fuels sprays to planet formation in galaxies has been addressed using these models. The literature is curiously divided between exact solutions of the equations, on the one hand, and scaling approaches, mainly due to Friedlander (1960) and Hunt (1982), on the other. The scaling approaches seem to hold the most promise for rocket applications, since it will be prohibitive in terms of computational resources to carry detailed information on the composition of a particle population from grid point to grid point. We have established two results that we believe to be new relating the scaling of the particle size distribution to the homogeneity index for the coagulation or fragmentation kernel.

Radiation

Norman and Hayes are developing a radiation model for the optically transparent region just above the propellant combustion interface (PCI) for integration into GEN2. It is known that the radiant flux produced by burning aluminum droplets will raise the temperature of the propellant, thereby altering the burn rate. In standard CFD models of the core flow, the mass flux injected through the PCI is parameterized as a function of the propellant density and gas pressure adjacent to the PCI, and radiation effects are ignored. By calculating the radiation flux on the PCI arising from the burning of Al droplets, we seek to augment the standard mass flux boundary condition by including an additional dependence upon the incident radiant flux incident there. This flux calculation will be provided by a formal solution to the transfer equation using appropriate data for the spatial distribution of burning aluminum droplets and aluminum oxide smoke. We tested our existing radiation solver by performing a simple calculation where the droplet/smoke distributions were given by simple functions of the cylindrical radius and the radiation field was assumed to be diffusive. This module was coupled to a 3-D hydrodynamics module and used to conduct a simple rocket simulation on eight processors of the NCSA Origin2000. The primary aim of the exercise was to assess the numerical behavior of our code when opacities and emissivities appropriate to the rocket problem were employed in the radiation prescription.