3.3 Fluid Dynamics

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Overview

There are four primary research and development activities being pursued in the Fluid Dynamics Group. These are the development and testing of the primary GEN1 fluid dynamics code, *Rocflo*; two-phase flow simulation and modeling to represent aluminum and aluminum oxide particles; turbulence simulation and modeling through large-eddy simulation; and modeling and simulation of radiative heat transfer. All of these activities are directed toward the requirements of the GEN1 and GEN2 simulation requirements for the core flow.

ROCFLO Code Development

The fluid dynamics code, *Rocflo*, continues to be developed, enhanced, and tested. A major milestone was passed in Y3 with the official (internal) release of the integrated GEN1 rocket simulation code, along with the GEN1 component codes, including *Rocflo*.

Validation and Testing (Alavilli)

Several small-scale laboratory rocket motors for which data are available have been simulated. Specifically, based on data provided by Fred Blomshield, (Naval Surface Warfare Center, China Lake) three different motors were simulated; two with cylindrical grains and the other with a six point star grain. The results are shown in Figure 3.3.1 comparing the *Rocflo* simulation to the experimental data for the evolution of head-end mean pressure. The pressure time history has been accurately captured for these motors, particularly the slope of the pressure-time curve arising due to propellant regression and the tail-off due to burn out are simulated accurately. However, since no ignition transient modeling is done in these simulations, the initial pressure buildup during ignition and flame spread is not accurate.

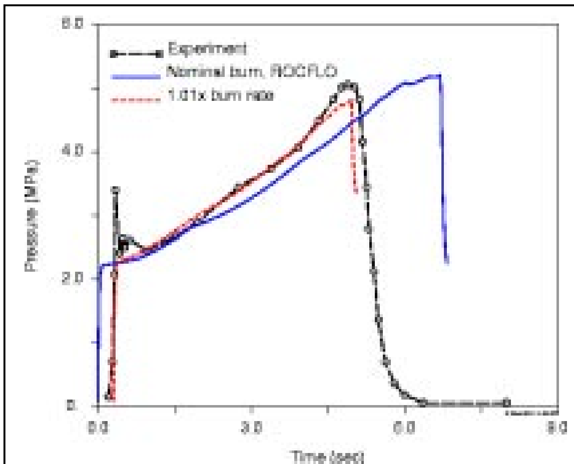

Fig. 3.3.1: Validation compares head-end pressure evolution to experimental data for lab-scale motor.

Ignition-transient Modeling for Solid Propellant Rockets (Alavilli, Buckmaster, Jackson, Short)

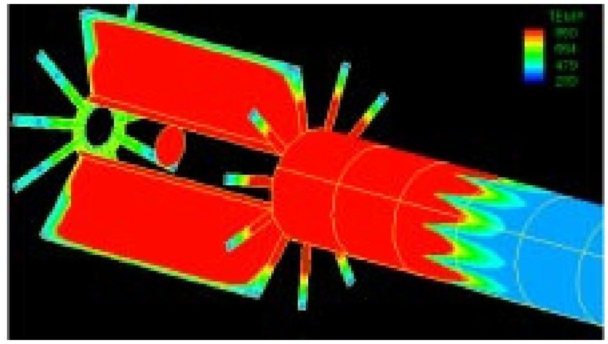

Fig. 3.3.2: Initial 3-D ignition transient simulation.

Ignition and flame spread modeling is critical to simulating the initial pressure buildup in a solid rocket motor. Currently available ignition transient models are inadequate to describe the detailed dynamics of ignition, especially in complex motors with star grain geometries such as the Space Shuttle booster. A large number of issues are considered and modeled in the current work; these include igniter flow, ignition criterion, flame spread and pressure seal rupture. The igniter flow is modeled as a specified inlet condition at the outlet of the igniter nozzle. Simulation of the igniter plume then captures the hot igniter gas impingement on the propellant and the shock patterns in the plume.

Heat flux to the propellant surface is computed by considering the conductive heat transfer to the propellant driven by wall-normal temperature gradients at the surface, and a specified auto-ignition temperature for propellant implicitly yields an induction period of propellant pre-heating, and flame spread is modeling through successive ignitions.

Adaptive Mesh Refinement and Dynamic Load Balancing (Alavilli)

Long time, or full burn, simulations of solid-propellant rocket motors must deal with the geometric and topological evolution of the computational domain due to the propellant regression and structural deformation induced by the gas loads. As the chamber volume increases during burning the computational blocks of *Rocflo* expand to fill in the entire chamber using an ALE formulation. Over long periods the cumulative effect of regression is to make the initial mesh discretization inadequate. To address this problem, dynamic and adaptive multi-block capabilities are being developed within *Rocflo*. This capability requires the ability to change block resolution, update topological interconnectivity across processors and balance the computational load. When fully developed this framework should allow optimal parallel performance for dynamic adaptive simulations.

Software Development

To support future fluids code development, several efforts in software and numerical methods development are being pursued. A few of these are listed here. Hybrid MPI/Open-MP parallel programming paradigms have been evaluated and benchmarked for scalability (Tafti, Najjar). Parallel I/O using HDF5 has been pursued in *Rocflo* (Tafti, Fiedler). New numerical techniques based on nodal integral techniques have been developed and evaluated for possible use in fluid simulations (Rizwan-uddin).

In Y4 the ignition transient model will be validated by comparison with experimental data for the Space Shuttle and other rocket motors, and the physical modeling of ignition will be improved by including augmenting mechanisms such as radiative heat transfer and flow turbulence. A large development effort is further required for the adaptive mesh refinement and load balancing implementation. A new effort is also beginning to develop, implement and integrate a fully three-dimensional unstructured grid capability into *Rocflo*, which will allow simulation of flows in extremely complex geometries, such as propellant cracks. Finally, several of the research efforts discussed below are producing models that will be or are being implanted into *Rocflo*.

Two-Phase Flow Simulation and Modeling

The core flow in a solid propellant rocket is multi-phase, with relatively large (~100 micron) burning aluminum droplets and relatively small sized aluminum oxide particles. Several modeling and implementation issues must be addressed if this complex multi-phase flow is to be accurately simulated. The modeling of large particles (droplets) and small particles (aluminum-oxide smoke) is handled differently because of the difference in time scale of their dynamics.

Large Particles, Aluminum Droplets (Balachandar, Bagchi, Ferry, Vanka, Najjar)

In a rocket core flow, the size of the Al droplets varies from a few tens of microns up to a few hundred microns. The Reynolds number (Re) based on the droplet diameter can be as high as a few hundred, so the low Re force law (Stokes drag) is not valid in this range. The standard drag law, which is valid at finite Re, cannot account for spatial variations in the surrounding flow. To obtain a generalized force law, we have performed high-resolution numerical simulations for time-dependent 3-D flow around a freely moving particle. The non-uniformity in the surrounding flow, e.g., straining or shear flow similar to rocket core flow, was found to have a profound effect on the drag and lift forces. An improved parameterization for force in a linearly varying flow was developed. It was also found that three-dimensionality in the wake of the particle has a profound effect on local heat transfer and evaporation rate compared with the axisymmetric solution.

The presence of heavy particles in a turbulent flow has a back effect on the flow that must be captured. This is being investigated using direct simulation in the somewhat simpler case of a turbulent pipe flow using three different sized particles. It was observed that two-way coupling reduces the preferential concentration of particles near the wall. Significant augmentation of turbulence, especially at the smaller dissipative scales, can be seen in the energy spectra at certain radial locations.

In a rocket core flow simulation, the treatment of large particle evolution involves several complications, all of which require further modeling. First, the actual number of particles present in the core flow is too large to allow simulation of each individual particle. A stochastic approach is being pursued in which a smaller number of “super particles” is tracked. The super particles provide the particle statistics required to determine the effect of the much larger number of actual particles. Second, the particles are acted on by turbulence, both the resolved and subgrid turbulence. To account for the effects of the subgrid turbulence, a modified Langevin model has been developed. Finally, the injection of aluminum particles from the propellant surface must be modeled, and a stochastic model of this process has been developed based on a model for the agglomeration and injection of aluminum droplets on the surface. These models are being further refined.

Small Particles, Aluminum Oxide (Balachandar, Ferry, Aref)

Due to their large number and small size, the aluminum oxide particles are treated as an Eulerian density field. A fast Eulerian method has been developed whereby a second order approximation to the particle velocity field is determined without solving the two-fluid particle velocity equations. This approximation has been evaluated and found to be accurate for the aluminum-oxide particles in the SRM core flow. A complication in the evolution of the oxide particle size distribution is that the particles can agglomerate and break apart. This is being addressed using asymptotic solutions of the Smoluchowski equation of particle coagulation and fragmentation. Studies of these solutions as steady states of a forced kinetics equation suggest that they are appropriate approximations for the rocket core flow. A similar analysis is being pursued to refine the aluminum droplet agglomeration model.

Implementation in *Rocflo* (Najjar, Balakrishnan, Alavilli)

To support the simulation of aluminum droplets, a Lagrangian particle tracking module, *Rocpart*, has been developed that works in concert with the Eulerian fluid solver *Rocflo*. The highly parallel implementation permits simulation for millions of fluid cells while tracking several millions aluminum droplets. The stochastic model for the injection of the particles has been implemented and tested in *Rocflo* over a wide range of parameters that define the injection process (Figure 3.3.3). To complete the representation of the aluminum droplets, a model for the evaporation and combustion of aluminum is needed. Models from the literature are currently being evaluated for this purpose in preparation for inclusion in *Rocflo*; also needed in this context is a representation for the oxidizer concentration in the core flow. This is also being implemented in *Rocflo*—as is a full gas-phase chemical reaction capability—to support equilibrium changes that occur in the nozzle.

The fast Eulerian technique for the simulation of oxide smoke as discussed above is being implemented in *Rocflo*. This effort has just begun and is the first step in integrating the fluid solver with a thermal radiation solver since the oxide smoke concentration determines the opacity of the gas to thermal radiation (see below). With support for aluminum droplets and their combustion, aluminum oxide smoke, and thermal radiation, a complete description of the physics of the burning of aluminized propellants will be possible.

Large Eddy Simulation and Turbulence

Large eddy simulation (LES) is the turbulence modeling technique we have chosen to use in the rocket simulation. However, LES subgrid modeling for such injection driven flows is not as well established as for other wall-bounded flows. Further, LES models suffer from a variety of shortcomings that we would like to improve. To address these issues, a new LES modeling technique called “optimal LES” has been pursued, both as standard model flows for turbulence research and in rocket-related flows. In addition, standard LES models are being implemented and tested in the *Rocflo* solver using an idealized rocket flow called the compressible periodic rocket (CPR).

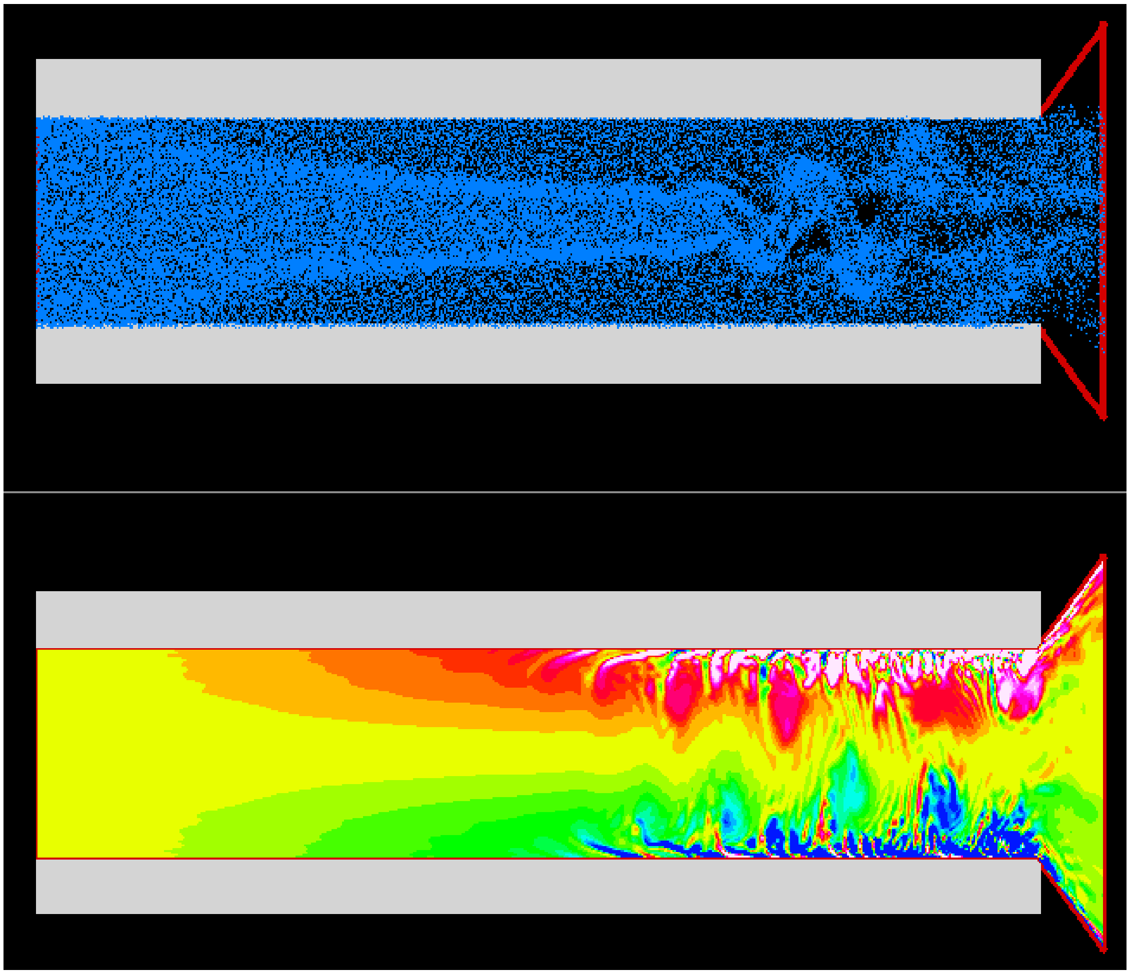

Fig. 3.3.3: Distribution of aluminum droplets in simulated core flow. Top image shows 90000 droplets tracked in computational domain. Bottom image shows spanwise vorticity. White/red represent positive vorticity, blue/green is negative.

LES Model Development (Moser, Najjar, Venugopal, Volker)

By applying the optimal LES modeling technique in which LES models are constructed by formal minimization of the error, we showed that modeling wall-bounded turbulence (channel flow) requires several properties of the subgrid term be represented in the model. These include the subgrid contribution to mean stresses, the subgrid contribution to the transport of energy, and the transfer of energy from the resolved to the subgrid scales. When optimal models that respected these requirements were used in channel flow LES, the results were remarkably good; better than any previous LES of this flow of which we are aware. This finding was determined to be directly applicable to the rocket core flow. DNS data from the incompressible planar periodic rocket (PPR), which is an injection driven flow in a planar channel with asymptotic treatment of streamwise acceleration, shows that inhomogeneities in the subgrid term similar to the channel are present in the injection driven flows. The PPR data will be used to develop optimal LES models specifically for such injection flows.

Through the study of isotropic turbulence, we also found that optimal LES models based on finite volume representations of the large-scale turbulence could be consistently formulated. Such models are currently being tested in actual LES.

LES Model Implementation and Testing (Moser, Najjar, Venugopal)

To develop and test LES models for use in solid propellant rocket simulations, a simplified model flow that retains the important features of the rocket is needed, such as the PPR discussed above. A compressible version of this model flow (the compressible periodic rocket, CPR) has now been devised and implemented in *ROCFLO*, so the LES models can be evaluated and tested in the context of the numerical discretizations used in the core flow simulation. An asymptotic treatment of acceleration and mass addition was devised to match the properties of known solutions for such injection driven flows. Preliminary 2-D simulations have now been performed, and the large-scale structures (Figure 3.3.4) are consistent with the simulation of a well-known ONERA experiment (see below). Three-dimensional LES simulations using intrinsic numerical dissipation as a subgrid model are underway. Implementation and testing of more sophisticated models, such as a dynamic model, a scale similarity model, and a stretched vortex model, are planned.

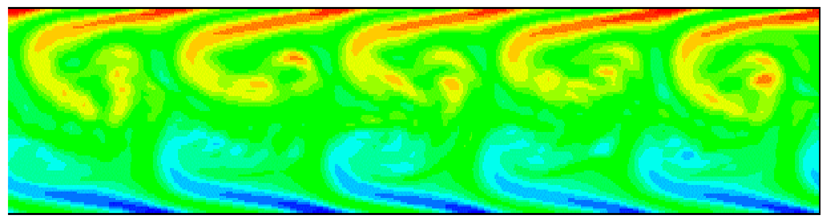

Fig. 3.3.4: Spanwise vorticity in compressible periodic rocket simulation.

To test the validity of the PPR and CPR approximations, temporal stability analysis of both flows was performed. The computed growth rates were found to be in excellent agreement with spatial stability analysis studies. The results from this study were also used to assess the growth of small amplitude perturbations in *Rocflo* and evaluate the minimum resolution requirements for performing turbulence simulations.

A high-resolution 3-D LES simulation of the ONERA experiment has been conducted using intrinsic numerical dissipation for the LES model. This simulation is being used as a test flow for Lagrangian particle simulations and as a validation point for the CPR formulation.

Turbulence Experiments (Adrian)

An apparatus to produce a non-reacting turbulent flow that simulates many aspects of the turbulence produced in a solid rocket chamber has been constructed, Figure 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 inviscid, laminar, self-similar solution (AIAA J. 4, 1462-64,1966). A 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 streamwise velocity flow field in Figure 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 theory or in the ideal boundary of the numerical simulations.

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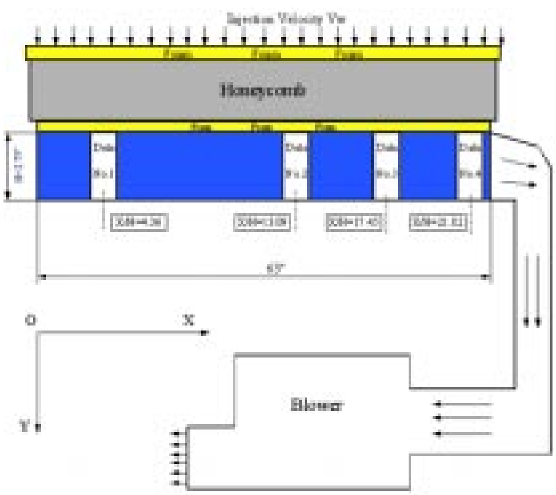

Fig. 3.3.5: Schematic of planar rocket chamber simulation experiment.

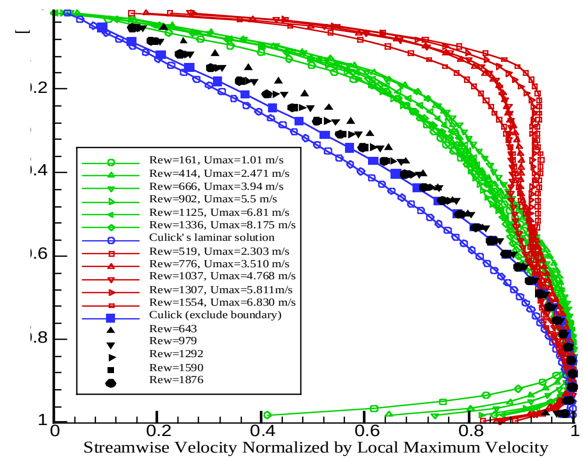

Fig. 3.3.6: Streamwise velocity profiles from planar rocket chamber simulation experiment.