3.4 Fluid Dynamics

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Overview

The Fluid Dynamics Group works on system-scale solid rocket motor multiphase compressible core flow code development as well as subscale model development relevant to the turbulent dynamics of the combustion interface. Research projects that will intersect with the integrated code some time in the future include work in injection, dispersion and combustion of Al droplets in the core flow; formation, dispersion and slag accumulation of aluminum oxide particles; and flow within cracks and other defects within the propellant.

Turbulence Research

Large Eddy Model Development (Moser, Najjar, Venugopal, and Zandonade)

To improve the veracity of large eddy simulation (LES) models in our solid propellant rocket simulations, and in general, we have been pursuing two different activities. In the first, a streamwise homogenized model problem for the simulation of turbulence in an injection driven compressible flow was developed. This is the so-called compressible periodic rocket (CPR) model. A module implementing the homogenization terms required to simulate this model in *Rocflo-MP* framework has been developed and tested. This allows LES of this problem to be performed in *Rocflo* for direct validation against direct numerical simulation (DNS) of the CPR. Large-scale production simulations of the DNS CPR are now being planned, and results from this effort will be reported on in the future.

The second area of LES development is the pursuit of optimal LES formulations appropriate for use in simulators such as *Rocflo*. A class of finite-volume optimal LES models are well suited for *Rocflo* implementation. Preliminary results from such finite volume models reported last year indicated that improvements were required. The models have since been refined, and the stability properties of the models were improved. Results for the refined models, both the spectrum and the third order structure function are in excellent agreement with the DNS. This along with previous excellent results from optimal LES in wall-bounded flows show that this modeling approach is indeed very powerful and worth pursuing further.

The primary drawback of the optimal LES models described above is their reliance on DNS data. A recent break-through in the theoretical formulation of these models promises to alleviate that problem. In this theoretical approach, much of the statistical information that is needed to formulate the model is determined from Kolmogorov inertial range theory, and the quasi-normal approximation. The one quantity that is not amenable to such modeling is obtained from the running LES via a dynamic procedure. The resulting model is valid in any situation in which the small-scales are approximately homogeneous and isotropic. For strongly inhomogeneous flows, more sophisticated modeling of the required correlations is being pursued. This modeling approach is currently being tested, and implemented in *Rocflu*.

Subgrid Turbulence Modeling (Moser, Najjar, and Wasistho)

We have been pursuing efficient implementations of subgrid scale turbulence model to account for turbulent motions smaller than the resolved scales in the core flow of the rocket. Four classical LES models have been implemented in redesigned *Rocflo-MP*: the basic and dynamic Smagorinsky model, scale similarity model and dynamic mix model. Validations in compressible periodic rocket (CPR) flow, ONERA-C1 (Figure 3.4.1) and ONERA-86, show that the models enable simulations using fairly coarse grids without any numerical dissipation and compare favorably with reference data. For example, in the ONERA-86-cold case using dynamic Smagorinsky model the mean axial velocity and pressure are in good agreement with experimental measurement (see Figure 3.4.1). In addition detailed evaluation of the numerical simulations of compressible rocket flows are conducted in laminar, transitional and turbulent regimes. It was found that the mean flow is in close agreement with the compressible theory than with the conventional Culick's solution. The oscillatory part of the flow agrees well with the acoustic layer model near the head end but the agreement with the simple theory decreases when the compressibility effect becomes important (see AIAA 2002-4344).

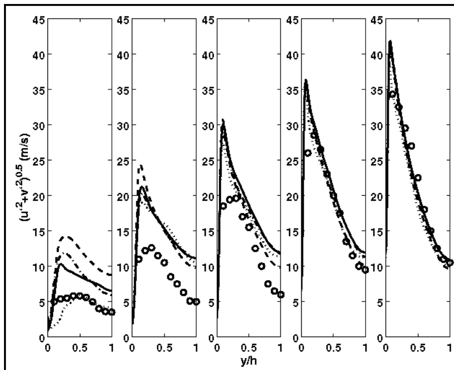

Fig 3.4.1: Comparison of LES results with experimental data.

Transpiration of hot gases from the burning solid wall of a SRM creates turbulence in the core flow. Experiments to study fundamental aspects of the turbulence production process have been conducted in a second-generation isothermal channel flow apparatus with two fully transpired walls. Results with different types of porous walls indicate that the core flow is extremely sensitive to the details of the wall boundary. Small changes in the hydrodynamic impedance of the wall can change the flow from almost laminar behavior to highly turbulent flow. Hence, good numerical simulation of the core flow requires accurate knowledge of the wall boundary conditions.

Experiments have also been initiated to determine the boundary conditions at the burning surface for use in computer simulations. To develop PIV methods to measure the hot gas flow above burning solid rocket fuels, initial work was done in the exhaust of a small rocket motor. It has been shown that PIV measurements can be made in 3,500 K^o, 1,000 m/s combustion gases. Future work will focus on determining the spatio-temporal character of the gas velocity just above a planar burning surface, using solid fuels with and without aluminum particles. These data will provide direct input for CFD boundary conditions in SRMs.

Multiphase Flow Modeling

Aluminum Droplets, Particles, and Smoke in Flow (Bagchi, Balachandar, Ferry, Rani, and Vanka)

The ongoing research efforts on microsimulation of aluminum droplet by Bagchi and Balachandar seek to address three specific problems: a) an accurate parameterization of forces acting on a droplet in a complex flow; b) micro-physics of the detailed interaction of a single particle/droplet with a complex flow; and c) a parameterization of heat transfer and evaporation rate of the droplet. In a rocket core flow, the size of the Al droplet varies from a few tens of microns up to about a few hundreds. The Al droplets account for nearly 20% of the heat generation. The standard drag law, widely used for tracking these particles, cannot account for the complex time and space varying fluid flow, especially near the rocket nozzle, where there is very strong streamwise acceleration of the flow and wall shear. In order to study the detailed interaction of a particle with such complex flows, we have developed a high-resolution, highly parallelized, direct simulation code. Using this code we have studied the effect of strong streamwise acceleration as in the nozzle, effect of near wall shear and associated particle rotation. The forces on the particle under such nonuniform flows are observed to be significantly different from the predictions using the standard law. An improved parameterization of force in several classes of linearly varying flow is developed.

More recent work is concerned with the effect of turbulent flows on the particle/droplet. A review of the existing literature reveals that not much is known on the effect of turbulence on the forces acting on a particle. The direct numerical technique developed here is used to parameterize the effect of turbulence. It is observed that turbulence has little influence on the mean drag (Figure 3.4.2) and lift force on the particle, but can significantly dictate the fluctuating forces. It is observed that rms force fluctuation scales linearly with both the mean drag as well as the level of free-stream fluctuation. It is also known that the presence of the particle can have a back effect on the turbulent flow itself. Understanding this effect is very important in many multiphase flows where the particulate and the continuum phases are strongly coupled (as in rockets). The detailed simulations considered here have greatly helped us to better understand and model of such droplet/particle-turbulence interaction. We are also pursuing the effect of surface evaporation from the particle on forces and heat transfer and the influence of three-dimensionality at higher Re.

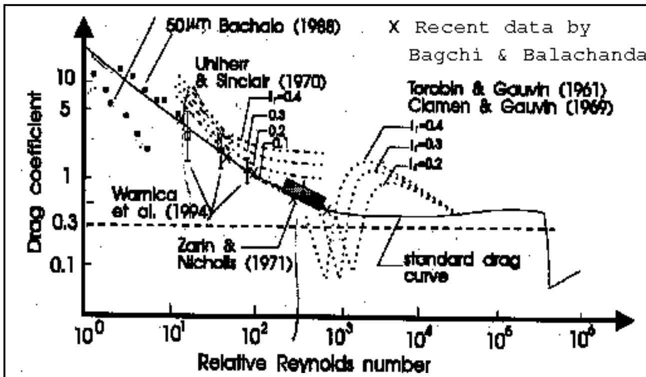

Fig 3.4.2: Compilation of mean drag coefficient in turbulent flow vs Re. Also shown are results of present DNS.

The primary focus of Ferry and Balachandar's research activities has been the continued development of the equilibrium Eulerian method in terms a semi-implicit improvement to the standard method, which has been thoroughly verified through various numerical experiments that incorporates additional physics into the model. The original formulation has been generalized to include more physics: e.g., two-way coupling, volumetric concentration dependence, and rotational forces. We have implemented the equilibrium Eulerian method in a DNS of isotropic turbulence turbulent channel flow to test the predictions made in our previous (Lagrangian) studies. We have also been investigating a novel idea to approximate the divergence of the particle velocity field for any particle size, generalizing Maxey's formula.

Rani and Balachandar are pursuing the idea of Equilibrium Eulerian particle velocity field for a fully-consistent two-way coupled multiphase isotropic turbulence simulation. The objective of the current effort is to use a two-fluid formulation that employs particle-fluid mixture governing equations to study two-way coupling between fluid turbulence and particles. These governing equations require closure, which will be provided by the Equilibrium particle velocity expansion. The advantage of this formulation is that there is no need to solve two sets of governing equations corresponding to the fluid and particle fields, as is the case with conventional two-fluid methods. Here, we focus attention to the limit where all the relevant length scales of the undisturbed flow are much larger than the particle diameter. This scale separation allows us to formally carry out an ensemble average over all the small-scale particle arrangements. Thus, we can ensemble average the fluid-particle mixture governing equations without losing any of the macroscopic turbulence scales (including the Kolmogorov scale).

The presence of heavy particles in a turbulent flow has a back effect on the flow that must be captured. This has been investigated by Rani and Vanka using two-way coupled direct numerical simulations in the case of a turbulent pipe flow. Particles are smaller than the Kolmogorov scale of turbulence. The continuous and the dispersed phases are treated using the Eulerian and Lagrangian approaches respectively. The effects of varying particle parameters such as response time, volume fraction and settling velocity on fluid turbulence are investigated. When the particle settling velocity is zero, variation of either the volume fraction or the response time has negligible effects on the fluid streamwise mean velocity profile. However, an increase in either the volume fraction or the response time augments the streamwise rms velocities and attenuates the radial and azimuthal rms velocities. Particles with positive settling velocity lead to a marginal increase in the streamwise mean velocities and a substantial increase in the streamwise *rms* velocities. A new, efficient and accurate particle collision algorithm has been derived. The effects of particle-particle collisions on fluid turbulence are also studied. Collisions are seen to reduce particle migration to the wall. A more comprehensive study of the effects of particle collisions on two-way coupling in a pipe flow has to be undertaken.

Coagulation and Fragmentation (Aref and Pushkin)

We are studying the equations describing coagulation and fragmentation phenomena with a view to applying the results to the aluminum particles used in solid-rocket fuels and the ash particles produced once these particles have burned. Modeling of the size and mass distribution of fuel and ash particles is an important input to the global simulation codes being constructed within CSAR, since it would potentially allow us not to have to gather such statistics via simulation. It is one element of a broader thrust within the particle group of CSAR. Pushkin has been looking at coagulation phenomena quite broadly and has discovered intriguing applications of the theoretical ideas developed well beyond the realm of rocket science. We are currently looking at extensions to multiple (more than binary) collisions, to effects related to differences in the particle relaxation time and the coagulation time scales, and to effects of particle anisotropy.

The main activity will be to bring the coagulation work to a fruitful and useful conclusion. Currently, several writing projects are underway: (1) An analogy between the scaling of coagulation kinetics and other phenomena exists. We have documented this in the distribution of the sizes of banks through mergers. A short paper is in preparation. (2) The expression for the spectral exponent, obtained for binary collisions, can be generalized substantially for other cases, and this is being written up. (3) A model of large particle growing by "scavenging" small particles has been obtained and is being pursued.

Integrated Code Development

Rocflo-MP (Blazek)

As we began incorporating more physics modules to the old fluid solver (*Rocflo*), it became obvious that a new flow solver was necessary in order to meet the future CSAR requirements. Our principal task has been the design and implementation of a new, 3-D structured multiblock flow solver (*Rocflo-MP*). It was also decided that an unstructured code will be needed to address even more complex geometric conditions such as flow in a propagating crack, joints and other accident scenarios. A new fluids framework was implemented to allow for substantial commonality between both the block-structured and the unstructured codes. The first full capable version of *Rocflo-MP* was released in March 2002. The new solver was subsequently tested and validated in a number of cases. One example is the ARC rocket, where the computed quasi-steady head end pressure was in close agreement with the experiment (44.7 versus 45 MPa). Another example is the Titan IV, the largest case so far (about 1.7M grid cells). The results of a run on 512 processors can be seen in Figure 3.4.3. *Rocflo-MP* was recently extended by a grid motion scheme and is being integrated into the coupled code (GEN2.5).

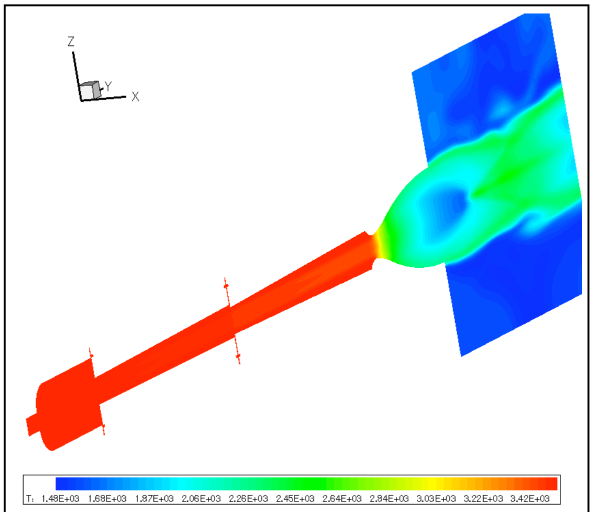

Fig. 3.4.3: contours of static temperature (in K) in cut through Titan IV motor.

The next step in terms of the structured code (*Rocflo-MP*) is to finish its integration into GEN2.5 and to validate the code for the case of fluid-structure coupling. After that, it is intended to enhance the simulation capabilities of *Rocflo-MP* by implementing: dual-time stepping — to increase the allowable time step, global grid motion scheme – to move also boundaries between grid blocks, discontinuous grid interfaces — to allow for a more general grid refinement/de-refinement strategy, coupling to unstructured grid interfaces – to treat complex geometries like the star grain or cracks, novel upwind spatial discretization scheme – to increase accuracy and robustness.

Rocflu (Haselbacher)

Alongside *Rocflo-MP,* Haselbacher is developing an unstructured fluid-dynamics code on the basis of common data structures, variable definitions, naming conventions, and coding standards. The main goal of increasing code reuse is to ease the integration of multiphysics modules. The current status of *Rocflu* is that a first-order accurate parallel version is running and has been tested on steady and unsteady inviscid flows. *Rocflu* was parallelized using the FEM framework and the *Charm++* library. *Rocflu* was also integrated with GEN2.5. We have also developed a new filtering method for unstructured grids, which is being used in *Rocflu* for

Large-Eddy Simulations. The most important tasks for the future are to extend *Rocflu* to second-order spatial accuracy, to incorporate a grid-motion capability, to couple it to *Rocflo*.

Together with Jiao and Geubelle, Haselbacher has developed a new framework for the communication of interface data between the application codes for GEN2.5. The main advantages of the new framework are increased modularity, flexibility, and simplicity. These are achieved through the concept of a manager module that orchestrates the interaction of the application codes. One example of the improved modularity is that the application codes no longer require rocket-specific code segments.

Multiphysics Modules (Ferry, Najjar, and Wasistho)

A fully integrated multi-physics flow simulation solver in solid propellant rockets has been achieved. It consists of a Lagrangian particle tracking module (*Rocpart*), an Eulerian fluid solver (*Rocflo*), an LES turbulence module (*Rocturb*) and an Equilibrium Eulerian smoke module (*Rocsmoke*). Fully coupled three-dimensional simulations have been performed showcasing the complex physical phenomena obtained within this framework construct (*Rocflo-MP*). Figure 3.4.4 shows the spanwise vorticity field, the particle location and the smoke concentration at one time instant. It is observed the highly unsteady flow nature where several large-scale vortices are convecting in the rocket core chamber. Further, significant wall-based structures are seen to evolve similar to the Parietal Vortex Shedding (VSP) phenomenon. Simulations have been conducted where approximately 1.8 million computational particles are being evolved with a superparticle loading factor of 90, hence representing over 160 million real particles.

The integration of the multiphysics framework will be undertaken under the newly developed *Rocfluid-MP* infrastructure. This allows evolution of Lagrangian particles in complex geometries and permits a much more robust and integrated tool to investigate multiphase flows in solid propellant rockets. It will include more sophisticated physical modules developed within the Fluids Group.

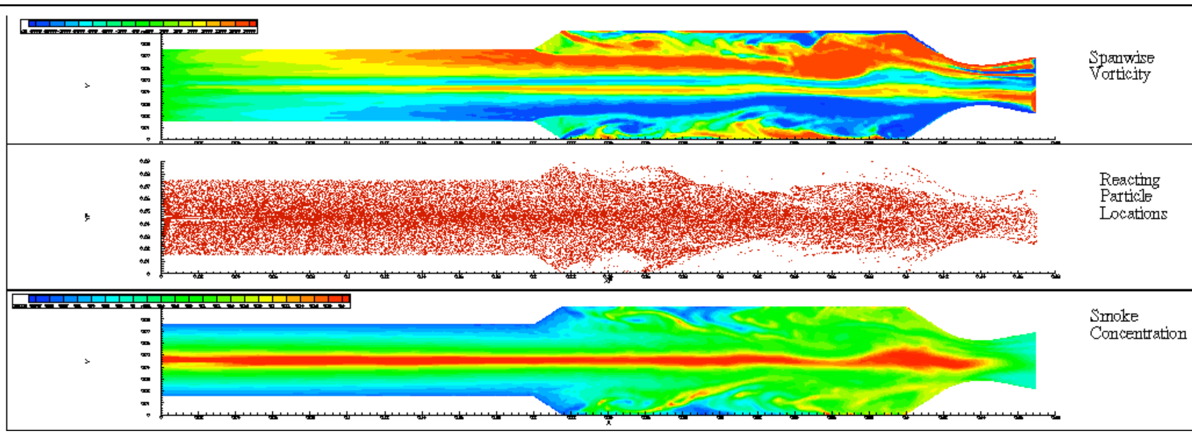

Fig 3.4.4: Spanwise vorticity, particle location and smoke concentration at one time for ONERA Hot-86 geometry.