3.3 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; injection, dispersion and combustion of aluminum droplets in the core flow, formation, dispersion and slag accumulation of aluminum oxide particles and flow within cracks and other defects within the propellant.

Large Eddy Simulation Model Development of Solid Rocket Core Flow (Moser, Najjar, Balakrishnan, Venugopal, Wasistho)

Moser and his coworkers have been pursuing two different activities to improve the veracity of large eddy simulation (LES) models in our solid propellant rocket simulations. 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 simulating 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 DNS of the CPR.

The second area of LES development is the pursuit of optimal LES formulations appropriate for use in simulators such as Rocflo. Langford proposed a class of finite-volume optimal LES models, and these are well suited for Rocflo implementation. Balakrishnan is pursuing a generalization of these models to arbitrary Reynolds numbers, and the models are being evaluated in isotropic turbulence. Results of the first LES with finite volume optimal LES models are shown in the figure below. Both the spectra and third-order structure function show good agreement with filtered DNS

Fig. 3.3.1: Three-dimensional large eddy simulation of channel flow with side wall injection (ONERA-86 cold case). Colors depict iso-vorticity contours and velocity magnitude.
data, though both could use improvement, particularly at high wavenumbers. It was observed that several of the model stencils proposed by Langford do not produce stable calculations. The cause of this is being analyzed so that the optimal LES can be constrained to produce stable simulations.

Another result of the optimal LES effort is an analysis of the effects of inhomogeneity on optimal LES models. It was found that in inhomogeneous flows, the optimal models must be constructed so that the subgrid contribution to Reynolds stress transport is correctly represented a priori. The consequences on the mean and rms velocities of not satisfying this are shown in the following figure. This has far-reaching consequences for LES model development in general. The implication is that LES models must represent much more than just subgrid energy transfer, they also contribute to mean Reynolds stress and to several terms in the Reynolds stress transport equations, and these aspects must be correctly modeled. In particular, this affects the simulation of the turbulence in a solid-propellant rocket, which is also strongly inhomogeneous.

Wasistho has 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 Rocflo: the basic and dynamic Smagorinsky model, scale similarity model and dynamic mix model. Validations in compressible periodic rocket (CPR) flow, ONERA-C1 (Figure 3.3.2) 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. The turbulence intensity, however, shows earlier transition and overprediction of the near head-end turbulence. A better turbulent injection model is needed to improve the result. In the future, the accuracy of the LES is to be improved by non-uniform filtering and full modeling of the energy subgrid terms. Moreover, Detached Eddy Simulation (DES) model in conjunction with zonal modeling is to be implemented, which is thought to be more suitable for flow in the nozzle.

Near-wall Turbulence (Adrian, Deng)

Adrian and Deng are concentrating on two areas relevant to CSAR. First is the better understanding of turbulence near the wall in the presence of strong injection from the wall. As outlined earlier this understanding is essential in being able to accurately simulate the turbulent flow within the rocket core. The second objective of the experiment is to investigate the turbulent flow within the rocket, against which the computational results can be validated. The experiments will produce data over a range of Reynolds numbers; this will allow for comparison with direct and large eddy simulations being performed within the center. Experiments are ongoing both in a channel and in a redesigned pipe configuration. For the for-
mer we have designed modifications of an existing wind tunnel to create a 2-D channel flow with one end sealed and blowing a porous section of one wall. Measurements are compared with those of Proudman-Culick solution for laminar injection-driven flow. The experimental results with different porous sections show the extreme sensitivity of the resulting mean flow to the nature of flow (and possibly turbulence) at the point of injection. These results are currently being validated with the new set of measurements in the pipe configuration.

Multiphase Flow Modeling for SRM (Balachandar, Bagchi)

The ongoing research efforts on microsimulation of aluminum droplet by Bagchi, Balachandar and Prof. Ha (Pusan National University, S. Korea) 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 linearly varying flows, such as shear and straining flows. 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 a linearly varying flow is developed. Figure 3.3.3 gives a comparison of the new parameterization with the full simulation and the results of standard parameterization.

The present 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 will be used to parameterize the effect of turbulence. 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 will help 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.
Fast Eulerian Method Development (Balachandar and Ferry)

The primary focus of Ferry and Balachandar’s research activities has been the continued development of the Fast Eulerian method. The original formulation has been generalized to include more physics, e.g., two-way coupling, volumetric concentration dependence, and rotational forces. The Fast Eulerian method has been implemented in a DNS of turbulent channel flow to test the predictions made in our previous (Lagrangian) studies. In other work, this group has developed a particle dispersion methodology based on autoregressive processes, and used turbulent statistics models to parameterize it. They have also investigated the super-particle problem, and found a way to minimize the effects of particle under-representation by an optimal choice of super-particle packet size.

In the near future we intend to test our expanded treatment of the Fast Eulerian method in the channel code. In particular we will demonstrate the importance of preferential particle concentration on the fluid motion. The code will also be used to test our non-linear diffusion model. We will use the idea of the “particle equilibrium velocity” (on which the Fast Eulerian method is based) to investigate turbulence attenuation by particles.

Particle-laden Fluid Flow Modeling (Balachandar, Vanka, and Rani)

The presence of heavy particles in a turbulent flow has a back effect on the flow that must be captured. Rani and Vanka have investigated this by using two-way coupled direct numerical simulations in the somewhat simpler 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. Results indicate that variation of either the volume fraction or the response time in the absence of gravity has negligible effects on the fluid streamwise mean velocities. 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. Increase in particle settling velocity leads to a marginal increase in the streamwise mean velocities and a drastic increase in the streamwise RMS velocities.

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).

Particle Coagulation (Aref, Balachandar, and Pushkin)

Several processes of particle coagulation and fragmentation occur during the process of rocket fuel combustion, e.g., a complicated process of melting and coalescence of Al particles embedded in the rocket fuel 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 important to the overall fidelity of the simulation. Pushkin and Aref have been studying the main coagulation model, due originally to Smoluchowski. Every instance of particle coagulation, from fuels sprays to planet formation in galaxies, is addressed using a form of this model. We have established a new result, which shows that the steady-state distribution of particle sizes is rather insensitive to the details of the actual coagulation interaction. In fact, a power-law distribution arises with the exponent of the power-law depending only on the degree of homogeneity of the coagulation kernel. This result suggests various modeling possibilities for the simulation of particle-laden flows with coagulation.

We are exploring extensions of the result in which the role of a background flow is included. Preliminary suggestions from numerical simulations are that the background flow will produce a steady-state distribution with a “knee,” with different exponents above and below a critical size. We are exploring how to derive such distributions theoretically. At the same time we are working with the code development group to see how the results obtained thus far can be incorporated into the particle-flow modeling. Pushkin is being co-advised by Aref and Balachandar to assure good integration of the theoretical work with the numerical simulation efforts.

Multi-physics Code Development (Haselbacher, Najjar, Blazek, Wasistho, Ferry, Jiao)

Haselbacher and Najjar have developed the Multi-Physics (MP) framework for the Rocflo fluids code used for core and nozzle flow computation. This framework allows simple integration of physical modules into Rocflo (Figure 3.3.5). Using this framework, we have successfully integrated particle module (Rocpart), turbulence module (Rocturb), and oxide smoke module (Rocsmoke) into Rocflo-MP during the last six months. Haselbacher’s involvement with the GEN1 effort concentrated on helping to support Rocflo and contributing to the further development of GEN1 in general. Furthermore, together with X. Jiao, he developed a new framework for the communication of interface data between the application codes for GEN2. The main advantages of the new framework are increased modularity, flexibility, and simplicity.
Haselbacher is also involved with the development of an unstructured flow solver, *Rocflu*, which will work in conjunction with the *Rocflo*. The idea being that while the core flow in general can be addressed with the block structured formalism of *Rocflo*, in order to treat more complex processes such as combustion and flow within propagating cracks within the propellant an unstructured flow solver, such as *Rocflu*, will be required and will need to perform along with *Rocflo*. The current status is that first-order accurate serial version of *Rocflu* is running and has been tested under both steady and unsteady inviscid flows. We have also developed a new filtering method for unstructured grids, which might be used in *Rocflu* for Large-Eddy Simulations. The most important tasks for the future are to extend *Rocflu* to second-order spatial accuracy, to parallelize it using MPI, to incorporate a grid-motion capability, to couple it to *Rocflo*, and to integrate it into GEN2. Accompanying research will investigate methods of obtaining higher-order accuracy on unstructured grids.

Wasistho has developed the code module *Rocturb*, which implements the different kinds of LES models addressed above within the framework of *Rocflo*. Najjar has developed the code module *Rocpart*, which handles the motion and burning of all Al droplets within the core flow and in the nozzle. A Lagrangian framework has been adopted to follow the time evolution of these droplets. An Eulerian framework has been adopted for the evolution of the much smaller smoke particles. Ferry has developed the module *Rocsmoke*, which handles the aluminum oxide evolution in the core and nozzle flow. It has been correctly coupled to the boundary conditions of *Rocflo*, to the source and sink terms in *Rocpart*, as well as to (in a rudimentary way) *Rocturb*. Ferry has also developed a version of *Rocspecies*, which handles the chemical composition of the gas. In the future it will be integrated into the framework of *Rocflo-MP*.

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**Fig. 3.3.5:** CSAR fluid dynamics framework provides structured and unstructured mesh environments driven by multiphysics subsimulations. New research results are routinely incorporated.