N91-13313

High Speed Turbulent Reacting Flows: DNS and LES

Peyman Givi
Department of Mechanical and Aerospace Engineering
State University of New York
Buffalo, NY 14260

Abstract

The objective of the research pursued during this summer was to continue our work on understanding the mechanisms of mixing and reaction in high speed turbulent reacting flows. Our efforts, in particular, were concentrated on taking advantage of modern computational methods to simulate high speed turbulent reacting flows. In doing so, we made use of two methodologies: (1) Large Eddy Simulations and (LES) and (2) Direct Numerical Simulations (DNS).

In the work related with LES our objective is to study the behavior of the probability density functions (pdf's) of scalar properties within the subgrid in reacting turbulent flows. The use of pdf methods in a stochastic description of reacting flows has proven valuable in Reynolds averaging turbulence modeling,[1] and it is expected that their implementation for subgrid closures in LES of reacting flows would also be beneficial. In our work, we used the the data base obtained by DNS for a detailed study of the pdf characteristics within the subgrid. This data base is generated by direct simulation of an initially unpremixed homogeneous turbulent flow under the influence of a chemical reaction of the type $A + B \rightarrow Products$. Simulations are performed for flows under various initializations to include the effects of compressibility on mixing and chemical reaction. As an initial effort, it is assumed that the chemistry is infinitely fast (i.e. Damkohler Number $\rightarrow \infty$); therefore a flame sheet approximation is employed. With this approximation, the transport of an inert scalar quantity is sufficient to portray the statistical behavior of the species field. Simulations are performed for both two- and three-dimensional homogeneous flows for several values of the turbulent Mach number. A spectral-collocation algorithm based on a Fourier expansion function[2] is employed in the numerical simulations.

After the generation of the data base on the fine grid, the results are statistically analyzed within an ensemble of these grids to describe the large scale conduct on the coarse grid[3,4]. The ratio of the mesh spacings (resolution) provided by the coarse and the fine grids is a measure of the size of the filter which would be used in LES. This analysis is done at intermediate computational times, at which the influence of the initial conditions (of the chemical field) is not substantial. The results indicate that the pdf of the inert scalar within the subgrid (of various filter widths) resembles that of a Gaussian distribution. This had been already surmised in incompressible flow simulations, as previous DNS results[5,6] had suggested. However, in present simulations this behavior is observed both in incompressible flows and in compressible flows dominated with shocklets. This observation is somewhat useful since it suggests that in subgrid modeling of an inert scalar property, the information on the first two moments of the variable is sufficient to parametrize the pdf within the subgrid. With the knowledge gained to date, it is anticipated that the approach based on pdf parametrization based on its first two moments may prove serviceable for turbulent combustion simulations. The approach based on the

solution of a transport equation for pdf, however, may not be practical at this stage. An estimate of computational requirements indicates that the cost associated with LES (a semi-deterministic solution of large scale with a probabilistic description of small scale by solving a pdf transport equation) is of the same order as that of DNS on the fine grids, unless the ratio of the fine to coarse grid is large. Our ongoing investigation is concerned with investigating the effects of finite Damkohler number, which is most appropriate for pdf modeling, and also on including the influence of the heat release. The statistical analyses are also being done for different flow types and for various filter widths.

In the work related with DNS, we considered a two-dimensional temporally developing high speed mixing layer under the influence of a second-order non-equilibrium chemical reaction of the type $A + B \rightarrow Products + Heat$. Simulations were performed with different magnitudes of the convective Mach numbers and with different chemical kinetic parameters for the purpose of examining the isolated effects of the compressibility and the heat released by the chemical reactions on the structure of the layer. A full compressible code is developed and utilized, so that the coupling between mixing and chemical reactions is captured in a realistic manner[7]. A computer code developed at NASA-Langley[8,9] was employed in the simulations. The results of numerical experiments indicate that at the initial stages of the layer's growth, the heat release results in an enhanced mixing, whereas at the intermediate and the final stages, it has a reverse influence. The effect of compressibility is the same in all stages of the development; increased compressibility results in a suppressed mixing and, thus, in a reduced reaction conversion rate. Mixing augmentation by heat release is due to expansion of the layer caused by the exothermicity, and mixing abation is caused by suppression of the growth of the instability modes due to increased heat release and/or compressibility.

Calculations are performed with a constant rate kinetics model and an Arrhenius prototype, and the results are shown to be sensitive to the choice of the chemistry model. In the Arrhenius kinetics calculations, the increase of the temperature due to chemical reaction is substantially higher than that of the constant rate kinetics simulation. This results in a more pronounced response of the layer in all stages of the growth, i.e., an increased mixing at the initial phase of growth, followed by subdued mixing at intermediate and final stages. Our ongoing work in this part of our research activity includes a study of the effects of harmonic forcing in mixing promotion in the case with Arrhenius kinetics and with moderate values of the heat release.

References:

[1] O'Brien, E. E., in *Turbulent Reacting Flows*, edited by P. A. Libby and F. A. Williams, Springer-Verlag (1980).

[2] Erlebacher, G. *et al.*, ICASE Report 87-20, NASA Langley (1987).

[3] Ebert, E. *et al.*, *J. Atmos. Sci.*, 46, 2178 (1989).

[4] Schumann, U. *et al.*, *Beitr Phys. Atmos.*, 60, 413 (1987).

[5] Givi, P. and McMurtry, P. A. *AIChE J.*, 34, 1039 (1988).

[6] Eswaran, V. and Pope, S. B. *Phys. Fluids*, 31, 506 (1988).

[7] Chu, B. T. and Kovasznay, L. S. G. *J. Fluid Mech.*, 3, 494, (1958).

[8] Carpenter, M. H. " *NASA TR*, in press (1990).

[9] Drummond, J. P., *NASA TM 4055*, Langley Research Center, Hampton, VA (1988).