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LES, DNS and RANS for the Analysis of High-Speed Turbulent Reacting Flows

by

Peyman Givi

Department of Mechanical and Aerospace Engineering
State University of New York at Buffalo
Buffalo, New York 14260-4400

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Peyman Givi

Department of Mechanical and Aerospace Engineering

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Abstract

The objective of this research is to continue our efforts in advancing the state of knowledge in *Large Eddy Simulation* (LES), *Direct Numerical Simulation* (DNS) and *Reynolds Averaged Navier Stokes* (RANS) methods for the analysis of high-speed reacting turbulent flows. In the first phase of this research, conducted within the past six months, we have focused our efforts in three directions: (1) RANS of turbulent reacting flows by Probability Density Function (PDF) methods, (2) RANS of non-reacting turbulent flows by advanced turbulence closures, and (3) LES of mixing dominated reacting flows by a dynamics subgrid closure. A summary of our efforts within the past six months of this research is provided in this semi-annual progress report report.

Summary of Accomplishments

In the past six months, we have conducted research in three areas: (1) the use of assumed PDF methods for RANS of turbulent reacting flows, (2) development of advanced turbulent models for RANS of non-reacting flows, and (3) development of a dynamics subgrid closure for LES of reacting turbulent flows.

In efforts related to (1), the recent experimental data in Ref.[1] pertaining to compositional structure of a turbulent reactive scalar mixing layer are reproduced by a mathematical-computational procedure utilizing the *Pearson* family (PF) of univariate and multivariate probability density functions (PDFs). By detailed comparisons against these data and some additional data generated by direct numerical simulation (DNS) of a spatially developing reacting mixing layer, an appraisal is made of the applicability and the extent of validity of PF for statistical description of reactant fluctuations. In accord with the experiment, a chemical reaction of the type $A + B \rightarrow Products$ is simulated in isothermal, incompressible flows. A wide range of the Damköhler number is considered including both frozen and equilibrium chemistry flows. The comparison of the results with laboratory data indicates that PF generated PDFs are very convenient, in the absence of better alternatives, for modeling the influence of turbulence on the reactant conversion rate. In particular, the *Dirichlet* frequency provides the most reasonable means of portraying the multivariate scalar PDF. The extent of agreement improves as the magnitude of the Damköhler number is increased. A more detailed comparative assessment of the model predictions against DNS data confirms the relative superiority of the Dirichlet PDF even though it is mathematically shown that this frequency is invalid in equilibrium flows. With the use of the PF generated PDF, the autospectral density function and the cross-spectra density function (including both the coherence and the phase) of the reacting scalars under equilibrium chemistry are related to frequency spectra of a conserved mixture fraction. This relation is very convenient and is favored over previous models for predicting the spectral characteristics of reacting scalars in the central region of the laboratory mixing layer and in any other homogeneous flow configurations.

Our efforts in (2) are devoted towards developing closures which can be used for modeling of the "second order moments" in the contexts of both RANS and LES. In particular, models are developed for predicting "velocity-scalar" and "scalar-scalar" fluctuations.

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Based on our earlier work, we feel that in the new era of LES a significant effort should be devoted to moment methods in addition to PDF closures. The importance of the these models have become very clear as the results of our most recent work on LES of turbulent reacting flows[2] indicate. It is demonstrated that many of the conventional closures which work reasonably well in RANS[3] fail in LES. Thus, it is very clear that the first step to be taken in any meaningful LES of reacting flows is to make sure that the moments up to the second order level are modeled accurately. It must be noted that in none of the previous contributions in LES, was this the subject of study. In fact, in almost all previous and current contributions, only the first subgrid scale moment of the transport variables have been the subject of modeling. Unfortunately the application of current closures of RANS for LES works only for the closure at the first moment. In its application for reacting flow simulations, the current RANS methodologies should be modified to be applicable for this purpose. In our efforts within the past six months, we have made use of the recent work of one of the Co-PI's of this proposal[4] in developing improved algebraic models. In his previous work, Taulbee[4] shows that with the modeled dynamics equations for the Reynolds stresses, it is possible to develop an improved explicit algebraic Reynolds stress model that can predict many of the flow features more accurately than the conventional models. This improvement is due to the fundamentals of the approach in that the model is based on the transport equations for the higher-order moments. Therefore, more physics is embedded in the equations. Furthermore, the extra degree of freedom provided by the closure allows more adaptability in its optimization for predictive analysis. In fact, some sample results in Refs.[2,5] do show that these new models are superior to previous closures in LES, even though the difference is not significant in RANS (also see Ref.[3]). Most of the work in the literature to date has been focused on the development of improved models for the Reynolds stress terms in LES. In our first step in implementing these models for our work we have made appropriate modifications to develop analogous closures

for velocity-scalar and scalar-scalar fluctuations. The results generated to date are very encouraging in that they compare better with experimental data than those obtained by standard closures.

Finally due to our recent progress in the area of diffusion flamelet modeling (DFM)[6-8] of nonpremixed reacting flows, we decided to devote a small portion of our time toward exploring the possibility of developing subgrid scale closures by means of DFM. Based on our findings reported in Ref.,[9] we expected that the model should work reasonably well in the flamelet region; that is when the chemistry is fast and the thickness of the flame is very small. In such cases, the LES methodology based on DFM is expected to be satisfactory. For this purpose we have initiated a task in which typical mixing controlled chemistry models such as those developed in Ref.[10] are used in a "dynamic" subgrid model for LES of homogeneous reacting flows. We have completed the "lengthy" mathematical formulation to accomplish this task; but we do not have any numerical data to report at the present time.

The results of our work in (1) are almost complete and a manuscript is being written. Our results in (2) will be reported in a full paper before the end of the first year of this research. Our results in (3) are preliminary and we do not currently know when a manuscript will be provided.

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