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# Time Accurate Simulations of Compressible Shear Flows

by

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# Contents

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**Abstract**

The objective of this research is to employ direct numerical simulation (DNS) to study the phenomenon of mixing (or lack thereof) in compressible free shear flows, and to suggest new means of enhancing mixing in such flows. The shear flow configurations under investigation are those of parallel mixing layers and planar jets under both non-reacting and reacting nonpremixed conditions. In the three-year duration of this research program, several important issues regarding mixing and chemical reactions in compressible shear flows are investigated. This Final Report provides a summary of our accomplishments under this research program.

This research has been supported by NASA Lewis Research Center under Grant NAG-3-1011. In the first year of this research, Mr. Russell W. Claus was the Technical Monitor of the Grant. In the second- and the third-year of this research, Dr. James D. Holdeman was the Technical Monitor.

# 1 Introduction

Traditionally, designers of internal mixers and nozzles [1, 2] have relied heavily on the use of turbulence models to predict the behavior of the flow in such devices [3, 4, 5, 6]. Despite their success, it is now widely understood that most of the turbulence models currently in use are not general and, in some cases, their application can lead to erroneous results [7]. An improvement of predictive capability of these models, together with a better understanding of the mixing mechanism are required before these models can be used for the design and manufacturing of the mixing device. In such analysis, the exact mechanism of micro and marco mixing, the coupling between large and small scale turbulent structures, and the influences of various mechanisms by which mixing is enhanced are a few examples of unsteady turbulence phenomena requiring further basis research.

In the past, the design and development of mixers has relied heavily on conventional laboratory experiments (*e.g.* [8]) and, to some extent, on flow visualization procedures. Recently, experimental efforts have been complemented by some computational analysis (*e.g.* [9, 10, 11, 12]) in order to gain a better feeling for the types of quantities that need to be measured; and to define, and perhaps to reduce, the number of parameters that characterize the flow behavior. Despite the success of the currently-used analytical tools in reducing the burden of experimental tasks, a major deficiency in these tools is due to their dependence on turbulence models. In these analysis, since most of the influences of turbulence are modeled *a priori*, the exact role of its transport cannot always be captured directly form the simulated results.

With the development of high speed, large memory computers it is now possible to examine to effect of turbulence and the evolution of the turbulence transport without resorting to turbulence closures. A recent computational methodology which has proven particularly useful in the investigations of turbulent flows is Direct Numerical Simulation (DNS) [13, 14, 15, 16, 7, 17]. This methodology involves the numerical solution of the appropriate transport equations of turbulent flow by means of very accurate and efficient numerical schemes. No turbulence modeling is used so that no restrictive assumptions regarding the structure of the turbulence transport are made. DNS has proven quite useful in the study and understanding of many important fundamental aspects of turbulence. Of primary significance is the ability of DNS to accurately describe the evolution of the large scale structure in flows of research interest, such as the shear layers [18]. The development of the large scale structures in the layer has been studied extensively through DNS, as has the development and influence of three dimensional small scale turbulence structures in such flows (see Refs. [7, 19] for reviews). Although only low to moderate Reynolds number flows have been considered in these simulations, the largest eddies are relatively independent of viscosity and, therefore, can be studied by DNS. The information gained by these simulations has been very useful in providing a better insight regarding some of the fundamental aspects of turbulent flows. Favorable comparisons between simulated flow fields and laboratory experiments has further justified the use of DNS for studying the physics of turbulence.

In the majority of previous applications, the implementations of DNS have been restricted to the analysis of idealized flows with very simplified boundary conditions. This has been primarily due to the limitations of the DNS methodology for the treatment of flows with complex boundary conditions. A major factor in imposing such restrictions is due to the fact that in most applications of *DNS* in turbulence simulations, a class of numerical methodology based on spectral methods [20] have been employed. Despite the attractiveness of spectral discretization in allowing a very fast convergence rate, such methods are not currently capable of dealing with flows of practical interest.[1]

[1]A recent technique which can overcome some of this difficulty is the spectral-element method [21, 22]. However, the implementation of this procedure is presently in formative stages, and they cannot be yet used for actual simulations.

The results of some recent efforts based on the more conventional finite-difference schemes have been very useful in providing algorithms with spectral-like accuracy, but without restrictive assumptions regarding the nature of the boundary conditions of the problems. For instance, the family of compact difference schemes based on the Pade approximations and the classes of high-order schemes are few examples of finite difference methodology which can be considered as viable tools for the simulations of high speed turbulent flows [23].

In the work supported under this grant, our objective has been to take advantage of available supercomputer capabilities to investigate the phenomena of turbulent mixing in compressible flows directly, without resorting to turbulence closures. Our particular objective has been to investigate various means of improving the mixing procedures in flows of interest in internal mixers. The effects of chemical reactions in such flows pertaining to the influence of chemistry on mixing enhancement and/or suppression have also been the objective of this investigation.

# 2 Summary of Accomplishments

During the course of this research, several aspects of mixing and chemical reactions in parallel shear flows have been investigated in detail. For a complete description of our findings, we refer the reader to our publications as listed in Section 4. Here, we provide a summary of our important findings:

## 2.1 DNS of Compressible Temporally Developing Mixing Layers

In the first year of this research, we initiated an investigation of the effects of mixing and chemical reactions in compressible mixing layers. The objective of this work was first to examine the role of compressibility in high speed flow in the most simplified configuration. For this purpose, we considered a temporally developing mixing layer. A write-up of the results obtained is provided in Ref. [24]. Below, the summary of our results is furnished.

A high order finite difference algorithm was employed for DNS of this flow. Within the framework of temporal approximation, periodic boundary conditions were employed in the streamwise direction eliminating the need for providing boundary condition in this direction of the flow. With such an approximation, the effects of large scale structures and the subsequent coupling between mixing and reaction in the unsteady compressible flow were simulated without addressing the asymmetric mixing phenomena which are observed in typical laboratory shear layers. With the accuracy of the numerical algorithm (second order in time, and fourth order in space), together with fine resolutions (both temporally and spatially), it was possible to perform accurate simulations of the reacting field with moderate values of the Reynolds, Peclet, Damköhler, Zeldovich, heat of reaction, and the convective Mach number. A full compressible code was implemented in order to allow for a reasonable and accurate simulation of the high speed reacting field. The main objective of the simulations was to examine the isolated effects of compressibility and the heat generated by the chemical reactions. A simplified reaction mechanism with idealized kinetics schemes was employed. Namely a finite-rate reaction of the type $A + B \rightarrow Products + Heat$ was the main subject under investigation. Two types of kinetics mechanisms were employed, one with constant rate kinetics, and another with an Arrhenius model. In both cases, the magnitudes of the Reynolds, Prandtl, Schmidt and Damköhler numbers were kept fixed, but the values of the convective Mach number and the heat release parameter were varied. In the constant rate reaction case, the Damköhler number is the only parameter which describes the chemistry, whereas in the Arrhenius model the Zeldovich number also is an important non-dimensional quantity to be considered.

The results of numerical experiments allowed a reasonable assessments of the roles played by the compressibility and the heat release. It was shown that both these factors have significant influences on the outcome of mixing, and modify the procedures by which the reacting species mix and convert to product species. This, in turn, was shown to influence the hydrodynamic transport within the flow and to modify the process by which the unsteady large scale vortical structures develop. These influences were captured in the numerical simulations by a careful examination of the global structures, as well as various integral and statistical properties.

In the range of parameters considered, it was concluded that heat release and compressibility generally result in decreased mixing with the exception of slight increase in mixing caused by volumetric expansion at high heat release rates. This was noted by the response of the layer to increased heat release and compressibility. As the magnitudes of the heat release parameter and the convective Mach numbers are increased, the layer becomes less responsive to background perturbations and it takes longer for the instability perturbations to grow. This was evidenced by both flow visualization, and by examining the statistical characteristics of the flow. The contour plots of various fluid mechanical and chemical quantities indicate that at low convective Mach numbers and low heat release rates, the instability modes grow at a faster rate, and the large scale coherent vortical structures are formed quicker. As the magnitude of the convective Mach number is increased, the layer becomes less sensitive to such perturbations. As a result, the layer grows at a slower rate and less mixing occurs. This was quantitatively demonstrated by examining the temporal variation of the vorticity thickness at different convective numbers which present a reasonable assessment of the effects of compressibility on mixing. Another feature of the increased compressibility was the formation of eddy shocklets as a consequence of increased compression after the formation of large scale structures (even though these structures are not very distinct at high convective Mach numbers). These shocklets were formed for both subsonic and supersonic free stream flows. As the layer is compressed, the flow in the low pressure regions outside of the mixing core was shown to go through a shock in order to adapt to the high pressure regions at saddle points at the braids of the vortical structures. These shocklets rotate in an opposite direction to the motion of large scale structures.

The heat release was shown to influence the formation of large scale structures and the subsequent evolution of the layer in two different ways. At the initial stages of mixing, the effect of heat release is shown to increase the volumetric expansion of the fluid. This results in thickening of the layer and in increasing the amount of products formed. After the initial stage, however, the heat release has a reverse influence. As the magnitude of heat release is increased, the layer becomes less responsive to the growth of perturbation, and it takes longer for the instability modes to grow. This delays the formation of large scale coherent vortices at high heat release and yields a substantial decrease in the magnitude of the total products formed. The contour plots of fluid mechanical/chemical quantities provide a valuable flow visualization tool in displaying the effect of heat release on the formation (or lack of formation) of large scale structures. The cross stream variations of the mean and the rms of the same quantities also show the augmentation or depression of mixing as a function of the heat release.

Another important feature of the results of reacting flow simulations is the effect of kinetics modeling. These results indicate that for the same values of the Damköhler and heat release parameter, the Arrhenius model of the reaction conversion has a more pronounced effect on mixing hinderance. The exponential temperature dependent reaction rate increases the magnitude of the temperature much faster, and therefore enhances the effects of heat liberation. In the case with a Zeldovich number of 10, it is shown that the temperature increase at the initial stages of the growth results in a rapid thickening of the layer. At the subsequent stages, the layer does not allow for the growth of instabilities, and large scale coherent structures are never formed within the time range of the simulations. This results in a substantial decrease in the amount of total product formation, and therefore yields a much smaller combustion efficiency. Future simulations with different magnitudes of the Zeldovich numbers, as well as the Damköhler numbers and the enthalpy of formation are required to examine the effects of these parameters on non-equilibrium behavior of the layer.

## 2.2 DNS of Compressible Spatially Developing Planar Jets

After the completion of the work in the first year, we decided to undertake the task of analyzing mixing characteristics of more practical spatially developing flows. At first, our intention was to simulate spatially developing circular jets equipped with "lobes" and also to assess the role of "swirl" on the jet mixing. However, with the advice of the Technical Monitor, it was decided to shift our attention to some other fundamental issues regarding the mixing phenomena in the absence of lobes and/or swirl. Therefore, we decided to perform DNS of spatially developing jets. The results of our findings are detailed in Ref. [25]. Below, a summary is provided.

In this work, a *Two-Four* compact parameter finite difference scheme was employed for DNS of a two-dimensional, compressible, planar jet flow. This scheme was employed in the context of time-marching differencing procedure with a body fitted griding system for the spatial discretization. The resulting computational tool is very suitable for simulating highly compressible flows with large magnitudes of localized gradients. The results obtained by these simulation were used to investigate the effects of the compressibility, the velocity ratio, and the density ratio between the two streams on the mixing characteristics of the jet. This investigation was conducted by analyzing both the instantaneous results and those obtained by statistical sampling.

It is shown that the convective Mach number, as defined in Refs. [26, 27, 28, 29]; also see Refs. [30, 31] is a key parameter in quantifying the effects of compressibility. These results show that an increase in the magnitude of the convective Mach number results in a decrease in the growth of the jet. This decreased growth is accompanied by a decrease in the amount of mixing. This finding is consistent with those of previous DNS of parallel mixing layers [28, 24, 32, 23] and those of early experimental investigations of compressible jets [33]. Therefore, it was concluded that the convective Mach number defined originally with the configuration of parallel mixing layers, is also a useful parameter in portraying the compressibility effects in planar jet flows.

The results also indicated that as the velocity ratio across the jet is increased, the mixing is enhanced. This mixing promotion is understandably more pronounced at low compressibility levels as compared to that at high compressibility.

Finally, it was illustrated that mixing can be enhanced by employing a non-unity density ratio across the jet. In the range of the parameters considered, this enhancement was achieved by employing density ratios both smaller and greater than unity. This finding is very valuable in devising a mechanism for mixing enhancement in high speed parallel flows. However, no correlations between the momentum ratio and the degree of mixing was established.

## 3 Continuation Efforts

This research identified the paths to be followed in the immediate future efforts. Therefore, after the termination of this grant by NASA LeRC, we continued our work in two directions under the support provided by the National Science Foundation. Since our recent findings are very related to the work sponsored by NASA LeRC, here we provide a summary of our most recent accomplishments:

## 3.1 Linear Stability Analyses of Parallel Shear Flows

Motivated by the results of DNS in Ref. [25], we decided to analyze the response of parallel mixing layers and jets from the point of view of inviscid linear stability analyses. For a detailed description of our results to-date, we refer to Refs. [34, 35]. Here a summary is provided.

In this part of our work, the inertial stability of several density stratified parallel planar mixing layers and jets was studied by means of a linearized analysis of the equations governing the transport of two dimensional inviscid flows. Additional analyses of compressible flows were also performed to assess the effects of non-zero Mach numbers. It is shown that at low Mach numbers, the linear analysis of incompressible flows may be used. DNS of inviscid density stratified shear layers and jets were also performed to verify the results of the analyses.

The results of the linear analysis indicated that density stratification can have a profound effect on the growth rate of the disturbances. For stratified flows where the high and low speed streams have different densities, it was found that the stratification can either have a mild stabilizing or destabilizing effect, depending on the magnitude of the density ratio and disturbance frequency (or wavenumber). Furthermore, the results demonstrated that the density ratio in such stratified flows can strongly influence the speed at which the large coherent structures propagate downstream. In general, it is shown that the convective wave-speed is biased to the velocity of the stream with the higher density. In order to assess the effect of heat release, shear layers and jets with a temperature spike were also analyzed. In all cases, the release of heat was shown to have a stabilizing effect. Much of the behavior of jet stability can be described at least qualitatively by examining asymmetric shear layer profiles. However such profiles are unable to determine the existence of two unstable jet modes. For this reason, several symmetric jet configurations were considered. Additionally, comparison of temporally evolving disturbances were made with spatially-developing disturbances.

In an attempt to assess the validity of the linearized theory, qualitative agreement with the growth rates obtained from DNS was found for both temporally and spatially evolving disturbances, except for spatial simulations at high frequencies. The discrepancy between the linear theory and the DNS at high frequencies was noted to be due to the pronounced non-linear interactions at such frequencies. This demonstrates a weakness of the linear theory. In order to capture such effects, it was necessary to perform a non-linear stability analysis. DNS can be considered as one form of such an analysis, since all of the terms in the equations governing the transport of the fluid are included. The behavior of the most unstable mode appears to be of prime importance. The results of the DNS go hand in hand with the behavior of the most unstable mode. The DNS and most unstable mode from the linear theory indicate that decreasing the density of the low speed stream has a destabilizing effect. This result could be applied to improve combustion efficiency by injecting a lighter fluid into a more dense fluid. For temporal simulations, agreement with the linear theory is found even at high disturbance wavenumbers. Concerning heat release, the simulations verify that high temperatures due to the exothermic reaction act to lower the growth rates.

Immediate future extension of this work is stability analyses of (1) axisymmetric jets and of parallel shear flows with (2) non-equilibrium chemical reactions and (3), externally applied magnetic fields. In all cases it would also be desirable to extend the analysis from two to three dimensions. The resulting eigenvalue problem would then involve partial differential equations. A substantial DNS data base which can be used for validity assessments of the stability analyses pertaining to these flows has already been generated and additional work in this area is in progress.

## 3.2 Modeling of Nonpremixed Reacting Turbulent Jets

Our most recent efforts on DNS of jets are concerned with the analyses of nonpremixed reacting jets. The results of our efforts in this investigation are reported in Ref. [36]; here a summary is provided.

In this work, a two-four compact finite difference algorithm is employed for DNS of a spatially developing planar jet flame under non-equilibrium chemical conditions. With the high numerical accuracy provided by this algorithm, it was possible to perform DNS under physically realistic conditions of variable density and exothermic reaction. The kinetic mechanism was assumed to obey the idealized model of the type $F + O \rightarrow$ Products. The data produced by DNS are statistically sampled to assess the compositional structure of the flame. The results of this analysis were shown to be consistent with those of laboratory measurements, even with the assumption of an idealized chemistry model. It is shown that as the intensity of mixing increases, the magnitudes of the ensemble mean and variance of the product mass fraction decrease whereas those of the reactants increase. This conclusion is only valid if the physical mechanisms by which the growth of instability waves is suppressed are masked. This was implemented by means of imposing a low amplitude random forcing at the entrance of the jet. The marginal and the joint PDF's of the reactants mass fractions, extracted from DNS data, showed features in accord with laboratory data. That is, as the relative intensity of mixing was increased and the value of the Damköhler number was decreased, the PDF's showed a lesser probability of product formation. The scatter plots of the instantaneous product formation indicated that the "laminar diffusion flamelet" model is capable of predicting the compositional structure of the flame when the magnitude of the Damköhler number is sufficiently large. Under this condition, the non-equilibrium effects are parameterized reasonably well by the instantaneous scalar dissipation rate in a simple laminar configuration with the same chemical characteristics. However, the flamelet library constructed in this way did not yield satisfactory results at low Damköhler numbers. The results further indicated that in the setting of a "turbulent" flame, exothermicity results in an enhanced reactant conversion and an increased rate of product formation. This trend is not in accordance with previous DNS and laboratory results. The factors resulting in this discrepancy are: (1) imposition of external forcing, and (2) the implementation of an Arrhenius kinetic model. Both of these factors are very important in diffusion flames in which the flow is fully turbulent and the chemical reaction rate can be assumed to obey the Arrhenius law. Therefore, we propose that in typical hydrocarbon turbulent diffusion flames, the effect of heat release is to increase the rate of product formation even though the rate of mixing may be somewhat reduced.

# 4 Publications

Several publications and M.S. Theses have resulted from our activities under this research program. NASA LeRC sponsorship is acknowledged in all the following papers, reprints, and reports:

## 4.1 Review Papers and Lead Articles

1. P. Givi, "Model-Free Simulations of Turbulent Reactive Flows," *Progress in Energy and Combustion Science*, **15**, 1-107, 1989 (invited).

2. P. Givi and J.J. Riley, "Current Issues in the Analysis of Reacting Shear Layers: Computational Challenges," chapter in *Major Research Topics in Combustion*, pp. 588-650, Editors: M.Y. Hussaini, A. Kumar and R.E. Voigt, Springer-Verlag, New York, NY, 1992 (invited).

3. P.A. McMurtry and P. Givi, "Spectral Simulations of Reacting Turbulent Flows," Chapter 9 in *Numerical Approaches to Combustion Modeling*, Progress in Astronautics and Aeronautics, **135**, pp. 257-303. AIAA Publishing Co., Editors: E.S. Oran and J.P. Boris, 1991

(invited).

4. P.A. McMurtry and P. Givi, "Direct Numerical Simulations of a Reacting Mixing Layer by a Pseudospectral-Spectral Element Method," Chapter 14 in *Finite Elements in Fluids*, **7**, pp. 361-384, Hemisphere Publishing Co., 1992 (invited).

## 4.2 Journal Publications

1. P. Givi, C.K. Madnia, C.J. Steinberger, M.H. Carpenter, and J.P. Drummond, "Effects of Compressibility and Heat Release in a High Speed Reacting Mixing Layer," *Combustion Science and Technology*, **78**(1-3), 33-68, 1991.

## 4.3 Conference Papers

1. C.J. Steinberger, "Model Free Simulations of a High Speed Reacting Mixing Layer," AIAA Paper *92-0257* (1992).

2. C.J. Steinberger and P. Givi, "Compositional Structure of an Unpremixed Reacting Shear Flow," Proceedings of the 25th Fall Technical Meeting of the Combustion Institute, Eastern Section, in *Chemical and Physical Processes in Combustion*, pp. 19.1-19.4, Ithaca, New York, October 14-16, 1991.

3. C.J. Steinberger, C.K. Madnia and P. Givi, "A Computational Study of Compressibility, Heat Release and Extinction in a High Speed Mixing Layer," Proceedings of the 24th Fall Technical Meeting of the Combustion Institute, in *Chemical and Physical Processes in Combustion*, pp. 99.1-99.4, Eastern Section, Orlando, Florida, December 3-5, 1990.

4. P. Givi, C.K. Madnia and C.J. Steinberger, "Heat Release and Compressibility in a High Speed Reacting Mixing Layer," JANNAF Scramjet Combustor Modeling Workshop, 26th AIAA/SAE/ASME/ASEE Joint Propulsion Conference, Orlando, Florida, July 19, 1990 (invited).

5. P. Givi and J.J. Riley, "Current Issues in the Analysis of Reacting Shear Layers: Computational Challenges," invited paper, "Combustion Workshop" organized by ICASE and Fluid Mechanics Division, NASA Langley Research Center, Oct. 2-4, 1990 (invited).

## 4.4 Theses

Two students completed their M.S. degrees under the support provided by this grant:

1. Craig J. Steinberger, "Mixing and Non-Equilibrium Chemical Reaction in a Compressible

Mixing Layer," M.S. Thesis, Department of Mechanical and Aerospace Engineering, SUNY at Buffalo, February 1991. Published as: *NASA Contractor Report 187084* (1991). Mr. Steinberger is currently a Ph.D. Candidate at SUNY-Buffalo.

2. Thomas J. Vidoni, "Mixing characteristics of a Compressible, Two-Dimensional Spatially Developing Planar Jet," M.S. Thesis, Department of Mechanical and Aerospace Engineering, SUNY at Buffalo, September 1992. Mr. Vidoni is currently a Ph.D. Candidate at Vanderbilt University in Nashville, TN.

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