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During the second year of this effort, we focused on introducing the effect of combustion in the computation of the spatially developing shear layer, and continued our analysis of the effect of density variation and upstream forcing on the growth of the mixing zone of the shear layer. We have developed a flame sheet model for the simulation of combustion at high Damkohler numbers where the application of the transport element method proves to be rather expensive. The model uses the instantaneous local strain rate as an input from the flow computations and, by integrating a one dimensional equation, computes the rate of burning within each flamelet within the domain.

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SECOND ANNUAL PROGRESS REPORT
ON

VORTEX SIMULATION OF TURBULENT COMBUSTION

(AFOSR Grant No. 89-0491)

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SUMMARY

During the second year of this effort, we focused on introducing the effect of combustion in the computation of the spatially developing shear layer, and continued our analysis of the effect of density variation and upstream forcing on the growth of the mixing zone of the shear layer. We have developed a flame sheet model for the simulation of combustion at high Damkohler numbers where the application of the transport element method proves to be rather expensive. The model uses the instantaneous local strain rate as an input from the flow computations and, by integrating a one-dimensional equation, computes the rate of burning within each flamelet in the domain. The coupling between the flow and combustion is also represented in the boundary conditions in each flamelet calculations. The coupling in the other direction is done as before, i.e. as volumetric expansion and baroclinic vorticity sources along the flame front. We are currently implementing this model in the vortex simulation of the reacting shear layer and comparing its results with those obtained using the transport element method. We have also continued our investigation on the effects of density variation, and its coupling with forcing on the growth of the layer. We find that while the growth of the unforced shear layer is a monotonic function of the density ratio, that of a forced shear layer is determined by the momentum ratio. It reaches a minimum when the two streams have equal momenta and grow substantially under other conditions.

I. OBJECTIVE

The objectives of this research are:

(1) The development and application of accurate and efficient numerical methods for the integration of the time-dependent, three-dimensional Navier-Stokes equations, the energy and species continuity equations at high Reynolds and Peclet numbers, moderate to high Damkohler numbers, and high rates of heat release. Solution methods are constructed for reacting shear flows at moderate to high Mach numbers.

(2) The investigation of mechanisms of flow-combustion interactions on the basis of the results of the numerical simulations, and the study of how these interactions can be exploited to control the combustion processes in turbulent shear flows. Numerical simulation results are also used to construct physical models which can be used in turbulent combustion closure.

Our work focuses on the development of grid free, Lagrangian field methods. In particular, we have extended the application of the vortex element method and formulated the transport element method for the simulation of compressible reacting flow. We have also formulated a compatible flame sheet model for the simulation of high Damkohler number combustion. To validate the numerical schemes and analyze flow-combustion interactions in shear flows, we have focused on simulations of shear layers in 2D and 3D, with particular emphasis on non-premixed, variable density cases. In analyzing flow-combustion interactions, we obtain solutions in which the effects of the velocity gradient, density gradient, heat release rate, pressure gradient and confinement are varied individually.

II. PERSONNEL

During the funding period of 1990-1991, two graduate students and a postdoctor were supported by this program:

(1) Marios Soteriou is expected to finish his Ph.D. thesis by the end of this academic year on the Simulation of Combustion in a Reacting Shear Layer.

(2) Van Luu started his Ph.D. work this summer on the Simulation and Mixing and Combustion in a Reacting Shear Layer with High Rate of Heat Release.

(3) Omar Knio spend a 9-month as postdoctor (50% support from this project) extending his work on the three-dimensional vortex schemes to handle compressible-shear flows.

III. WORK STATUS

III.1. Unsteady Flame Sheet Model for Reacting Flow

The simulation of combustion in the reacting shear layer has so far been accomplished using the transport element method in which the species continuity equations are integrated along with the momentum and energy equations to determine the local rate of reaction at different points in the field. This method provides a direct simulation type approach, i.e., assumptions regarding the structure of the reaction zone and the modes of interaction between the flow and combustion are not made apriori. Instead, the simulations have been used to determine the structure of this zone under conditions of low and moderate Damkohler numbers.

As the Damkohler number increases, it has been found that the thickness of the reaction zone becomes much smaller than the typical flow scale as determined by, e.g., the local vorticity thickness of the vorticity layer. This substantially increases the number of computational elements required to resolve both the flow and species gradients simultaneously leading to a sharp rise in computational cost. In the application of a direct method such as the transport element method one needs to transport all the species. This increase in cost is compounded by the need to extend the models to accommodate multi-step chemical kinetics. If a flame sheet model is sufficient, then only the local concentrations of the minor species are needed.

The unsteady flame sheet model we have developed will be described in detail in an upcoming publication (which will be submitted to the 24th Symposium). It is based on assuming a one-dimensional flame structure in the direction normal to the local flame front. The formulation is developed as an extension of the Carrier, Fendell and Marble original formulation of a strained flame with infinite rate chemistry. In our model we allow for finite diffusion and finite kinetic rates. We have used the model to study the effect of unsteady, primarily periodic strain on the flame development and to prove, or otherwise, some of the basic assumptions in the flame sheet closure models of turbulent combustion. The results are summarized next.

In the flame sheet closure model, one assumes that the total burning rate is the local burning rate corresponding to the mean strain rate multiplied by the average area of the flame. Using the mean strain to compute the burning rate assumes that the flame does not respond to the unsteady component of the strain. We find that to be incorrect in cases when the local strain exceeds the quenching strain and when the frequency of the oscillating flame is comparable with the flow time scale. A strain generated by a turbulent flow can be decomposed into two components: a mean value, ε_m, and a root-mean-square, ε'. When the flame is strained such that the maximum strain, $\varepsilon_m+\varepsilon' < \varepsilon_q$, where ε_q is the mean strain which quenches a flame, we find that applying the results of steady calculations leads to a reasonable approximation of the burning rate. However, when $\varepsilon_m+\varepsilon' > \varepsilon_q$, substantial reduction of the burning rate below the value computed using the mean strain and the possibility of complete extinction are encountered. The reduction depends on the frequency of the oscillations. Moreover, when $\varepsilon_m-\varepsilon' < 0$, the reaction zone may experience extinction due to the rapid depletion of one of the reactants. These results are very important in reaction closure models.

We are currently implementing this unsteady flame sheet model into the vortex computations and comparing its results with those obtained using the transport element method. Results are being documented in a paper which will be presented at the Aerospace Sciences Meeting in January, 1992.

III.2. Baroclinic Effects in a Variable-density, Spatially Developing Layer

We continued our investigation on the effects of variable density across the shear layer on its growth rate, entrainment ratio and motion of individual eddies within the mixing zone. During this period, we focused the effect of upstream forcing, in the form of harmonic modulation of the flow rates, on these parameters by comparing results of an unforced layer with those of a forced layer. There are some striking qualitative and quantitative differences between the two cases. The preliminary results have been included in recent AIAA paper, with is attached to this report. The main conclusions are listed below.

In the unforced layer, there is a monotonic dependence of the growth rate on the density ratio between the two streams. As the density of the slow stream increases beyond that of the high speed stream, the growth rate of the layer increases, the volumetric entrainment ratio favors the high speed fluid and individual eddies move, with respect to the mean flow speed,.in the direction of the slow stream. These results are in agreement with the experimental measurements and agree also with the conclusions of the linear stability theory of variable-density-shear layers. Models based on the redistribution of the vorticity within the large structures by the action of the baroclinic torque were constructed to physically explain the observed trends, which as mentioned before are well correlated by the density ratio (at a constant velocity ratio).

In the forced layer, there is an interesting and unexpected non-monotonic dependence of the growth rate on the velocity ratio, although the other two characteristic parameters, the entrainment ratio and eddy motion, behave in the same way as in the unforced case. The best parameter space which we found for characterizing the behavior of the layer in this case is the momentum ratio. We found that the smallest growth rate (at all velocity and density ratios investigated) occurs at momentum ratio of unity. The growth rate increases for momentum ratios smaller and larger than unity. This behavior has been observed before in the case on a jet issuing into an atmosphere with a different density. The mechanism leading to this critical dependence on the momentum ratio was found to be the pairing of the eddies which can no longer be described as vortex monopole but as vortex dipoles.

Future work.on this subject will consider the effect of different forms of forcing using different combinations of the fundamental and subharmonic frequencies organized at different phasing relationships. Extention to 3D spatially developing layer will follow.

III.3. Mixing and Combustion between two Concentric Jets

With partial support from the Gas Research Institute, we have applied the methodologies developed during the course of this research project to investigate the mechanism of mixing between two concentric jets and the formation of large unsteady structures which appear to govern the burning process. This problem has been the subject of several experimental investigations in the Air Force Laboratories and Sandia Laboratories since it represents a generic configuration of combustors in propulsion and industry. It also lends itself well to the analysis techniques which we have developed.

The results of this project have appeared in several recent publications. One of these papers is attached in the back of this report. We find that as the velocity of the inner jet increases, it penetrates the recirculation zone of the outer flow and causes its shear layer to become unstable. This instability is manifested in the shedding of large-scale structures form the shear layer between the outer recirculation zone and the free stream. As the jet velocity increases further, the inner stream breaks through the recirculation zone and large eddies are shed from both the inner and the outer shear layers. The eddies are subsequently paired, forming mixed structures downstream. These structures, which form at a finite regular frequency that depends on the velocity ratio of the two streams, resemble the flame turbules which have been observed in the reacting flow experiments. We plan to extend these computations by adding a combustion model to understand how heat release affects this mixing mechanism.

IV. PUBLICATIONS DURING 1990-1991

1. Ghoniem, A.F. and Krishnan, A. "Vorticity-combustion interactions in a turbulent reacting jet," *Dynamics of Deflagration and Reactive Systems: Flames*, Progress in Astronautics and Aeronautics, **131**, ed. by Kuhl, Leyer, Borisov and Sirignano, 1991, pp. 237-256.

2. Ghoniem, A.F., Knio, O.M., and Heidarinejad, G., "The structure of the reaction zone in a reacting shear layer;" *Dynamics of Deflagartion and Reactive Systems: Flames*, Progress in Astronautics and Aeronautics, **131**, ed. by Kuhl, Leyer, Borisov and Sirignano, 1991, pp.220-236.

3. Knio, O.M., and Ghoniem, A.F., "Three-dimensional vortex simulation of roll-up and entrainment in a shear layer," *J. Comput. Phys.*, 1991, in press.

4. Ghoniem, A.F., and Heidarinejad, G., "Effect of Damkohler number on the reaction zone in a reacting shear layer," *Combust. Flame*, **83**, pp. 1-17, 1991. (*)[1]

5. Ghoniem, A.F., "Vortex Simulation of Reacting Shear Flow," Chapter 10 in *Numerical Approaches to Combustion Modelling*, ed by E. Oran and J. Boris, Progress in Aeronautics and Astronautics, Vol. 135, 1991, pp. 305-348. (*)

6. Ghoniem, A.F., "Numerical Simulation of Turbulent Combustion using Vortex Methods," *Fluid Mechanics of Combustion*, Springer-Verlag, 1990, in print.

7. Knio, O.M. and Ghoniem, A.F. "Three-dimensional vortex simulation of the reacting shear layer," *AIAA Journal*, in press 1991.

8. Ghoniem, A.F., Knio, O.M., and Krishnan, A., "Lagrangian simulation of the initial stages in a reacting jet," *The 23rd Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, pp. 699-705, 1990. (*)

9. Martins, L.-F., and Ghoniem, A.F., "Numerical simulation of the nonreacting flow in a bluff-body burner; effect of the diameter ratio," Heat and Mass Transfer in Fires and Combustion Systems, ed by W.L. Grosshandler and H.G. Semerjian, HDT-Vol. 148, ASME Publications.

10. Ghoniem, A.F., Knio, O.M. and Soteriou, M., "Effect of variable density on Mixing and Combustion in turbulent shear flow," presented at *the 29th AIAA Aerospace Sciences Meeting*, Reno, Nv, January 1991. **AIAA-91-0081**. (*)

11. Ghoniem, A.F. and Martins, L.-F., "Effect of the velocity ratio on the wake flow behind an axisymmetric bluff-body," *the 29th AIAA Aerospace Sciences Meeting*, Reno, Nv, January 1991. **AIAA-91-0580**. To appear in AIAA Journal. (*)

12. Ghoniem, A.F., Martins, L.-F., Rotman, D.A. and Kelly, J., "The dispersion of the jet fluid due to the large-scale motion in bluffbody flows," AIAA/SAE/ASME 27th Joint Propulsion Conference, June 24-26, 1991/Sacramento, CA, **AIAA-91-1861**.

References marked with (*) are appended to this report.

13. Najm, H., and Ghoniem, A.F., "Modeling pulsating combustion due to the flow-flame interactions in vortex stabilized pre-mixed flames," the International Symposium on Pulsating Combustion, August 5-8, 1991, Monterey, CA. (*)

V. SEMINARS AND LECTURES DELIVERED DURING 1990-1991

1. Gas Research Institute, Chicago, IL, 1991.
2. National Center for Supercomputer Applications, Champain, IL. 1991.
3. AMSE Local Chapter, Boston, MA, 1991.
4. Northeastern University, Boston, MA, 1991.
5. Ch. Michelson Institute, Bergen, Norway, 1991.

VI. INTERACTIONS WITH INDUCTRAIL AND GOVERNMENT LABORATORIES DURING 1990-1991

1. General Electric Corporate Research and Development Center, with Dr. Sanjay Correa.
2. Altex Technologies (small R&D Business), with Drs. M. Namazian and J. Kelly.
3. Ford Motor Company, with Dr. Chris Kent.
4. General Motors Co., Allison Gas Turbine Division, with Dr. N. Rizk and H. Mongia.
6. Army Atmospheric Research Laboratory, with Mr. R. Meyers.