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A study of fuel disintegration and mixing in a supercritical environment was undertaken. The approach was based on a model describing a supercritical, temporal mixing layer and on the utilization of Direct Numerical Simulations (DNS). The database from a DNS of a temporal, binary species, initially density stratified, excited mixing layer that did not reach transition was enlarged and scrutinized. The scrutiny was based on the development of the entropy equation for a supercritical fluid and on the examination of contributions to the irreversible entropy production (the dissipation). The lack of transition was due to the formation of regions of large density gradients that damped the emerging turbulent scales. To obtain transition, the Reynolds number, as well as the amplitude of the initial excitation, were increased. Two new databases were created for initial Reynolds numbers of 500 and 600. The two new databases were examined to determine the phenomena responsible for vorticity production. Most of the spanwise vorticity production was due to stretching/tilting, and most of the contribution to the vorticity magnitude was due to the viscous terms. The regions of large density gradients created during roll-up and pairing persisted at transition, and the fluid in these regions was non-ideal and consisted primarily of the entrained fluid, with small amounts of entraining fluid dissolved in it.

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LARGE EDDY SIMULATIONS OF SUPERCRITICAL MULTICOMPONENT MIXING LAYERS

(Contract Number: AFOSR-ISSA-00-0012)

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ABSTRACT

A study of fuel disintegration and mixing in a supercritical environment (relative to the fuel) was undertaken in order to determine parameter regimes advantageous to mixing. The adopted approach was based on the development of a model describing a supercritical, temporal mixing layer and on the utilization of Direct Numerical Simulations (DNS) as an investigation method.

During the current year, the database from a DNS of a temporal, binary species, initially density stratified, excited mixing layer that did not reach transition was enlarged and scrutinized to determine the reasons for the lack of transition. The scrutiny was based on the development of the entropy equation for a supercritical fluid, and on the examination of the various contributions to the irreversible entropy production (the dissipation). The results showed that the lack of transition was due to the formation of regions of large density gradients which damped the emerging turbulent scales. To obtain transition, the Reynolds number, as well as the amplitude of the initial excitation were increased, producing two simulations in which transition was attained; two new databases were thus created, for initial Reynolds numbers of 500 and 600, respectively. Since vorticity is known to play a crucial role in turbulence, the two new databases were examined to determine the phenomena responsible for vorticity production. Examination of the vorticity budget at transition revealed that most of the spanwise vorticity production was due to stretching/tilting, and that most of the contribution to the vorticity magnitude was due to the viscous terms. It was also shown that the regions of large density gradients created during roll-up and pairing persisted at transition, and that the fluid in these regions was non-ideal and consisted primarily of the entrained fluid, with small amounts of entraining fluid dissolved in it.

TECHNICAL DISCUSSION

The first year of this investigation was devoted to developing a database of a three-dimensional, supercritical, transitional temporal mixing layer. The mixing layer was composed of a lower stream containing the fuel (n-heptane) and the upper stream containing nitrogen; supercriticality was initially measured with respect to the pure fuel. The mixing layer was chosen as the simplest configuration from which one may obtain results that will establish, through DNS, a framework for understanding mixing of supercritical fluids at small scales.

Following previous modeling performed at JPL for isolated fluid drops (Harstad and Bellan, 1998, 2000), the model of supercritical behavior was based upon fluctuation-dissipation theory (Keizer, 1987). The advantage of this theory was that it inherently accounted for nonequilibrium processes and naturally led to the most general fluid equations by relating the partial molar fluxes and the heat flux to thermodynamic quantities. Thus, Soret and Dufour effects (potentially important at supercritical conditions) were taken into account from first principles through the transport matrix where they complemented the traditional Fick's mass diffusion and Fourier thermal diffusion terms. Results from the recent supercritical simulations of Harstad and Bellan, 2000, using heptane drops in nitrogen have already been validated with the microgravity data of Nomura, 1996, within an average of 15%, thereby showing that the fluid model was correct. This model was here adapted to the shear layer configuration. However, there were specific issues that were considered in the DNS of a three-dimensional (3D) shear layer and that had not been relevant to the drop model:

(a) In contrast to the drop study, the treatment of the transport coefficients cannot be exact in the context of DNS since the Reynolds number, *Re*, would be far too large to make the computations feasible. Since it was required that the Batchelor scales (the smallest scales associated with scalar mixing, $\eta_B \sim \eta_K / Sc$ where η_K was the Kolmogorov scale and *Sc* was the Schmidt number) be resolved, this dictated the maximum *Sc* which could be used in the particular calculation. For example, for heptane/nitrogen, *Sc* was too large for any domain size since heptane had a liquid-like density. The strategy was then to calculate these numbers based upon the observations that the viscosity was primarily a function of *T*, whereas *Sc* and *Pr* were primarily functions of the mass fractions, and to find approximate fits for these quantities in the range of parametric interest.

(b) It was here unpractical to use the very accurate and computationally efficient non ideal EOS's employed in Harstad and Bellan, 2000, because these could still be too computationally intensive when performing 3D simulations. Instead, the Peng-Robinson EOS was used, based on pure species reference states accurate to better than 1% relative error (on pure reference states) through comparisons with highly accurate EOS's (Harstad et al., 1997) over the range of variables used in this study.

The shear layer equations were coded using a fourth order Runge-Kutta scheme for advancing in time, and an eight-order compact method for spatial discretization. The implemented boundary conditions were those of Poinsot and Lele, 1992, for compressible flows. Since those boundary conditions were developed for perfect rather than real gases, they were adapted for the present real gas computations by calculating an 'equivalent gas constant' from the EOS; the accuracy of this simplistic substitution is discussed in more detail below. Also, the layer was perturbed in the mean velocity using the most unstable wavelength of Moser and Rogers, 1991, found in the context of atmospheric, incompressible gases.

Results from the 3D shear layer (initial conditions: Reynolds number of 400, Mach number of 0.4, 60 atm, lower stream at 600K, and upper stream at 1000K) showed that the density stratification was stabilizing the layer and preventing it from achieving the transitional regime at a nondimensional time at which a transitional state had been reached by a layer whose lower stream was initially laden with drops. One intriguing feature of the layer was the appearance of regions of high density gradient magnitude which were not merely the distortion of the original density interface. The appearance and geometry of these regions of high density gradient magnitude was intriguing because it corresponded to the wispy threads of fluid emanating from a supercritical nitrogen jet in gaseous nitrogen as observed by Chehroudi et al., 1999. These features were absent at subcritical conditions either in the experiment or in atmospheric air DNS simulations, indicating that they may be specific to the supercritical situation. These results were all documented in Miller, Harstad and Bellan, 2000.

Since the layer did not achieve transition in a physical time comparable to that, for example, of a drop laden mixing layer, the calculations were pursued with the goal of achieving transition at a later physical time. However, this did not occur for the chosen initial conditions, and moreover, the layer reached a culminating point in the averaged positive spanwise vorticity. The averaged positive spanwise vorticity was considered to be a good indicator of transition since the initial mean velocity profile was such that the spanwise vorticity was negative everywhere; transition would occur if the positive spanwise vorticity exhibited and continued to display a large increasing rate. The results illustrated in Fig. 1, together with the momentum thickness, the product thickness and the enstrophy (another indicator of transition), indicated the lack of transition.

To investigate the origin of the stability preventing transition in a physical time larger than that, for example, of a drop laden mixing layer, the entropy equation was derived for a supercritical fluid and the irreversible entropy (i.e. the dissipation) production was examined. For supercritical fluids, the dissipation was shown to contain three contributions: viscous, Fourier heat flux and molar flux contribution. The molar flux contribution contained both the effect of the mixture nonideality and that of the Soret term. The database from the long-time run was used to compute the budget of the small scale dissipation by calculating the difference between the DNS (i.e. unfiltered) and that of the filtered flow field. The results from plane averages and RMS of the three terms showed that the dominant contribution to the small scale average dissipation was from the viscous term, but that the major RMS contribution was from the molar flux term at all times except at the culmination of the averaged positive spanwise vorticity. Since the molar flux contribution to the dissipation contained six terms, a budget of the molar flux dissipation was calculated to identify which of the terms was the principal contributor to the molar flux dissipation magnitude. It was found that the non-ideality term was the major contributor in the heptane stream, whereas the nonideality and Soret terms tended to be of same order of magnitude in the nitrogen stream. These calculations as well as contour plots showed that the RMS of the molar flux dissipation correlated with the regions of maximum density gradient magnitude. Moreover, it was also noticed that the DNS dissipation RMS, as well as each of its contributions was larger than the respective average value, indicating that there was considerable backscatter in the flow.

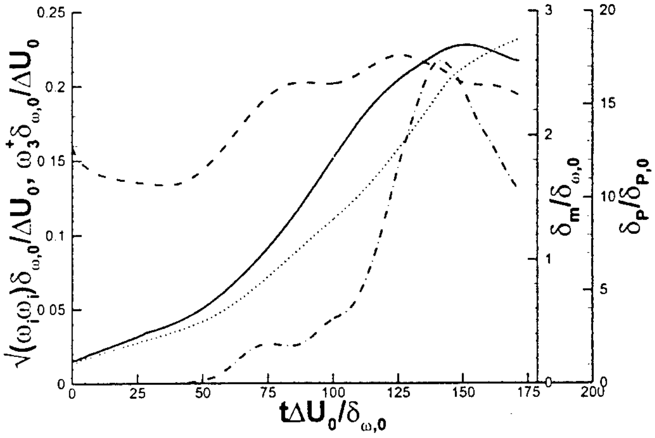

Figure 1. Momentum (——) and product (• • •) thickness, enstrophy (-- -- --) and averaged positive spanwise vorticity (--•--•--) as a function of time.

The results concerning the hindering of transition due to the presence of a large density gradient region were found consistent with the experimental results of Hannoun et al., 1988, who found that large eddies impinging on a density interface 'bounce' back without significant entertainment of unstirred fluid instead of overturning. Since the layer growth is known to depend primarily on entertainment, and since this accelerated growth is known to promote the appearance and evolution of the small turbulent scales, this damping mechanism may be enhancing the effect of density stratification in hindering transition.

The calculation of the dissipation was valuable not only in elucidating the responsible mechanisms impacting the stability characteristics of the flow, but also in pointing out that at large simulation times the mass fractions and temperature displayed large gradients at the upper and lower boundaries of the computational domain; these were the only locations where non-periodic boundary conditions were applied. This provided the motivation to re-examine the implementation of the boundary conditions according to Poinsot and Lele, 1992, and Baum et al., 1994. Thus, the 'characteristic' boundary conditions were derived for a general fluid having a real gas equation of state. This derivation was consistent with the fact that for $Re \rightarrow \infty$ the conservation equations including the Soret and Dufour effects were an incomplete elliptic set. In fact, the elliptic character was determined to be the result of the value of the effective thermal conductivity which was always enhanced, while the effective diffusivity was always reduced (see Harstad and Bellan, 1999) when comparing to atmospheric flows. Simulations of a one-dimensional propagation of acoustic waves in a two-dimensional domain using subsonic non-reflecting boundaries were conducted with the new, fundamental boundary conditions, and compared with the previous simulations based on the 'simplistic' effective gas constant (see above). The results revealed that whereas using the fundamental analysis induced the acoustic waves to properly pass through the boundaries without reflections, the use of the simplistic approach yielded significant reflections at the boundaries. Most discrepancies occurred when a source term was added to the mass fraction equations, where additional to the reflections at the boundaries, the solution within the entire domain was different in the simplistic and fundamental approaches. This work will be enlarged in the near future to consider two-dimensional wave propagation, and the results will be further documented in a manuscript.

The fundamental boundary conditions were implemented in the code, the discretization was changed to a sixth-order compact scheme, and two simulations were performed for initial Reynolds numbers of 500 and 600, respectively. Given the large initial density stratification (12.88 for the initial conditions of the calculation: 60 atm, lower stream at 600K, upper stream at 1000K, and Mach number of 0.4), it was deemed important to increase the amplitude of the layer excitation, so as to increase the entertainment of the heavier, lower stream n-heptane. With these new initial and boundary conditions, transition was achieved in both simulations. Portrayed in Fig. 2 are the global characteristics of these two layers.

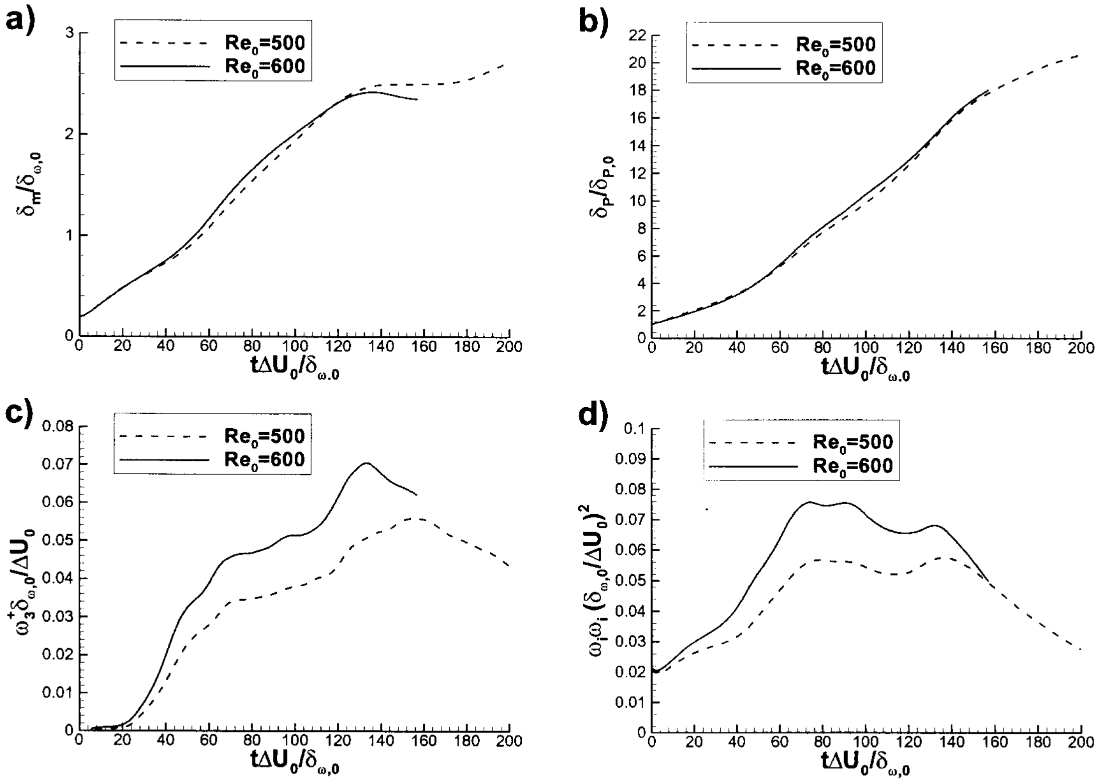

Figure 2 Time Evolution of Global Quantities for Re_0=500 and Re_0=600 a) Momentum Thickness b) Product Thickness c) Positive Spanwise Vorticity d) Enstrophy

The momentum thickness based Reynolds numbers were 1250 and 1452, respectively, at transition. These values are smaller than the traditional magnitudes of measured transitional Reynolds numbers due to the reference viscosity being here four orders of magnitude larger than the species viscosity; this is an artifact of DNS designed to allow the attainment of large Reynolds numbers in domains of physical interest.

Since vorticity is known to play a major role in turbulent flows, the phenomena predominantly responsible for vorticity production were identified by analyzing the budget of the vorticity equation at the transitional state. It was found that, on average, the stretching/tilting term dominated all other effects in the production of spanwise vorticity, but that the viscous term dominated the vorticity magnitude production. In this respect, the major difference identified between the layer that did not reach transition and the present case was the dominance of the stretching/tilting term in the former resulting in the production of turbulent scales, and the dominance of turbulence destruction through the action of viscosity in the latter. This conceptual picture was supported by the dominance of the viscous terms in the irreversible entropy production.

Visualization of the layer at the transitional state (braid and between braid planes) revealed the existence of convoluted regions of large density gradient magnitude; no such convolutions had been observed in the layer that did not reach transition. Moreover, it was also observed that parcels of heptane seemed to have 'broken off' from the lower stream and entered the upper stream. The striking visual correlation between the regions of large density gradient magnitude, the desintegrated heptane and the regions of minimal mass diffusion factor (which measures the departure from mixture ideality; it is unity for ideal mixtures), provided the motivation to examine the composition and thermodynamic characteristics of the fluid in the region of large density gradient. Conditional averages revealed that the fluid in these regions was mostly heptane, but with a small amount of nitrogen dissolved into it. Mixing of this fluid was observed to be inhibited, as evidenced by the smaller that unity mass diffusion factor. With increased cutoff for the proportion of the value of the maximum density gradient magnitude on which the heptane mass fraction and mass diffusion factor averages were conditioned, the fluid composition became closer to heptane and the molecular mixing became increasingly hindered.

Departures from the perfect gas behavior were also identified in contour plots of the compression factor (which is unity for a perfect gas). Whereas both pure streams were close to perfect gases, the mixed fluid showed strong departures from perfect gas behavior. These departures were further quantified through plots of the local difference between the fluid temperature and the local critical temperature, and the fluid pressure and local critical pressure of the mixture. The temperature was found to be supercritical everywhere; therefore the entire field is at supercritical conditions (identified as the absence of a two-phase region). However, the pressure was found to be supercritcal in the pure species regions, and subcritical in the fluid mixture region; this subcritical pressure was attributed to the change in composition of the fluid (the critical point being mixture dependent).

Further studies will elucidate some aspects of the assumed PDF representation of a supercritical mixing layer, before addressing the issue of SGS modeling.

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