Modeling of Three-Dimensional Mixing and Reacting Ducted Flows

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Theme

A NUMBER of reactive flow systems, e.g., chemical lasers and scramjet combustors, are characterized by flow processes that are predominantly three-dimensional in nature. In a chemical laser device, lasing typically occurs in a direction normal to the mixing plane, whereas, the predominant flow direction is in the third direction. In many scramjet designs, hydrogen injection is made typically from rows of orifices mounted flush and normal to the combustor wall or in fins spanning the combustor inlet. The objective of this study[1] was to: a) develop an analysis capability that considers in detail the three-dimensional mixing and reacting flow processes occurring in confined environments, e.g., scramjet combustors or laser optical cavities and b) base line the analysis by comparing theoretical predictions with existing three-dimensional flow measurements.[2-4] Also, the analysis was used to examine the three-dimensional density distribution in a continuous wave DF laser optical cavity.[1]

Contents

The system of partial differential equations governing three-dimensional, confined unidirectional flows of a compressible, reacting fluid is obtained as an approximation to the full three-dimensional Navier-Stokes equations. This approximation, referred to as the "parabolic Navier-Stokes equations," describes steady, confined three-dimensional flows wherein a) a predominant flow direction is uniformly discernible; b) diffusion processes in the predominant flow direction are negligible compared with convection; and c) no disturbances are propagated upstream, e.g., recirculation is not considered.

The resulting equation system consists of three momentum equations, a total enthalpy equation, N species equations, plus the following relations.

1) A turbulence model is used to close the governing equations. Three different approaches are used. The first uses simple mixing length theory (MLT) to compute the turbulent eddy viscosity (ϵ). The second also uses MLT to compute ϵ, but assumes that the diffusion coefficient in the (x_1x_2) plane is ϵ, and that in the (x_1x_3) plane it is $C\epsilon$, where C is a constant. See Fig. 1 for the definition of the (x_1x_2) and (x_1x_3) planes. The third approach is the two-equation model $(k+d)$ for computing the turbulent kinetic energy (k) and the turbulent dissipation rate (d). For this model, the turbulent eddy viscosity is given by $\epsilon = C_\tau K^2/d$, where C_τ is a constant equal to 0.09.

2) Pressure variations in ducted flows are computed using a quasi-one-dimensional integral[5] equation treatment for computing the mean-pressure gradient in the axial direction. If the pressure distribution is known a priori, i.e., for boundary-layer flows, then this computation is not required. For cases where the pressure field is computed, the analysis is limited to regions outside of the transonic flow regime.

3) A simplified reaction model was used to obtain an upper limit on the effects of heat release on the flowfield development. By neglecting the mole fractions of the dissociated species, it is assumed that the complete reaction, e.g., $2H_2 + O_2 = 2H_2O$, characterizes the heat release.

4)The turbulent Lewis number for all cases considered in this report was assumed to be unity. This assumption requires the turbulent Prandtl number be equal to the turbulent Schmidt number. The turbulent Prandtl number may be expressed as a constant or given by an empirical relationship (e.g., see Ref. 6).

5) An equation of state, using perfect-gas behavior for each species and applying Dalton's law was also used.

The sensitivity of the predicted flowfield solution to a number of key parameters was studied. Specifically, those parameters examined were discretization, eddy viscosity model, tensorial character of eddy viscositiy, turbulent Prandtl number, and transverse velocity. The detailed experimental results of Rogers[2,3] for a single- (Fig. 1) and mulitiple-orifice injection of hydrogen into a supersonic air boundary layer provide the necessary data base for comparison of predictions. Initial conditions for the predictions were established from these data, and the downstream station at $x_1/d = 30$ was selected as the initialization station.

The two-equation turbulence model $(k+d)$ has enjoyed considerable success in modeling two-dimensional turbulent flows. In this study, initial values for k and d were obtained by computing an eddy viscosity ϵ and a length scale ℓ from MLT, and using the relationship, between k, d, ℓ, and ϵ. As shown in Fig. 2, a modest improvement in the correlation between theory and experiment was obtained using the $k+d$ model to predict the H_2 concentrations. To be noted, however, is that the introduction of two additional equations increased computer run time by approximately 30% and leads us to conclude that use of higher order turbulence models for the problem of interest herein are somewhat premature at this time.

In general, the level of agreement between predictions and experiment for seven additional cases considered were similar to those obtained in Fig. 2. Specifically, the predicted H_2 mass fractions were greater than the experimental values in five of the seven cases. A means for accounting for this effect through the mixing model would be to employ the $k+d$ tur-

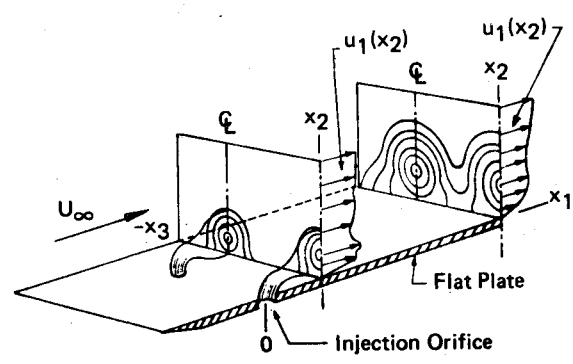

Fig. 1 Three-Dimensional flowfield downstream of transverse injection from discrete orifices.

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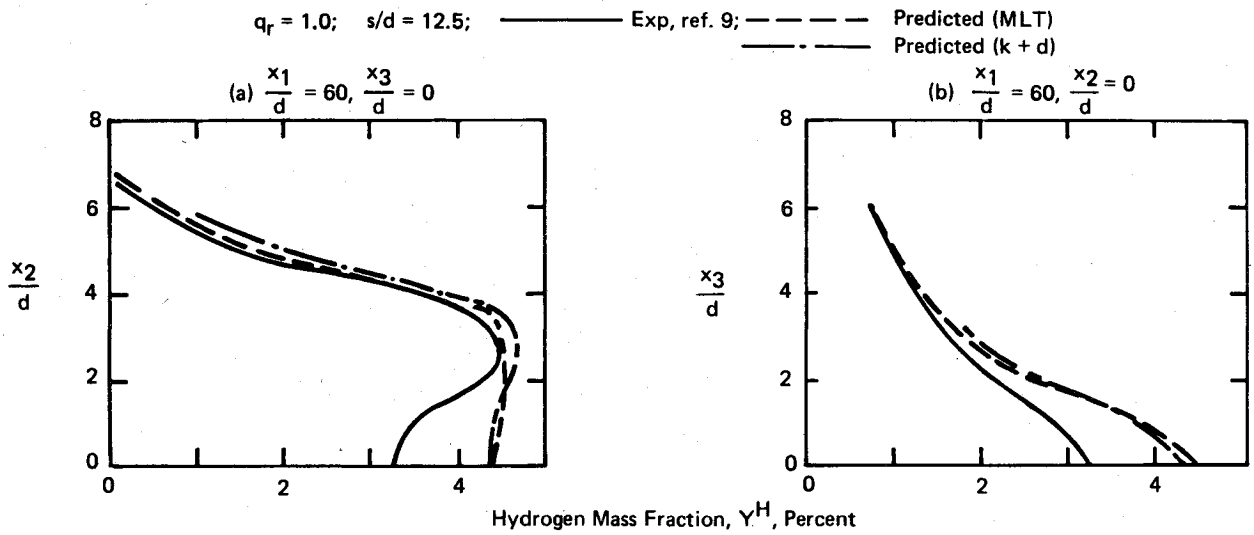

Fig. 2 Comparison between experimental and predicted H_2 mass fraction profiles along center plane ($x_3/d=0$) and wall ($x_2/d=0$), using two equation turbulence model, case 1-6.

bulence equations and relate the initial turbulence kinetic energy to the H_2 injection parameter, q_r i.e., as q_r increases the turbulence level in the boundary layer increases. The computer code was not exercised to further explore this concept, since the results would represent only a data fit and not provide any new information. Detailed turbulence data would be required to test the ability of the $k+d$ model to characterize the dominant turbulent mixing processes. However, from the comparisons between data and theory, it is concluded that the COMOC code, even with the simplest turbulence model considered, gives correlation with experimental data with sufficient accuracy to provide useful engineering design guidance.

A task in the early phases of the study was to evaluate the concept of a numercial "virtual source" as a means of eliminating the requirement for detailed initial conditions. The validation of this concept was accomplished using the detailed cold-flow experimental data. After marching 30 diam downstream from the point of injection, good agreement was obtained between the predictions and the data location and magnitude of peak H_2 concentration predicted to within 10% of data. At the final station $x_1/d=120$, agreement between the virtual-source simulation and the data is excellent, being essentially identical with the results starting with data at $x_1/d=30$.

Computations of reacting flow environments are reported in Ref. 1 to demonstrate the ability of analysis to provide insight into the details of laser cavity and scramjet combustor flowfield structure. Efforts are in process to tie or baseline these analytical results to experimental data to provide a basis from which to interpret the theoretical predictions for reacting flows.

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