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Combustion Research for Gas Turbine Engines

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Abstract

Research on combustion is being conducted at Lewis Research Center to provide improved analytical models of the complex flow and chemical reaction processes which occur in the combustor of gas turbine engines and other aeropropulsion systems. The objective of the research is to obtain a better understanding of the various physical processes that occur in the gas turbine combustor in order to develop models and numerical codes which can accurately describe these processes. Activities include in-house research projects, university grants, and industry contracts and are classified under the subject areas of advanced numerics, fuel sprays, fluid mixing, and radiation-chemistry. Results are highlighted from several projects.

Introduction

As we enter into the age of the computer and the laser, new opportunities are emerging to make significant advances in the understanding of the physics of combustion. These advances are needed in the gas turbine engine industry. Development costs and maintenance costs are prevalent factors when considering the next generation of gas turbine engines. The costs associated with the design and development of engine components, including the combustor, are alarmingly high using today's design methodology.[1] Also, the ever-increasing operating pressures and temperatures of new engines for increased performance and better fuel economy are having adverse effects on durability of hot section components. This results in high maintenance costs. Clearly what is needed is an improved design methodology which can allow the design engineer to converge to the optimum design in a much shorter development cycle.

At NASA Lewis Research Center, combustion research is integrated into activity in internal fluid mechanics. The objectives of the research are to advance the understanding of flow physics, heat transfer and combustion processes which are fundamental to aeropropulsion, and to translate this knowledge into models and numerical codes of aerothermodynamic phenomena. The overall goal is to bring internal computational fluid mechanics to a state of practical application to propulsion systems. These models and numerical codes would then be available to the industry to incorporate into their own engine/component design systems.

The approach at Lewis is to establish an integrated computational-experimental research program. The activity consists of research on numerical methods, well-defined experiments for code and model verification, and the demonstration of computational codes for propulsion system components. In the area of combustion, research has been underway for some time in these three areas.[2,3] With a recent reorganization in the Aeronautics Program at Lewis, this research activity has been consolidated with similar research in other components such as compressors, turbines, and transition ducts and is continuing in the internal fluid mechanics research program. Although the amount of work currently being supported in combustion has been decreased in the new organization, the prime research needs in combustion are recognized and the program is focusing on them.

Figure 1 is a cut-away view of a ficticious combustor which illustrates the complex fluid mechanics and combustion features. The flows are highly three-dimensional with turbulence levels in many cases comparable in magnitude to the bulk velocity. Liquid fuels are injected as a spray which then undergoes vaporization and mixing. Chemical reaction occurs which causes changes in density and fluid mechanics properties and can cause the formation of a solid phase (soot) with its attendant high radiation heat transfer. The understanding of these physical processes is needed before accurate numerical codes can be built and used as a predictive tool in the design process. In addition the numerical methods for three-dimensional flows need improvements in accuracy and efficiency in order to properly simulate the features of these flows. This then is the framework of the current combustion research program. As shown in Fig. 2, the activities are focused in four areas: advanced numerics, fuel sprays, fluid mixing, and radiation-chemistry. Both experiments and computational research are being conducted, with the long range objective of providing the numerical codes that can be used with confidence as a predictive tool in the industry's design system. In this report a research project from each of these areas will now be highlighted as examples of the kinds of work currently being supported at Lewis.

Advanced Numerics: Error Reduction Program

A major restriction to the development of a computer based design methodology is the accuracy of the numerical methods used in combustor flow codes. The upwind differencing currently used in these flow codes,[4] introduces an appreciable error in the calculated result. This error (or numerical diffusion) is frequently of such a large magnitude that it obscures the turbulence model used in the calculation.

To alleviate this problem, NASA has conducted a program to identify and incorporate an improved accuracy differencing scheme into a combustor flow code. Under a portion of this program a variety of differencing schemes were examined in several test calculations. The schemes examined included QUICK (Quadratic Upstream Interpolation) and SUD (Skewed Upwind Differencing). QUICK differencing was developed by Leonard.[5] This scheme improves the accuracy of convective differencing by performing an upwind biased quadratic interpolation. This scheme is second order accurate and can produce nonphysical oscillations in the solution. SUD, developed by Raithby,[6] attains high accuracy by differencing in an upwind manner along the flow streamlines. While maintaining the same formal accuracy as upwind differencing the truncation error in SUD is smaller in magnitude. As with QUICK, SUD can produce nonphysical oscillations in the solution, therefore, a scheme to "bound" SUD was also examined. This scheme employs the concept of flux-blending,[7] wherein a bounded flux determined from upwind differencing is blended with the unbounded - but more accurate - SUD flux. The main factor is to blend as little of the lesser accurate scheme while still maintaining a properly "bounded" solution. This procedure called BSUDS, starts from an initial, totally skew differenced estimate and blends an upwind flux if the solution is out of the range of neighboring values. If the solution is in range, i.e., bounded, then no blending is performed.

An illustration of the accuracy of the upwind, QUICK, and SUD schemes is seen in Fig. 3. The figure displays the results of a single point scalar transport calculation made for various flow angles. All schemes agree with an exact solution (no error) at a flow angle of zero, but departing from this each scheme displays some degree of error relating to numerical diffusion. The error displayed by upwind differencing increases with flow angle up to a maximum at 45°. QUICK displays a similar behavior but the overall level of error is much less. SUD displays an error maximum around 15° but tends to zero at angles approaching 45°. Both QUICK and SUD display a much higher level of accuracy than upwind.

A scalar transport calculation is useful for generally examining some aspects of differencing scheme performance, but a more complete test is a laminar flow calculation. The results of a series of laminar flow calculations from Ref. 8 are displayed in Fig. 4. In this figure axial velocity profiles at a distance of one-half a duct height from the inlet are shown for two different computational meshes. In these calculations an indicator of accuracy is the steepness of the velocity profile. Steep velocity profiles are exhibited by QUICK and BSUDS with the upwind profiles exhibiting a high degree of numerical diffusion. On the coarse mesh, BSUDS appears to be more accurate than QUICK, while on a fine mesh there is not much of a distinction between the two schemes.

An important aspect of improved accuracy is the effect that the differencing scheme has on the rate of convergence. The computational times to converge the system of governing equations in the previous laminar calculations is shown in Table 1. The convergence times are ratioed to the upwind convergence times to clearly illustrate the computational penalty paid to attain improved accuracy. Generally, the improved accuracy schemes required from 3 to 15 times longer to reach a converged solution. To a degree one can hope that this computational penalty can be offset with the use of coarse meshes to achieve the same overall level of accuracy. In reality it appears that a relatively fine mesh is needed even with the high accuracy schemes. In any case the need for improved solution algorithms with these more accurate differencing schemes is strongly demonstrated.

Fuel Sprays: Study of Dilute Turbulent Particle-Laden Jets

A research topic of current interest in computational fluid mechanics is spray processes in combustion chambers. However, due to the complications involved in the spray processes, e.g., hydrodynamics of spray atomization, polydisperse drop diameter distributions, drop shattering and coalescence, and evaporation and combustion of drops, spray processes in combustion chambers are excessively complex for systematic model development and evaluation. In contrast, injection and mixing of monodisperse solid particles is a much simpler process, and facilitates the modeling of the underlining physics involved in practical multiphase flows.

The objective of this work was to evaluate models of dilute turbulent particle-laden jets. Dilute solid-particle-laden jets in a still environment were considered. These flows are relatively simple and only involve interphase momentum exchange. Modeling efforts concentrated on effects of turbulent fluctuations on momentum transfer between the phases, as well as the dispersion of the particles by turbulent fluctuations. Three typical models of the flow processes were considered: (1) a locally homogeneous flow (LHF) model, where slip between the phases was neglected; (2) a deterministic separated flow (DSF) model, where slip was considered but effects of turbulence on particle motion were ignored; and (3) a stochastic separated flow (SSF) model where effects of both interphase slip and turbulence on particle motion were considered using random-sampling techniques.

The LHF model represents the simplest treatment of a multiphase flow. In this model, the particles and the continuous phase are assumed to have equal rates of turbulent diffusion. This implies that interphase transport rates are infinitely fast, so that both phases have the same velocity at each point in the flow. The LHF approximation is valid only for flows containing small particles, where characteristic response times of particles are small in comparison to characteristic times of turbulent fluctuations. Faeth[9] has indicated that LHF models only yield accurate predictions for particle sizes smaller than most practical applications. Despite the limitations, LHF models have some important advantages. They require minimal information concerning initial conditions of particle properties, which are often difficult to obtain for practical flows. The theoretical model of the flow is equivalent to that of a single-phase flow and effects of multiple phases only appear in the representation of state relationships, bypassing the difficulties involved with modeling interactions between the phases.

The DSF model considers slip between the phases but neglects turbulent particle dispersion. In this model particles follow deterministic trajectories and only interact with mean properties of the continuous phase. The computation involves dividing the particulate phase into representative samples whose motion and transport are tracked through the flow field using a Lagrangian formulation. An Eulerian formulation is employed to solve the governing equations for the continuous phase. The effect of interphase transport is considered by inserting appropriate source terms in the governing equations for the continuous phase. The source terms are determined using the "Particle Source in Cell" technique. Neglecting turbulent dispersion is appropriate for flows containing large particles, where particle response times are large in comparison to characteristic turbulent fluctuation times.

Most practical particle-laden flows and sprays, however, exhibit properties between the two limits represented by LHF and DSF models and therefore require consideration of turbulent particle dispersion. The stochastic separated-flow (SSF) approach, first proposed by Gosman and Ioannides[10] and subsequently developed by Faeth and coworkers,[9,11,12] was adopted to study the effects of turbulence on particle dispersion. The SSF model involves finding trajectories of statistically significant samples of individual particles as they move away from the injector and encounter a random distribution of turbulent eddies. Particle trajectory computations are similar to the DSF model, except that instantaneous eddy properties replace mean-gas properties. Eddy properties are obtained by constructing the probability density function (PDF) of velocity, assuming isotropic turbulence, and random sampling to find each velocity component.

The three models of particle-laden jets have been systematically evaluated and some typical results are shown here. Comparisons of model predictions with experimental data are shown in Figs. 5 and 6, taken from Ref. 13. Figure 5 presents radial profiles of mean and fluctuating properties for the gas phase, and Fig. 6 presents radial profiles for the particle phase. Since this jet has a relatively low particle loading, gas phase properties are relatively independent of model type and both the LHF and SSF models are in good agreement with the measurements. For the particle properties SSF predictions agree reasonably well with the data. Predictions of the LHF model for particle properties are not at all satisfactory, since neglect of slip overestimates particle fluctuations levels and rates of spread. The DSF model also yields poor results because neglecting particle dispersion by turbulence causes the rate of spread of the particles to be substantially underestimated. Similar results were found throughout the data base used in the study.

For the two separated-flow models used in this study (DSF and SSF) the model predictions are relatively insensitive to the specification of gas-phase initial conditions. The specification of initial particle properties, however, exerts much more pronounced effects on predictions. Accurate measurement of particle initial conditions, e.g., particle size, mean and fluctuating velocities and particle mass flux, is essential to obtain meaningful predictions of separated-flow models, especially when particle relaxation time is large compared to particle residence time in the flow field.

Practical particle-laden flows and sprays usually involve regions where the dilute flow approximation is not appropriate, such as near the injector. Phenomena to be considered for future model extension in application involving dense particulate flows include: the finite volume fraction of the dispersed phase, effects of nearby particles on particle transport properties, and effects of particle collision and coalescence. There is also a pressing need to overcome the experimental difficulties encountered in the dense flow region so that further progress can be made toward developing reliable models for this region.

Fluid Mixing: Direct Numerical Simulations of Chemically-Reacting Mixing Layers

The advent of high speed vector processing computers has made possible the study of turbulence and turbulence-chemistry interactions via computational "experiments." One promising approach that has been supported at NASA Lewis[14] is Direct Numerical Simulation (DNS). Direct Numerical Simulations solve the complete time-dependent, Navier-Stokes equations at a range of flow Reynolds number wherein all the scales of turbulence can be fully resolved on a computational mesh. This typically requires the calculation of flows where the Reynolds number based on the Taylor macroscale is of the order of 100. The key assumption involved is that the large scales of turbulence which can be represented on the computational mesh will not significantly vary with Reynolds number. While this may not be true for all the aspects of turbulent flow which one might desire to study, a previous study of incompressible turbulent flows[15] has indicated that a great deal of insight into the structure of turbulent flows can be obtained. One of the main goals is that this information will be effective in developing turbulence-closure models.

Incompressible turbulence models typically require information on fluctuating pressure-velocity correlations that are difficult to measure experimentally. Reacting flows further complicate the problem with the need for an instantaneous measure of density and the number of double and triple correlations rapidly becomes overwhelming. Indeed, even the form of averaging (Fauvre or Reynolds) to be used in constructing the governing equations is not straight-foward.[16] The promise of DNS is that it can provide complete flow field values that can be processed to provide any necessary correlation or test various closure models.

The above states the promise of DNS, but there are a number of "realities" which should also be mentioned. The first has already been noted: simulations must be made at low Reynolds number. This is primarily a numerical resolution limitation. Even employing highly accurate psuedo-spectral methods[17] and large computational meshes (typically 64 by 64 by 64 for the results reported herein) the range of turbulent scales that can be represented is limited. A second limitation is that the numerical methods used restrict the calculation to relatively simple

geometries. The numerical calculations discussed here are of a time-evolving shear layer as opposed to the experimentally measured spacial mixing layer. The time-evolving mixing layer is not a direct analog of the spacial mixing layer, and some physical phenomenon cannot be represented. For example, the flow streamlines in the time-evolving case are not aligned along the flow direction as they are in the spacial case. A final limitation relates to the statistical nature of DNS results. One simulation must typically run for several CPU hours to simulate a small fraction of physical time (on the order of a second). Statistics sensitive to scale variation may not be adequately sampled. It is easily seen that more small scales of turbulence can be represented on a finite computational domain than larger scales and this can bias the statistical results. These factors require care in the sampling of simulation results to obtain statistically stationary information.

Despite the current limitations inherent to DNS a number of turbulent flow phenomenon can be well represented. An example is the experimental versus computational flow visualization results shown in Fig. 7. The experimental flow visualization was provided by Koochesfahani[18] and displays a flow structure resulting from the merging of two discrete vortices. This flow structure is strikingly similiar to the results of a two-dimensional numerical simulation. The experiment was conducted at a Reynolds number and with fluids differing from the computation, yet the comparison is encouraging.

Another favorable aspect of DNS results is displayed in Fig. 8. Similarity theory predicts that the mean velocity half-width of the shear layer should grow linearly. As seen in Fig. 8, the time evolution of the velocity half-width grows linearly with time in the numerical simulations. If a transformation relating space and time is performed[17] the time evolving results are found to be in good agreement with similarity theory. This agreement is favorable for a large range of initial conditions as shown on Fig. 8.

A final comparison between simulated results and experimental data is shown in Fig. 9. The experimental data, Mungal,[19] is of a mildly exothermic chemical reaction. The similarity plot of integrated product level from a numerical simulation agrees fairly well with the shape and peak of the experimental data. The shape of the product profile is somewhat sensitive to the initial conditions used in the simulation and current research is being conducted to assess whether alternate initial conditions might clear up the small discrepancy displayed.

The overall agreement between DNS results and experimental information is strongly encouraging. The highlights of the current research is merely illustrated here and Ref. 14 is recommended for further details.

From this array of favorable initial results it appears that this approach can provide insights into the physics of turbulent chemistry which will one day lead to improved closure models usable by combustor designers.

Radiation, Chemistry: Fast Algorithms for Combustion Kinetics Calculations

The ordinary differential equations (ODE's) describing complex chemical reactions are characterized by widely different time constants. Although the ODE's are stable, standard numerical techniques such as the popular explicit Runge-Kutta and Adams methods are prohibitively expensive to use because of the severe steplength restrictions imposed by the requirements for numerical stability.[20] Such systems of ODE's are commonly referred to as "stiff" systems.[21]

The aim of the present investigation was to examine currently available integration techniques for solving chemical kinetic rate equations. The motivation behind this work is the increasing interest in (1) modeling the reaction mechanisms describing the consumption of fuels and pollutant formation and destruction, and (2) multidimensional modeling of reactive flows, which includes the equations of fluid motion. The former results in the need to integrate large systems of nonlinear ODE's. The latter results in the need to integrate the ODE's at several thousand grid points. To make such calculations practicable, it is necessary to have a very fast homogeneous batch chemistry integrator.

The techniques examined include two general-purpose solvers, EPISODE[22] and LSODE,[23] developed for an arbitrary system of ODE's, and the specialized techniques CHEMEQ,[24] CREK1D,[25] and GCKP84,[26] developed specifically for chemical kinetics applications. Testing of these codes was accomplished by application to two practical combustion kinetics problems. Both problems described adiabatic, homogeneous, gas-phase, transient, batch combustion reactions at constant pressure. Test problem 1 described the ignition and subsequent combustion of a mixture of 33 percent carbon monoxide and 67 percent hydrogen with 100 percent theoretical air. It consisted of 12 reactions among 11 species. Test problem 2, involving 30 reactions among 15 species, described the ignition and subsequent combustion of a stoichiometric hydrogen-air mixture. Both problems were integrated over a time period of 1 msec, which encompassed all three combustion regimes: induction, heat release, and equilibration.

In using LSODE, EPISODE, and CHEMEQ the temperature was calculated by employing two different methods. In method A the temperature was evaluated via an iterative solution of the algebraic enthalpy conservation equation. In method B the temperature was computed by solving its ODE. Both CREK1D and GCKP84 were written explicitly for non-isothermal chemical reactions and therefore include calculation procedures for the temperature.

Figures 10 and 11 present the variation of the local error tolerance with the computer (i.e., CPU) time required to solve test problems 1 and 2, respectively. In these figures CPU is the computer time (in seconds) required on the NASA Lewis Research Center's IBM 370/3033 computer. All results were obtained using single-precision accuracy, except GCKP84 which was in double-precision. The error control performed is different for the different codes. Consequently, the local error tolerance, EPS, does not have the same meaning for all the codes. For LSODE, GCKP84,

CREK1D, and CHEMEQ, EPS is the local relative error tolerance.[20] For EPISODE, however, EPS is a mixed relative and absolute error tolerance - relative for species with initially nonzero mole fractions (i.e., reactants) and for the temperature, and absolute for species with initially zero mole fractions (i.e., intermediate species and products).

Figures 10 and 11 show that LSODE is the fastest code currently available for solving combustion kinetic rate equations. Because GCKP84 has been designed for a variety of chemical kinetics problems it requires more work per step than LSODE and is hence slower. CREK1D and, especially for test problem 2, EPISODE are attractive alternatives to LSODE. However, there are many problems associated with using EPISODE for solving combustion kinetics rate equations - details are given in Ref. 20. Figures 10 and 11 show also that the use of temperature method A does not result in significant inefficiency. On the contrary this method can be significantly faster than evaluating the temperature by integrating its ODE (Fig. 11).

For multidimensional chemically reacting flow calculations computational speed is of primary concern and moderate accuracy is adequate. However, in developing and validating reaction mechanisms, accuracy is of critical importance. An accuracy comparison of the techniques examined in this study was made as follows. For each test problem a mean integrated root mean square error (E_{rms}) was estimated. E_{rms} is approximately the average true error incurred by a technique in solving the complete problem. Figures 12 and 13 present the variation of E_{rms} with the user-supplied value for the local error tolerance, EPS. Note the significant discrepancies between values specified for EPS and the errors actually obtained. For both problems temperature method A is as accurate as temperature method B - in many cases, it is significantly more accurate. LSODE is the most accurate code for solving chemical kinetic rate equations. However, GCKP84, CREK1D, and CHEMEQ-A compare favorably with LSODE for small values of EPS. EPISODE is significantly less accurate than the other codes because the error control used in it is inappropriate for chemical kinetics applications.[20]

The present study has shown that LSODE is the fastest and most accurate code currently available for solving chemical kinetic rate equations. However, it is recognized by combustion device modelers that LSODE is not fast enough for economical calculations of multidimensional reacting flows. Current research efforts at NASA Lewis are aimed at further speeding up codes for solving chemical kinetic rate equations.

Concluding Remarks

The four research activities highlighted above are examples of NASA Lewis sponsored work which are building blocks toward achieving computational codes of combustion and fluid mechanics which can be applied by industry as predictive tools in their design system. Much work remains to be done in this area and NASA Lewis will continue to commit itself to using its resources in working with other segments of the technical community in achieving these research objectives.

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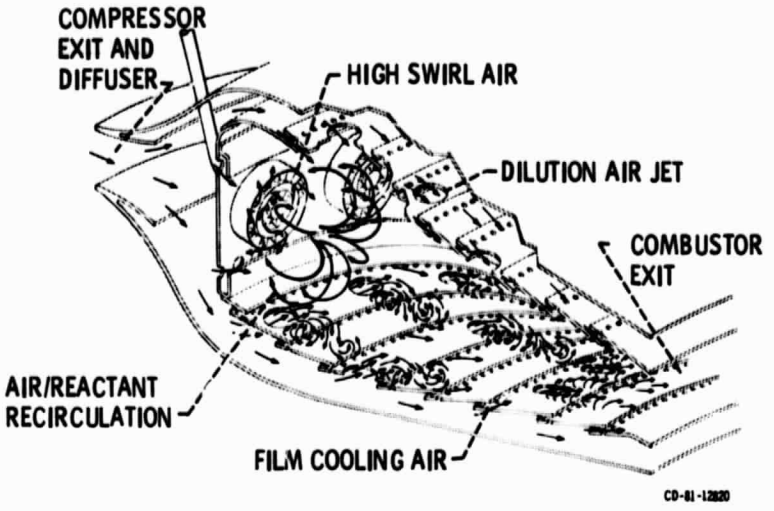
TABLE I. - RATIO OF CONVERGENCE TIMES
FOR VARIOUS DIFFERENCING SCHEMES
WITH UPWIND CONVERGENCE TIMES
USED AS THE STANDARD

Mesh	Upwind	BSUDS	QUICK
Coarse (30 by 22)	1	6.4	3.2
Fine (58 by 38)	1	14.7	15.7



- FULLY 3-DIMENSIONAL FLOW
- CHEMICAL REACTION/HEAT RELEASE
- HIGH TURBULENCE LEVELS
- 2 PHASE WITH VAPORIZATION

Figure 1. - Cutaway illustration of a portion of a full annular combustor system, with major features highlighted.

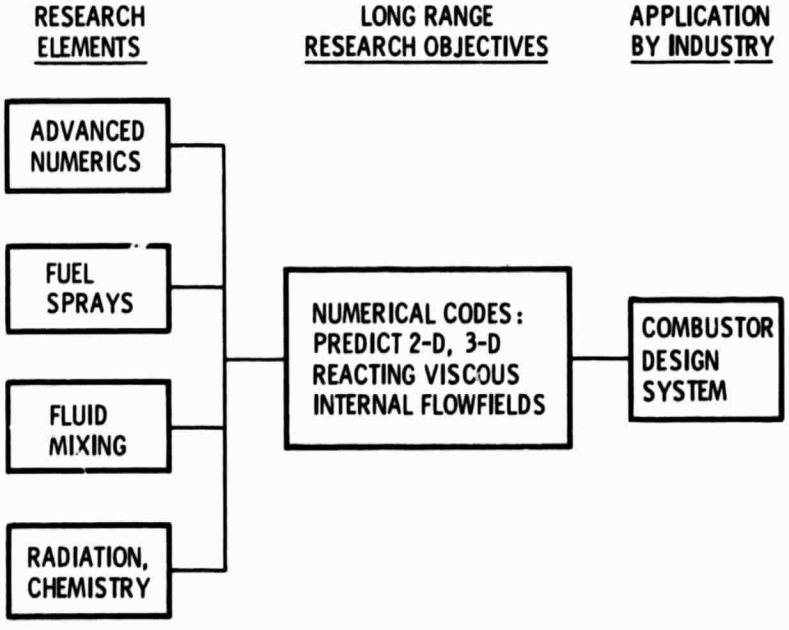


Figure 2. - Combustion research has long range objectives to produce predictive numerical codes that have practical application in engine manufacturer's combustion design system.

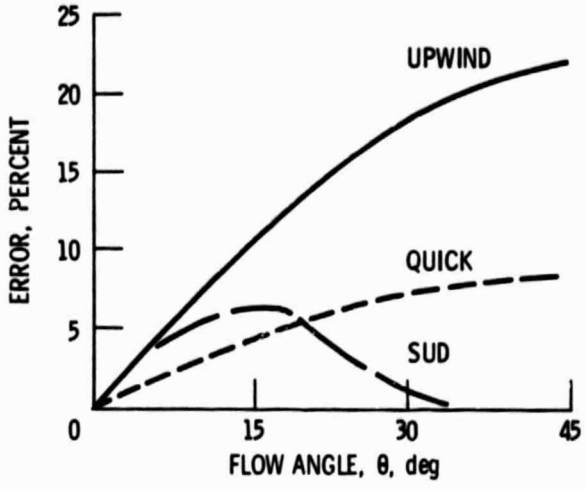
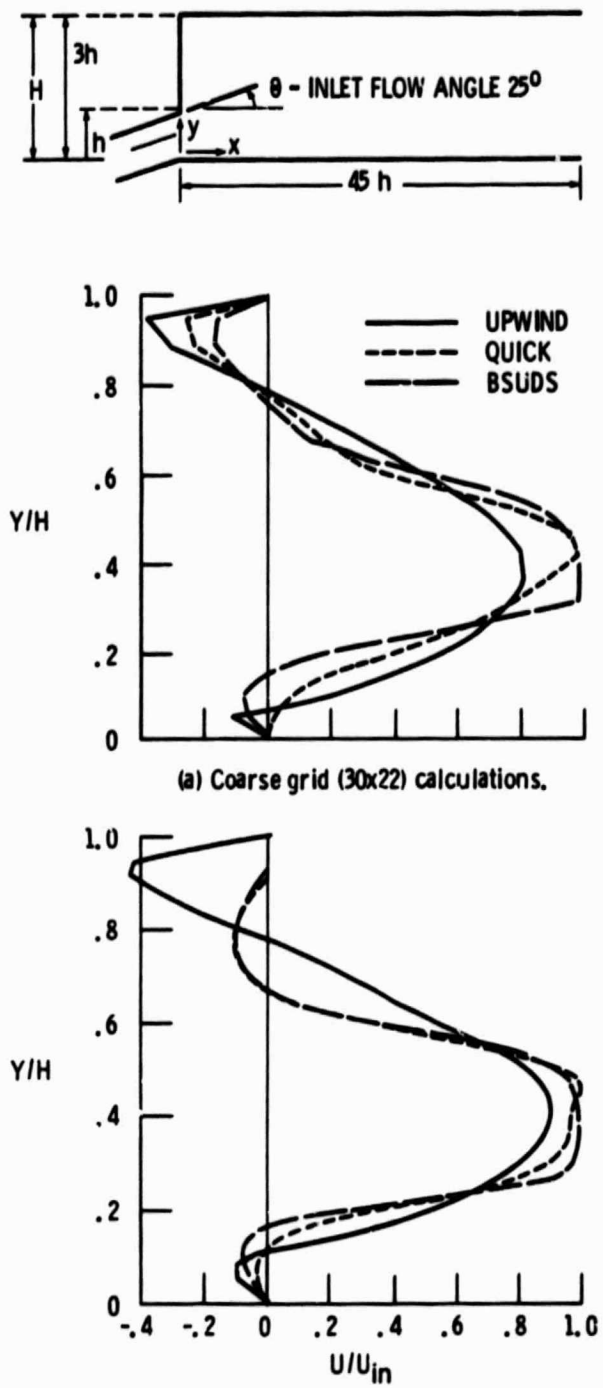


Figure 3. - Results of a scalar transport test calculation for various differencing schemes. Error from an exact solution is displayed versus flow angle.



(a) Coarse grid (30x22) calculations.

(b) Fine grid (58x38) calculations.

Figure 4. - Laminar flow test calculations comparing upwind, QUICK, and BSUDS. Inlet flow angle of 25°.

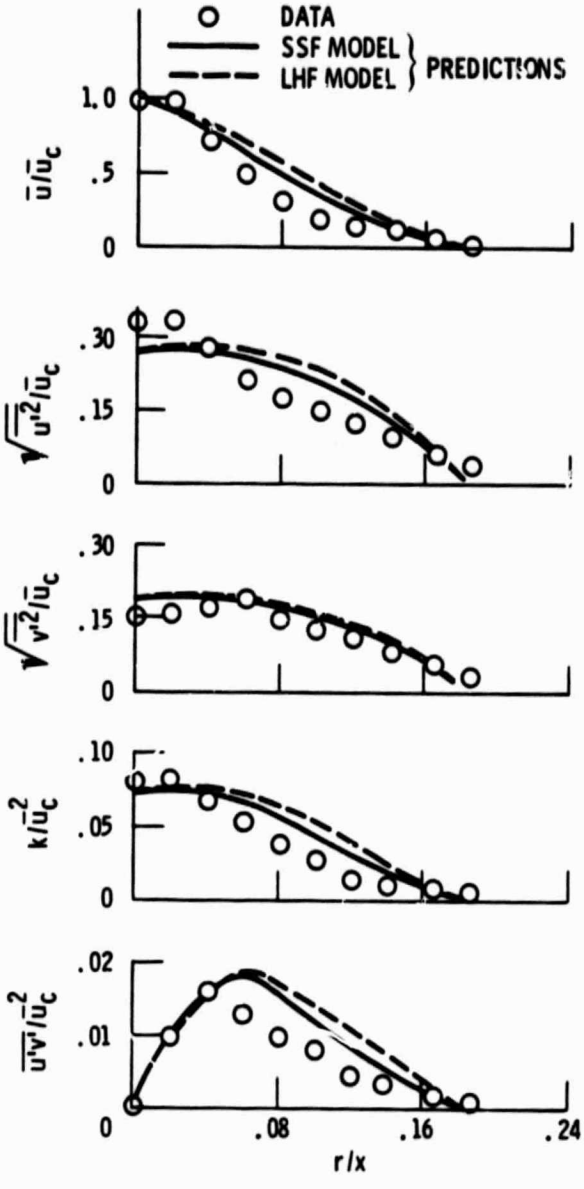


Figure 5. - Radial variation of gas-phase mean and turbulent quantities in case 3 particle-laden jet. x/d = 40, SMD = 119 μm, LR = 0.66.

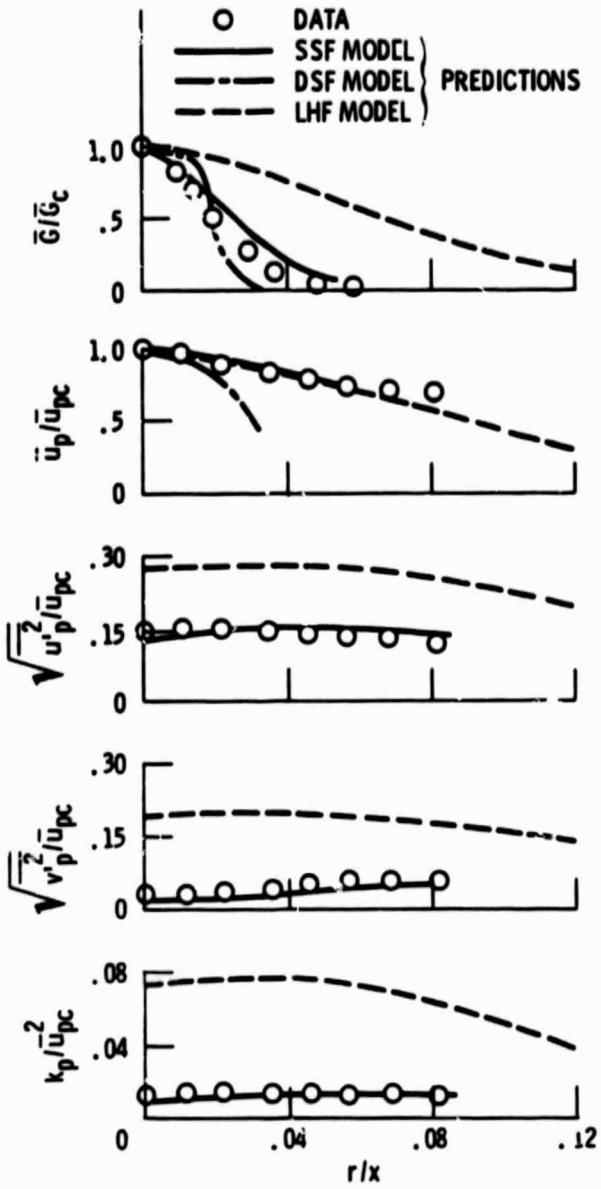
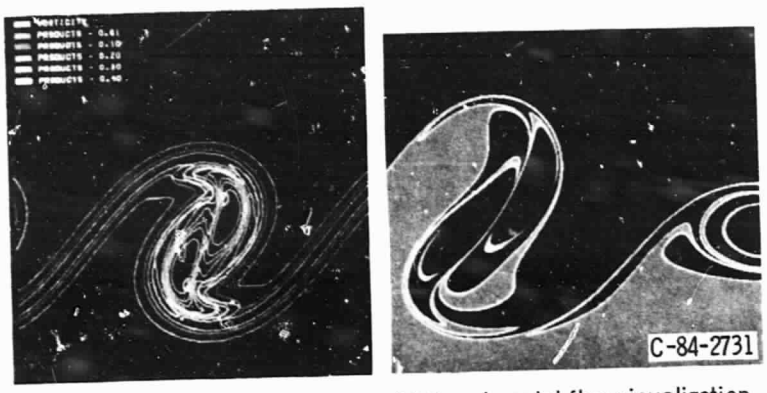


Figure 6. - Radial variation of solid-phase mean and turbulent quantities in case 3 particle-laden jet. x/d = 40, SMD = 119 μm, LR = 0.66.



(a) Computational results. (b) Experimental flow visualization.

Figure 7. - Flow structure comparison between direct numerical simulation and experimental flow visualization.

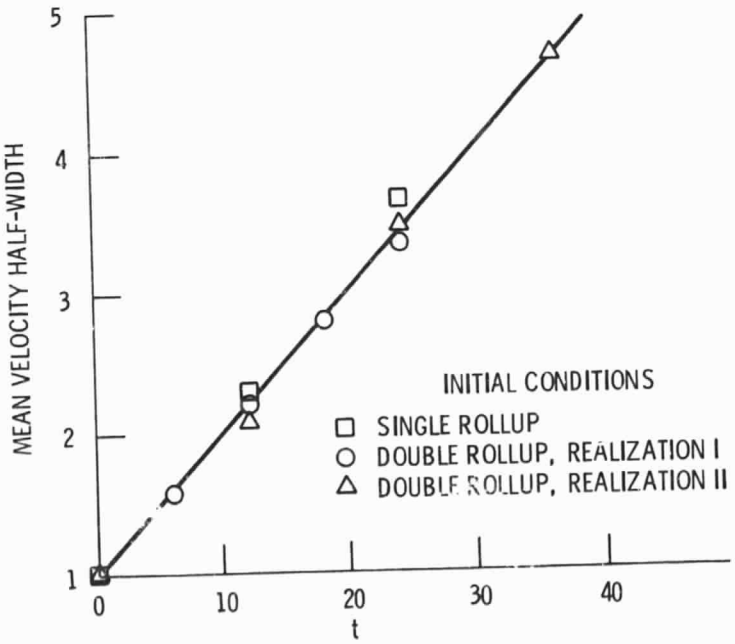


Figure 8. - Mean velocity half-width, z_M (= $z_{1/2}$), versus time - three-dimensional simulations.

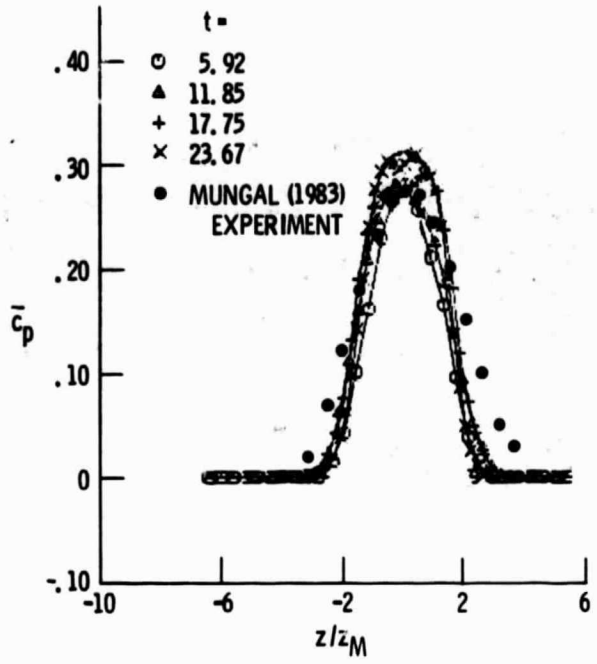


Figure 9. - Similarity plot of integrated product level versus radial location, 3-D simulation.

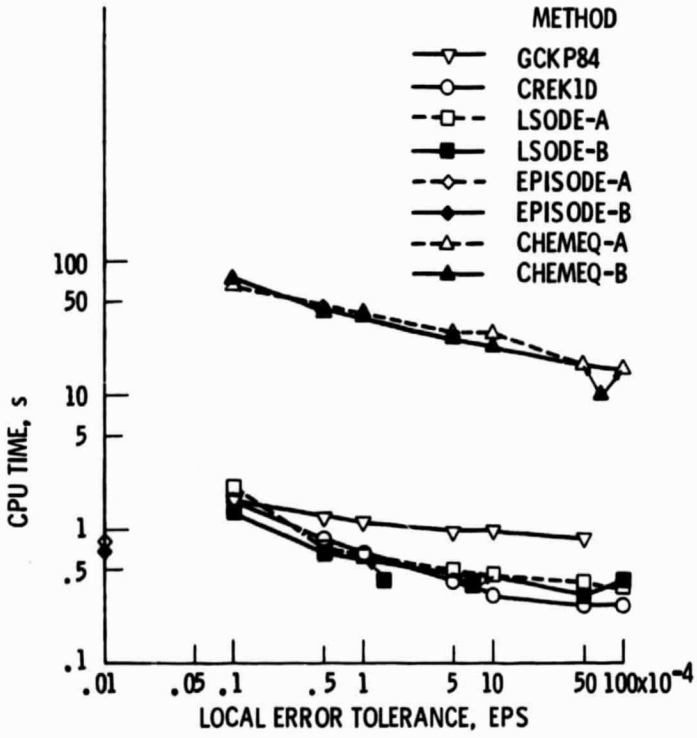


Figure 10. - Variation of the CPU time(s) with error tolerance, EPS, for test problem 1. All runs on IBM 370/3033.

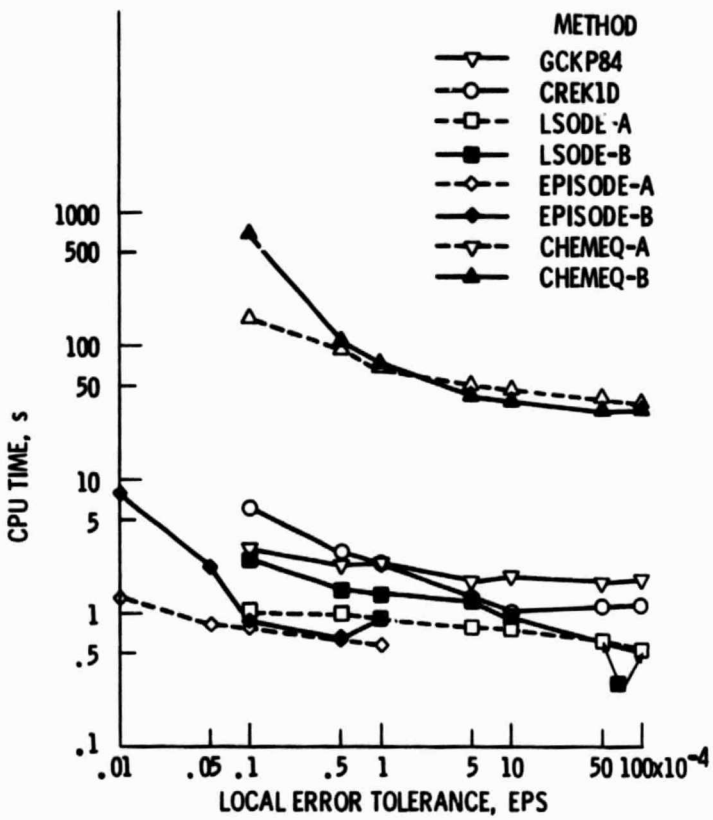


Figure 11. - Variation of the CPU time(s) with error tolerance, EPS, for test problem 2. All runs on IBM 370/3033.

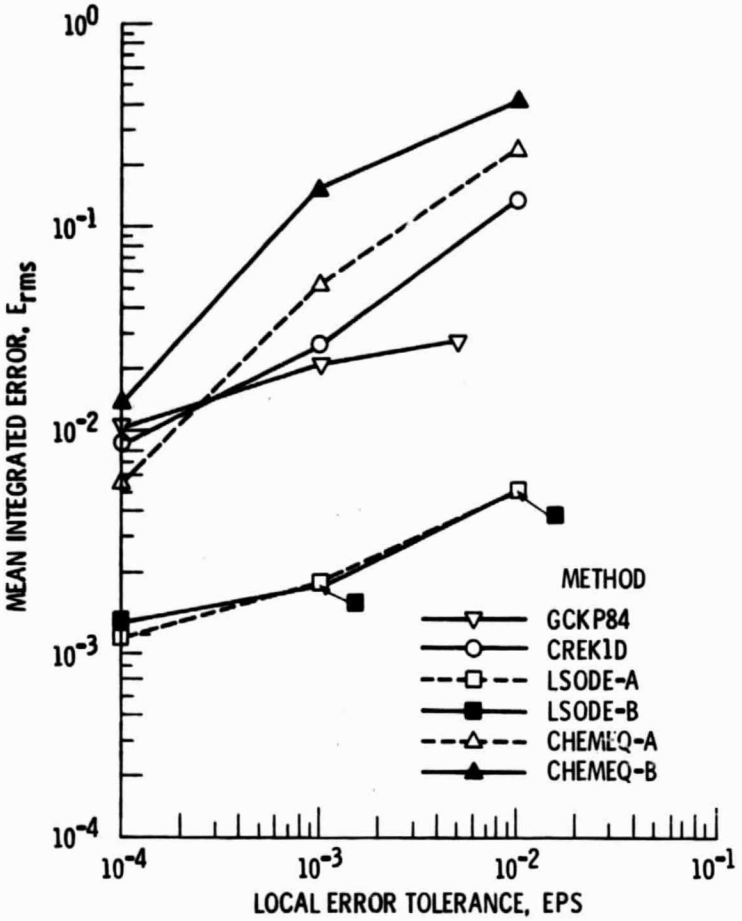


Figure 12. - Variation of the mean integrated global error (E_{rms}) with the local error tolerance (EPS) for test problem 1.

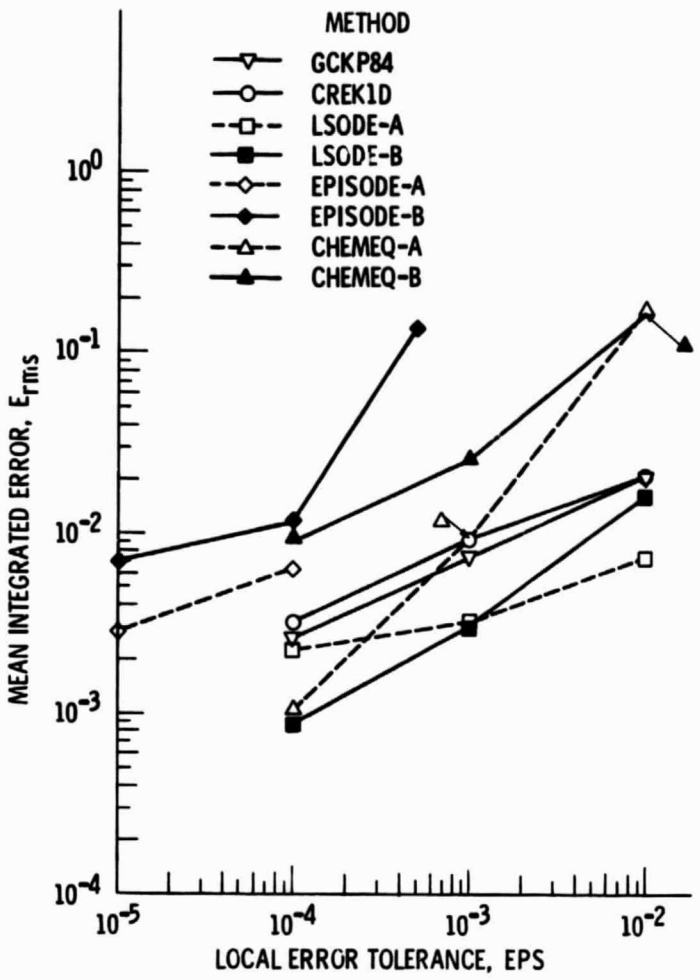


Figure 13. - Variation of the mean integrated global error (E_{rms}) with the local error tolerance (EPS) for test problem 2.