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CFD APPLICATIONS IN CHEMICAL PROPULSION ENGINES

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Charles L. Merkle
Department of Mechanical Engineering

I. Research Objectives and Potential Impact on Propulsion

The present research is aimed at developing analytical procedures for predicting the performance and stability characteristics of chemical propulsion engines. Specific emphasis is being placed on understanding the physical and chemical processes in the small engines that are used for applications such as spacecraft attitude control and drag make-up. The small thrust sizes of these engines lead to low nozzle Reynolds numbers with thick boundary layers which may even meet at the nozzle centerline. For this reason, the classical high Reynolds number procedures that are commonly used in the industry are inaccurate and of questionable utility for design. A complete analysis capability for the combined viscous and inviscid regions as well as for the subsonic, transonic and supersonic portions of the flowfield is necessary to estimate performance levels and to enable trade-off studies during design procedures.

Most engines that are used for auxiliary propulsion operate at efficiencies that are considerably below those reached by larger engines. Although a portion of this efficiency decrement is due to the reduced Reynolds number conditions, a substantial fraction can also be attributed to the design processes which fail to take into account properly the viscous nature of the flow. Improved design and analysis capabilities should allow considerable performance improvements in these small engines. Higher performance in turn means that a reduced amount of propellant is needed to keep the spacecraft on orbit, thus leading to longer spacecraft life without increased launch weight. This potential for increased on-orbit time is the justification for the present research effort. Additional areas that are being considered include CFD modeling of combustion instability. These efforts are directed, for the most part at larger engines, but again, the application of CFD here promises to provide increased understanding of the physics that control engine design.

The numerical analyses of compressible flows has progressed rapidly in the past two decades,and it is presently routine to compute two-dimensional steady flows, while two-dimensional unsteady and three-dimensional flows are feasible in a research environment. Although two-dimensional computations are within the reach of day-to-day design procedures, no particular attention has been given to the computation of rocket flowfields and care must be taken to develop a procedure that is accurate and efficient enough for design use. Similarly, the areas of combustion instability is one that has received little attention from full CFD formulations. In addition to the computational aspects, major modeling issues exist with regard to the spray atomization and vaporization processes as well as the turbulent combustion processes and the heat release rates in the combustor. Three-dimensional and unsteady flows are also of downstream interest. The present effort is directed towards these issues.

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II. Current Status and Results

At present, coordinated efforts are going on in several areas. The first has to do with the application of CFD methods to the prediction of mixing and combustion in auxiliary propulsion engines . Our efforts here have started from an existing code for hypersonic reacting flows. This code uses an LU-SSOR central-difference algorithm with a complete chemistry and physical properties formulation for hydrogen-oxygen reactions and kinetics. Turbulence is modeled by the simple Baldwin-Lomax mixing length model. Although this procedure is effective for hypersonic flows, it has some shortcomings in the low-speed subsonic regime that is characteristic of the heat release regions in chemical propulsion engines. Several enhancements are being investigated to increase the robustness and efficiency of the code in this lower speed regime.

The first enhancement in the code was to switch from the LU solution algorithm to a fourth-order, explicit Runge-Kutta procedure with an implicit treatment for the axisymmetric and chemical kinetics source terms. The implicit treatment of the source terms enables larger time steps in applications where the source terms are stiff. All terms are still centrally differenced on a finite volume grid in a manner identical to the original LU formulation. Some representative results comparing the new RK4 procedure with the LU method are presented on Fig. 1. These results show that the Runge-Kutta method converges approximately twice as fast as the LU procedure in terms of iterations, in addition to showing faster CPU times per iteration. The LU procedure requires about 135 μsec. per grid point per iteration on the CRAY-YMP, while the RK method requires only 98 μsec.

Other enhancements to the code include the implementation of characteristics-based boundary conditions on the inflow and outflow boundaries (which also enhance the convergence of the original LU method as Fig. 1 shows). In addition to implementing characteristic techniques, boundary procedures were also added to enable the specification of the incoming mass flow rather than only stagnation quantities. This enhancement enables the user to mimic the experimental procedure where upstream conditions control the incoming flow rates of fuel and oxidizer while the choked throat in the nozzle sets the chamber pressure. Experience to date with the RK method shows that it is more robust than the LU method for this problem, and, in addition, requires smaller amounts of artificial viscosity to be added, thus enhancing the accuracy of the results, particularly in the steep gradient regions near the wall.

Some representative solutions for a gaseous hydrogen-oxygen engine are shown on Figs. 2 to 4. Figure 2 shows the overall geometry of the proposed station-keeping engine for the Space Station, while Fig. 3 shows the computed temperature contours and Fig. 4 the corresponding Mach number contours in the downstream mixing region of the low Reynolds number combustor. The computational grid used for these results is given in Fig. 5. The results show that the hydrogen stream from the outer periphery of the nozzle undergoes little reaction with the internal oxygen-rich core stream. Although these predictions could be correct, the present turbulence model is not sufficient to predict accurately the mixing and combustion processes in this complex boundary-layer/free-shear-layer region. For this reason we are currently adding a k-ε turbulence model to the code to enhance these predictions.

At the present time the k-ε model has been coded and is being debugged and validated. The model is presently working for the boundary layer in the outer hydrogen stream alone, and current efforts are directed toward demonstrating it for the shear layer region as well. The model is formulated with low Reynolds number terms to enable the profiles to be computed all the way to the wall. Preliminary results suggest that this more complex turbulence model will predict substantially faster mixing and combustion processes than the present mixing length model, although comparison of the code predictions with hydrogen-oxygen flame measurements obtained from the literature is necessary to verify its accuracy. Downstream plans include extension to a complete PDF model of the turbulent combustion process.

Additional efforts on the low Reynolds number nozzle problem include the implementation of a flux-difference-split, upwind-biased, finite volume method with TVD capabilities for the flowfield. Results to date show that the upwind-finite volume method is considerably more robust than the centrally differenced methods, and should result in a more reliable code. The use of third-order biased differencing provides accuracy that is similar to that obtained with central differences. All results to date are for air chemistry, and again for the Baldwin-Lomax turbulence model, and are based on an alternating direction implicit (ADI) solution procedure. Modifications for the chemistry and physical properties of hydrogen-oxygen mixtures is nearly complete and results should be available shortly. The incorporation of an LU time marching procedure, that is also underway, should provide a further improvement in computational efficiency over the RK4 method. Although the LU procedure is not efficient for centrally differenced schemes, it is quite effective for upwind schemes, and substantial improvements in speed are expected.

A third effort in developing robust procedures for the small rocket engine application is adaptation of a parabolic Navier-Stokes (PNS) based algorithm to fully elliptic flow in the supersonic portion of the nozzle. This method has been demonstrated for perfect gas flows and is currently being extended to the full hydrogen-oxygen kinetics scheme, again using the same kinetics package that was used above. Our current efforts here are on the development of the space-marching PNS procedure. Later extensions will add a reverse iterative sweep to incorporate the complete elliptic Navier-Stokes effects. Some representative results for the perfect gas case in a contoured, high expansion nozzle, including the effects of expansion to a non-ideal back pressure are shown on Figs. 6 and 7. The PNS method, being a single pass method, is much faster than iterative methods, and the forward-backward sweeping procedure for the full Navier-Stokes equations is again much faster than classical time-marching algorithms.

Other efforts include the addition of a time derivative preconditioning method for enhancing convergence in low speed regimes such as occur in rocket combustors and the development of an Eulerian-Lagrangian method for oxidizer droplets. The convergence rates of most time-marching procedures scale inversely with the flow Mach number because of the stiff eigenvalues in the low speed regime. Because most rocket combustion occurs at these low Mach numbers, it is imperative that methods be developed to retain fast convergence rates especially when complex chemistry models are in use. The present effort is based on extending earlier preconditioning methods by the author for inviscid flows to flows where diffusion is significant. Figure 8 compares the convergence rates with and without preconditioning for typical low speed conditions.

The work on two phase flows is in an early stage with efforts currently focussed on reviewing current state-of-the-art modeling procedures for liquid spray combustion. At present a first generation liquid propellant model has been developed and applied to one-dimensional flows. Our immediate plans are to extend this analysis to two dimensions by combining our existing Eulerian methods for the gas phase with Lagrangian droplet models developed elsewhere.

Finally as a last effort, a CFD-based combustion instability model is being developed for predicting finite amplitude waves in rocket combustors. At present, efforts are concentrated on developing accurate procedures and we are therefore employing simple combustion models (equivalent to n-τ models) with perfect gas conditions. Later extension to more realistic combustion models is planned. The model is based on an iterative, implicit time-marching method with capabilities similar to those described above for low speed flows. At present we are comparing one and two-dimensional oscillatory wave calculations with test cases based on linearized stability results that have been recommended by the current JANNAF Combustion Instability Panel as the result of recent JANNAF workshops.

III. Proposed Work for Coming Year

For the coming year our efforts are to be divided among several fronts. Primary emphasis is to be placed on enhancing and upgrading the turbulent combustion model and validating the code. Of secondary interest is a continuing effort to make the algorithm more robust and reliable both through day-to-day running, and through the addition of algorithm enhancements. Additional improvements are also planned to enable a wider, choice of wall boundary conditions and geometrical configurations. Low level efforts are also planned for the continued development of a liquid spray capability in the code. The final item to be addressed is the continued development of a combustion instability model based on CFD procedures.

The efforts on improved turbulent combustion models will focus on completing the incorporation of a two-equation model of turbulence to enable us to represent the boundary-layer-shear-layer more realistically. This model will then be augmented by a turbulent combustion model, most likely of the PDF variety using existing techniques from the literature. The validation of the code by comparison with experimental data will also be an area of focus. In conjunction with advanced turbulence modeling, we will also look for methods for enhancing the mixing and combustion processes in the rocket combustor. This will probably necessitate the use of three-dimensional phenomena, and, in particular, will include an assessment of the effect of discrete hole injection of hydrogen fuel (as is presently being done in the experimental configuration) on the mixing and combustion of the Space Station engine. These discrete holes are presently being modeled in two-dimensional fashion as a slot, and this simplified treatment may be underestimating the degree of mixing and combustion. Improved methods for treating this three-dimensional injector pattern without going completely to three-dimensions will also be sought, including efforts for estimating the errors introduced by the use of the current two-dimensional predictions instead of the more realistic three-dimensional geometry.

In terms of a continued upgrade of the code, the results of other companion studies concerning various methods for enhancing the present algorithm will be integrated into the model as appropriate. Specific issues to be considered include the efficacy of switching to the flux-difference-split method, the enhancements to be gained through the use of low Mach number preconditioning, and the desirability of incorporating the PNS-based Navier-Stokes algorithm for the supersonic portion of the nozzle flowfield. The emphasis in these code improvement issues will be to evolve the code steadily into a more reliable procedure, as capabilities dictate. In addition, the extension of the method to other chamber geometries will also be undertaken, with the purpose of determining the capabilities of the method for predicting thrust and specific impulse accurately.

Additional capabilities to be included in the analysis include the addition of regenerative and radiation wall cooling procedures so the nozzle flowfield calculations will predict both the wall temperature and the heat flux distribution. The accurate prediction of wall heat transfer is an important issue in the design of small rocket engines, and requires an adequate model of turbulent wall heat transfer as well as some estimate of the locations of transition to turbulence. The improved turbulence model should provide some help in this area also.

Efforts to model the two-phase liquid spray combustion process will continue, although at a lower level of effort than the above topics. The purpose here will continue to be focussed on identifying the appropriate levels of technology and assessing the degree to which the spray combustion process can be predicted. Only representative solutions of simpler combustion processes are expected to be completed this year. A major emphasis will be placed on assessing the degree of reliability that can be expected as a stepping stone for planning the following year's effort.

In the related area of combustion instability, primary emphasis will be placed on demonstrating the accuracy that can be expected from a CFD analysis of combustion instability using a global model for the combustion process. Emphasis will be placed on estimating the effect of distributed heat release on disturbance growth, the effects of finite nozzle lengths of representative size, and other similar analyses based on simple phenomenological combustion models. These calculations will center around two-dimensional, radial-tangential modes, but additional studies of complete three-dimensional models based on the numerical solution of the linearized equations will be obtained as a precursor to incorporating three-dimensional disturbances in the complete nonlinear solution. Additional emphasis will be placed on the effect of finite amplitude disturbances on the growth of waves. An assessment of the advantages of CFD analyses over classical linear stability procedures will also be a goal of this research along with a comparison of the relative merits of the CFD predictions.

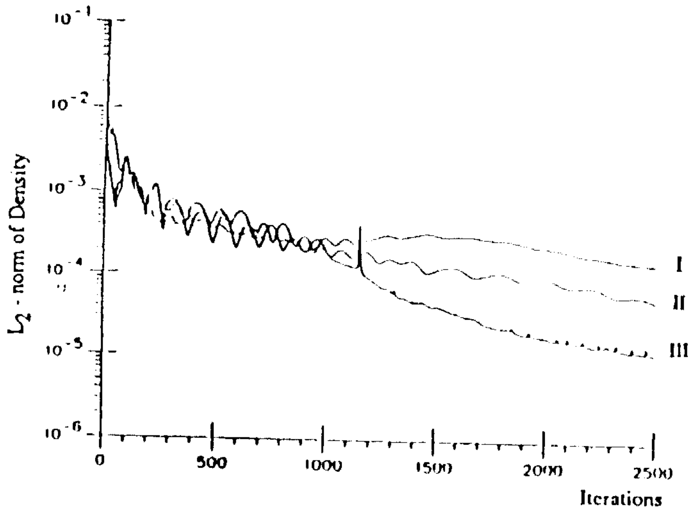

Figure 1. Convergence Histories: I) Original LU scheme (135 μs/grid point/iteration), II) Modified LU (123 μs/pt-iteration), III) Four-step Runge Kutta (98 μs/pt-iteration).

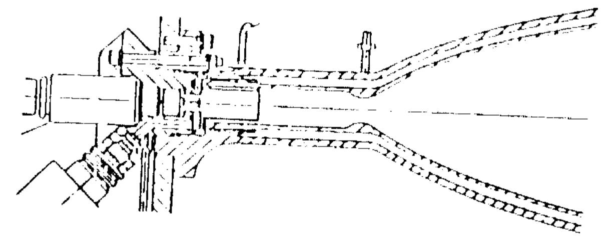

Figure 2. Aerojet Space Station Thruster #2

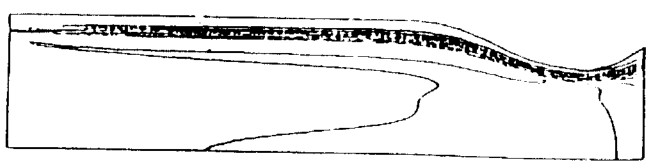

Figure 3. Temperature Contours

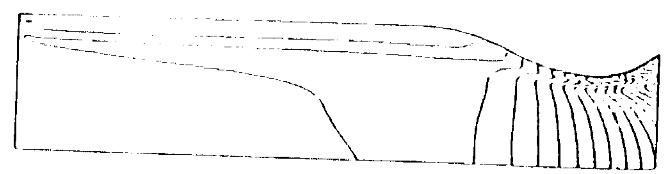

Figure 4. Mach Number Contours

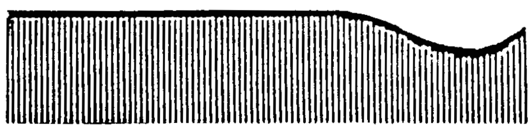

Figure 5. 90 x 60 Computational Grid

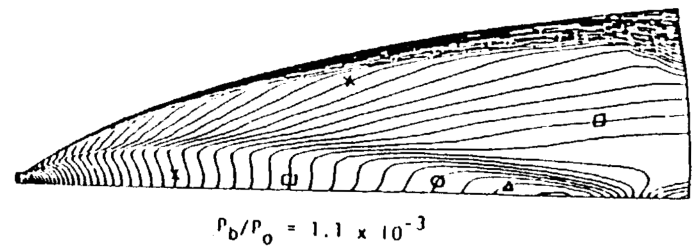

Figure 7. Mach Number Contours for Turbulent Flow in Overexpanded 272:1 Contoured Nozzle.

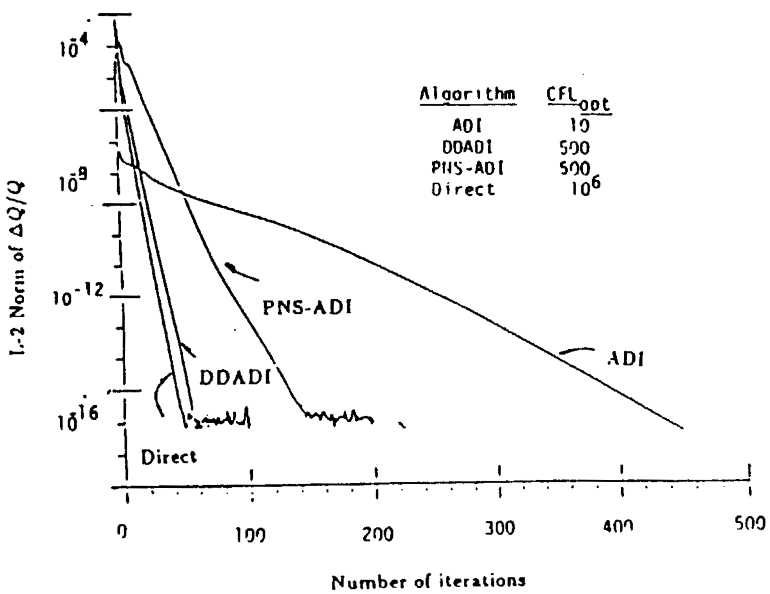

Figure 6. Comparison of Convergence for PNS-ADI Scheme with ADI Method for Supersonic Nozzle Flow.

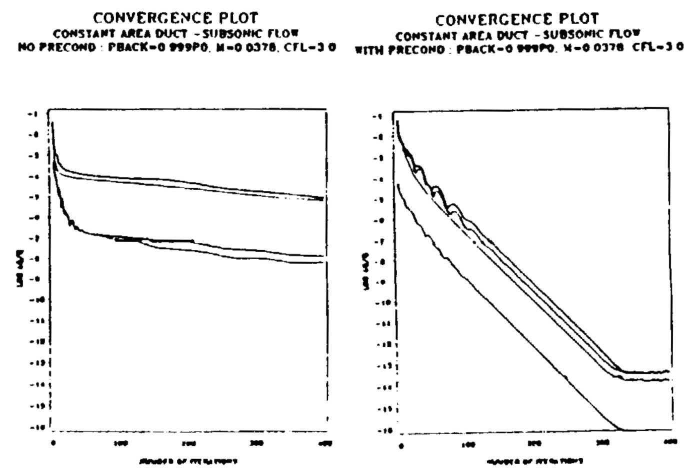

Figure 8. Effect of Time Derivative Preconditioning on Convergence in Low Mach Flows Representative of Combustor Conditions.

III. Proposed Work for Coming Year

1. Complete the development of the droplet temperature measurement technique and its integration with the droplet size and velocity techniques in order to obtain the capability to make simultaneous droplet size, velocity and temperature measurements in liquid hydrocarbon sprays.

2. Complete the fabrication, assembly and testing of the 70 atm, 300°C turbulent flow system and single droplet generator.

3. Obtain a set of simultaneous droplet size and velocity measurements in a vaporizing liquid hydrocarbon spray, at atmospheric pressure and room temperature, and at one laminar and one turbulent flow condition.

4. Obtain a set of droplet size and temperature versus time measurements for the case of individual liquid hydrocarbon droplets injected into the same two flow conditions used in task 3.

5. Make a preliminary study of the behavior of individual liquid hydrocarbon droplets injected into a supercritical environment using high speed, back lit photography.

6. Make a preliminary investigation of the feasibility of using two-dimensional Raman scattering to visualize supercritical liquid hydrocarbon droplets.

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