Final Technical Report

for

COMPUTATION of REACTING FLOWS in COMBUSTION PROCESSES

Theo G. Keith, Jr.
Principal Investigator
Kuo-Huey Chen
Co-Principal Investigator

Department of Mechanical, Industrial and Manufacturing Engineering
University of Toledo
Toledo, Ohio 43606

December 1997

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NASA Grant Number NAG3-1219

Abstract

This final report summerizes the research activities sponsored under the NASA grant number NAG 3-1219 during the period of time spanning from January, 1991 to November, 1996. The main objective of this research is to develop an efficient three-dimensional computer code for chemically reacting flows. The main computer code developed is ALLSPD-3D. The ALLSPD-3D computer program is developed for the calculation of three-dimensional, chemically reacting flows with sprays. The ALLSPD code employs a coupled, strongly implicit solution procedure for turbulent spray combustion flows. A stochastic droplet model and an efficient method for treatment of the spray source terms in the gas-phase equations are used to calculate the evaporating liquid sprays. The chemistry treatment in the code is general enough that an arbitrary number of reaction and species can be defined by the users. Also, it is written in generalized curvilinear coordinates with both multi-block and flexible internal blockage capabilities to handle complex geometries. In addition, for general industrial combustion applications, the code provides both dilution and transpiration cooling capabilities. The ALLSPD algorithm, which employs the preconditioning and eigenvalue rescaling techniques, is capable of providing efficient solution for flows with a wide range of Mach numbers. Although written for three-dimensional flows in general, the code can be used for two-dimensional and axisymmetric flow computations as well. The code is written in such a way that it can be run in various computer platforms (supercomputers, workstations and parallel processors) and the GUI (Graphical User Interface) should provide a user-friendly tool in setting up and running the code.

Summary

The ALLSPD-3D code has evolved from the two-dimensional version released in June, 1993. Besides extension to the three dimensions, the new code features several improvements, including a user-friendly graphical user interface (GUI), multi-platform capability (supercomputers, workstations, and parallel processors), improved turbulence and spray models, generalized chemistry, a new solution procedure, and more general boundary conditions. In this summary, a brief description of the numerics and physical models of the ALLSPD code is discussed. More information about the code can be accessed through internet at the following address:

http://www.lerc.nasa.gov/WWW/IFMD/allspd

The numerics of the ALLSPD code is based on modern compressible algorithms to take advantage of advances made in CFD in the past two decades. It is well known that numerical methods developed for compressible flows are often ineffective at low Mach numbers. There are two main reasons for this difficulty. First, the system's eigenvalues become stiff at low flow velocities. In theory, this can be circumvented by using a large CFL number in implicit numerical schemes. In practice, however, a large approximate factorization error in multi-dimensions limits an optimal CFL number beyond which convergence slows down. At low Mach numbers, there are large disparities among CFL numbers based on each eigenvalue and the numbers can not become the same optimum number simultaneously. Second, the pressure term in the momentum equations becomes singular as the Mach number approaches zero, yielding a large roundoff error. This behavior smears the pressure variation field and often produces inaccurate solutions. These difficulties are circumvented in the ALLSPD code by the pressure decomposition and the eigenvalue rescaling techniques. The results of these treatments show that the convergence characteristics of the code are indeed independent of the flow Mach numbers.

Chemically reacting flows exhibit another category of numerical difficulties because of the wide range of time scales involved in the calculation. To avoid this chemical stiff problem, the chemical source terms are treated fully implicitly. This measure is equivalent to preconditioning the time derivative terms of the species conservation equations so that all chemical and convective processes proceed at approximately the same numerical rate.

The numerical issues relating to solving this set of governing equations are robustness, CPU time requirement, implicitness, stability, equation coupling and memory.

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Some of the issues are very closely related; such as robustness, implicitness, stability and equation coupling. During the past two decades, the development of numerical algorithms and the usage of solvers in CFD have been pretty much dependent on the availability and accessibility of computer resources. The trend evolves from explicit, decoupled schemes to strongly implicit and fully coupled strategies. The pros and cons among various schemes may depend on the problems of interest and sometimes the vectorization and/or parallelization on computer platforms as well. Nevertheless, the strongly implicit, fully coupled schemes, in general, give better stability, robustness and convergence for at least steady state calculations although they usually take more CPU time per iteration compared to explicit schemes. For combustion flow computation, due to the strong coupling nature of the chemical source terms in detailed chemistry treatment, the equation-wise coupling (at least for species equations) is inevitable.

In order to make comprise between degree of coupling and the total memory requirement, the partially decoupled numerical scheme is adopted. This procedure divides the whole set of equations into three groups. The first group is the five flow equations, the second group is the two turbulent equations and the third group is the species equations. Each group of equations is solved in a coupled manner and the subsequent sweep to the three groups completes one iteration. This arrangement provides us great flexibility in various types of flow calculations while maintaining the strongly coupled and implicit manner within the existing combustion code structure. The solver in the ALLSPD-3D code has been modified to include the LU scheme which is thought to be more suitable for solving large set of coupled three-dimensional reacting flow equations.

A recently developed low Reynolds number κ-ϵ is used to represent the effects of turbulence. In this model, the κ and ϵ equations are solved all the way down to the wall and the conventional wall function treatment of near wall regions is not needed. Some variations of implementing this model, especially the near wall treatment, are also available as an option to alleviate the fine grid requirement near the walls typically a heavy burden associated with this type of model for three-dimensional calculations. Although the turbulence is included, the mean flow quantities are still used in the chemistry calculations (laminar chemistry) in the current version of the code. A simple eddy breakup model (EBM) is use to model the turbulence effect on the combustion.

The liquid phase is treated by solving Lagrangian equations of motion and transport for the life histories of a statistically significant sample of individual droplets. This involves dividing the droplets into n groups (defined by position, velocity, tem-

perature and diameter) at the fuel nozzle exit and then computing their subsequent trajectories in the flow. The spray model used in this study is based on a dilute spray assumption which is valid in the regions of spray where the droplet loading is low. The liquid fuel is assumed to enter the combustor as a fully atomized spray comprised of spherical droplets. The present model does not account for the effects due to droplet breakup and coalescence processes which might be significant in a dense spray situation. A stochastic process is included in the spray calculation to account for the turbulence dispersion on the spray trajectories. Also the temperature within each droplet is non-uniform and the vortex model is used to compute the internal temperature distribution.

Most combustors in aero-propulsive engines involve very complex geometries. To enhance geometrical flexibility, the ALLSPD code is written in generalized curvilinear coordinates and is equipped with multi-block grid and internal blockage capabilities. These features allow the users to handle complex geometries.

Some main features of the ALLSPD-3D code are listed in the following table and can also be accessed at the World Wide Web at the following address:

http://www.lerc.nasa.gov/WWW/IFMD/allspd

The code is freely distributed to the US users. There are more than one hundred copies of the code distributed to the general users within the US. The Web site of the ALLSPD code contains many pictures of flow applications that were part of the test cases during the ALLSPD code development. For each code distribution, the package contains a source code, a user manual, a complete suite of test cases. Limited user support is provided through NASA Lewis Research Center.

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ALLSPD-3D Main Features
● 3D/2D/axisymmetric/overset grid topology capabilities
● Finite-difference, compressible flow formulation with low Mach number preconditioning (current version intended for subsonic flow simulations and uses central-differencing for convective and viscous terms on right ans left-hand sides)
● Strongly coupled, implicit steady-state and unsteady algorithm
● Generalized finite rate chemistry
● Generalized properties and chemical reaction database
● Eddy dissipation model for turbulence-chemistry closure
● High and low-Reynolds number k-e turbulence models
● Realistic multiblock spray combustion model (a stochastic separated flow model with vortex model for droplet internal temperature distribution)
● Radiative heat transfer model (accounting for exchange between surfaces, gaseous species $H2O$, $CO2$, and particulates)
● Serial & parallel versions (using PVM for message passing) on various platforms (IBM, SGI, SUN, HP workstations, CRAY)
● Various boundary conditions (multiple inlets/outlets, dilution holes, transpiration holes, periodic, symmetry far-field, slip, wall function, adiabatic or isothermal walls, centerline singularity, and overset iterpolation)

Figure 1: ALLSPD-3D Main Features

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Publications

During the grant period, publication activities are listed as follows:

1. Chen, K.H. and Keith, T., "Numerical Study of Three-Dimensional Air Flow Characteristics in a Throttle Body with Chimera Grid," Conference Proceedings, pp. 487-492, 2nd Asian Computational Fluid Dynamics Conference, Tokyo, Japan, 15-18, Dec. 1996.

2. Chen, K.H., DelSignore, D. and Keith, T., "Numerical and Experimental Study of Three-Dimensional Air Flow Characteristics in a Throttle Body," Conference Proceedings, pp. 439-448, International Congress on Fluid Dynamics and Propulsion, Cairo, Egypt, 29-31, Dec. 1996.

3. Chen, K.H. and Bulzan B., "Numerical Study of Cooling System Design in a High Pressure Combustion Rig with Chimera Grids," AIAA 96-3126, presented at the 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, July 1-3, 1996/Lake Buena Vista, FL.

4. Chen, K.-H., Duncan, B., Fricker, D., Lee, J. and Quealy, A., "ALLSPD-3D, Version 1.0a," NASA TM 107204, April, 1996.

5. Yungster, S. and Chen, K.H., "Application of Chimera Grid Scheme to Combustor Flowfields at all Speeds," AIAA 96-0731, presented at the AIAA 34th Aerospace Sciences Meeting & Exhibit, January 15-18, 1996/Reno, NV.

6. Chen, K-H, Shuen, J.-S. and Mularz, E., "A Comprehensive Study of Numerical Algorithms for Three-Dimensional, Turbulent, Non-equilibrium Viscous Flows," AIAA 95-0800, presented at the AIAA 33rd Aerospace Sciences Meeting & Exhibit, January 9-12, 1995/Reno, NV.

7. Chen, K-H, "A Diagonally-Dominant Coupled Strongly Implicit Procedure for 3D Viscous Flows," Conference Proceedings, Vol. 1, pp. 325-333, 1st Asian Computational Fluid Dynamics Conference, Hong Kong, 16-19 Jan. 1995.

8. Chen, K.-H. and Shuen, J.-S., "Three-Dimensional Coupled SIP Method for Spray Combustion Flows at All Speeds," AIAA 94-3047, presented at the 30th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, June 27-29, 1994/Indianapolis, IN.

9. Chen, K.-H. and Pletcher, R.H., "Numerical and Experimental Study of Three-Dimensional Liquid Sloshing Flows", *J. of Thermophysics and Heat Trans.*, **8**, 507 (1994).

10. Pletcher, R.H. and Chen, K-H., "On Solving the Compressible Navier-Stokes Equations for Unsteady Flows at Very Low Mach Numbers," AIAA-93-3368 and NASA TM 106380, presented at the AIAA 24th Fluid Dynamics Conference, Orlando, FL, July 6-9, 1993.

11. Mularz, E. J., Bulzan, D. L. and Chen, K.-H., "Spray Combustion Experiments and Numerical Predictions," NASA TM 106069 and AGARD-CP-536, pp. 35-1 to 35-22, presented at the Propulsion and Energetics Panel 81st Symposium held in Fiuggi, Italy, 10-14 May, 1993.

12. Chen, K.-H. and Shuen, J.S., "A Coupled Multiblock Solution Procedure for Spray Combustion in Complex Geometries", AIAA Paper No. 93-0108, presented at the AIAA 31st Aerospace Sciences Meeting & Exhibit, January 11-14, 1993/Reno,NV.

13. Shuen, J.-S. Chen, K.-H. and Choi, Y., "A Coupled Implicit Method for Chemical Non-Equilibrium Flows at All Speeds," *J. Comput. Phys.*, **106**, 306 (1993).

14. Chen, K.-H. and Pletcher, R.H., "Simulation of Three-Dimensional Liquid Sloshing Using a Strongly Implicit Calculation Procedure", *AIAA Journal*, May 1993.

15. Chen, K.-H. and Pletcher R.H. , "A Primitive Variable, Strongly Implicit Calculation Procedure for Viscous Flows at All Speeds", *AIAA Journal*, Vol. 29, No. 8, 1991.