Development of Methods to Predict High-Speed Reacting Flows in Aerospace Propulsion Systems

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This paper discusses the current state-of-the-art of computational capabilities for predicting reacting flows in high-speed aerospace propulsion systems with an emphasis on the flow fields in scramjets. We begin with a review of the history of efforts to model the scramjet environment and then concentrate on more recent activities that lead to today’s capabilities. The NASP technology program provided strong motivation for advancing the computational capabilities of the country in both the government and private sectors. Required ground test facilities with sufficient test times were limited to around Mach 8, and higher Mach numbers, achievable in pulse facilities, could only be maintained for the order of milliseconds. In addition, the number of facility cycles available to parameterize a given engine flow path were limited, and the facilities were expensive to operate. Computational capabilities were needed to fill both of these gaps. While the NASP program was not successful in developing a vehicle, it did spawn the development of new computational algorithms. The Hyper-X Program beginning in 1995 revived high-speed computational research and development. A flight program is the catalyst that drives technology development and synthesizes all of the efforts into a unified tool for development of the ultimate experiment, the flight of a hypersonic vehicle. The genesis of most of the current day state-of-the-art computational tools for scramjet research and development began with this program. This paper attempts to cover this story from NASP and Hyper-X to the present day.

I. Introduction

Research to develop a high speed airbreathing aerospace propulsion system was underway in the late 1950’s. A major part of the effort concentrated on the supersonic combustion ramjet, or scramjet, engine. Work had also begun to develop computational techniques for solving the equations governing the flow through a scramjet engine. Scramjet technology and the computational methods to assist in its evolution would remain apart another decade, however. The principle barrier was that the computational methods needed for engine evolution lacked the computer technology needed for solving the discrete equations resulting from the numerical methods. Even today, computer resources remain a major pacing item in overcoming this barrier. Significant advances have been made over the past thirty five years, however, in modeling the supersonic chemically reacting flow in a scramjet combustor. To see how the two fields finally merged, we briefly trace the evolution of the technology in both areas.

Following pioneering efforts of Ferri1 and Digger2 in the 1950’s, a significant increase in the research to develop scramjet engine concepts occurred in the 1960’s. In 1965, the NASA Langley Research Center initiated the Hypersonic Research Engine (HRE) Project to develop a high-speed airbreathing technology for application in the propulsion systems of hypersonic cruise vehicles.3 The goal of the HRE Project was to flight test a regeneratively cooled, hydrogen fueled, pylon mounted scramjet on the X-15 research airplane and demonstrate design performance levels. The HRE did not reach the flight demonstration stage due to cancellation of the X-15 program, but the ground-based program did continue and resulted in the development and construction of two variable geometry engine models. Work with these models significantly increased the scramjet technology base to be applied in more advanced configurations.

Following completion of the HRE Project, attention moved to propulsion concepts that would provide high performance when installed on a vehicle. The original concept, a pylon mounted HRE, would have resulted in excessive levels of external drag, so the pylon was removed and work began to highly integrate the engine with the airframe of candidate vehicles. In addition, engine weight was reduced by moving from a variable to a fixed geometry which reduced the engine structure. Out of this activity, the Langley airframe integrated scramjet engine concept was conceived. This program has continued to the present day, and has resulted in the successful demonstration of the concept to produce net thrust in subscale hardware. A detailed review of this program was given by Northam et al.3

In addition to the NASA scramjet research and development program, other government activities included a Navy sponsored scramjet program at the Applied Physics Laboratory of the Johns Hopkins University (JHU/APL)4.5. This work also increased in the 1960’s and was directed towards the development of an air-breathing shipboard missile using a scramjet propulsion system. Development of this concept continued until 1977. At that time, concern over the storage of the highly reactive and toxic fuels to be used forced a change to more conventional but safer fuels.

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This change resulted in the development of an integral-rocket/dual-combustor ramjet concept that used a fuel-rich gas generator to preburn the fuel for a main supersonic combustor, thus allowing the use of hydrocarbon fuels.  

The Air Force also sponsored scramjet research and development during the 1960's. They continued the support of several programs that were initially funded by the HRE program. In 1964, a program was started at the General Applied Science Laboratory to continue development of a low-speed fixed-geometry scramjet engine. A dual-mode scramjet program was continued with the Marquardt Company at the same time. Soon thereafter in 1965, the Air Force began an effort with the United Aircraft Research Laboratory to continue development of a water cooled variable geometry scramjet design. These three efforts ended in 1968, and only the NASA and JHU/APL programs continued into the 1970's. 

During the 1970's, computational techniques were first applied to study the supersonic reacting flow found in a scramjet combustor. A detailed review of those activities is given by White, et al. A summary of that discussion and additional work is now provided. Some of the earliest work to model supersonic reacting flows was by Ferri and his colleagues, Morretti, Edelman, and Dash. They employed an explicit viscous characteristics method that split the governing equations into hyperbolic and parabolic parts, followed by a coupled numerical solution of each part at each integration step. Modeling multistep finite-rate chemistry was also included in their solution strategy. Spalding and his colleagues then took Ferri’s splitting-based approach and improved its efficiency by developing a fully implicit solution procedure for solving the governing equations. Spalding then developed several implicit parabolized Navier-Stokes programs for modeling scramjet combustor flow fields. These codes included the CHARNL two-dimensional axisymmetric program and the SHIP three-dimensional program. Both programs used the well known SIMPLE solution procedure for spatially marching the governing equations in the parabolized direction while employing a tridiagonal matrix solution procedure to perform repetitive sweeps for solution of the equations in the cross-plane(s). These programs assumed that a state of chemical equilibrium always existed, but they were later modified by Evans to include the effects of finite-rate chemical reactions. The modified programs were still being used in the mid-2000s for studies of mixing and reaction in combustor configurations. 

The work of Ferri and Spalding was then adapted by Dash to develop the SCORCH program that used a hybrid explicit-implicit procedure for modeling supersonic reacting flows. The method again split the governing equations into hyperbolic and parabolic parts. The hyperbolic part was solved using a viscous characteristics approach that employed an upwind finite-difference procedure. The parabolic part was solved using an implicit finite-difference procedure. Work on this program and its application to supersonic combustion problems has continued to the present day. 

While Ferri, his colleagues, and Spalding were developing analysis techniques for direct application to the supersonic reacting flow problem in a scramjet, other algorithm developments were underway, directed primarily at solving high-speed external flow problems. These techniques ultimately found their way, however, into the internal reacting flow arena. The first of these algorithms was the MacCormack explicit, unsplit predictor corrector method initially developed to model the hypervelocity impact cratering problem. The MacCormack method was a variation of the Lax-Wendroff second-order accurate scheme that could be applied to complex geometries. Because of these qualities, the algorithm was readily adopted and used to study a wide class of external flow problems. Implicit algorithms were also developed for external flow problems in the 1970’s, motivated by the need to resolve the high gradients present in wall boundary layers. The resolution of boundary layers requires fine computational grids, resulting in a severe stability constraint on the marching time step size of an explicit method. Where only a steady state solution was required and time accuracy was not necessary, implicit methods converged much more rapidly. Early work to develop implicit solution techniques for the Navier-Stokes equations was carried out by Brilley and McDonald and Beam and Warming. Both approaches used a spatial factoring procedure that reduced the multidimensional problem to one of sequentially solving a set of one-dimensional spatial implicit operators. Using this computationally efficient procedure, convergence rates one to two orders of magnitude faster than the explicit method were achieved for steady-state problems on highly stretched grids. 

While the application of implicit methods was generally limited to scramjet inlet flow fields through the late 1970’s and early 1980’s, explicit methods were applied extensively in studies of combustor flow fields. In 1977, Drummond developed the two-dimensional TWODLE combustion program, based on the MacCormack method, to model internal scramjet combustor flow fields. The code used an equilibrium chemistry scheme to model $H_2$-air reaction and several algebraic eddy viscosity methods to model the turbulence field. The program was applied to several scramjet combustor component problems. Particular emphasis was given to the scramjet fuel injector problem in an attempt to better understand the complex flow field in this region of the engine. Development on the program continued into the early 1980’s when the program was used to carry out the first simulation of a scramjet flow field using a two-dimensional model engine module. Detailed studies to optimize the configuration of the scramjet fuel injectors were also completed during this period. 

An explicit solution procedure was also employed by Schetz during the early 1980’s to model the APL dual-combustion ramjet described earlier. He employed a modular approach to carry out his analysis. The mixing and burning of the center jet from the fuel-rich gas generator was calculated with a jet mixing code that was modified to include a turbulent kinetic energy mixing model, a chemistry model, and other improvements. Because of the high
static pressures and temperatures that were present in the device, a local diffusion-controlled, equilibrium chemistry model was used to model reaction in the combustor. Schetz’s procedure for modeling combustor flows was ultimately combined with an inlet analysis procedure to compute performance estimates for the dual-combustion ramjet.29

While numerical methods for modeling scramjet flow fields were developing through the 1960’s, 1970’s and early 1980’s, there was a parallel growth in computer hardware upon which these methods could be applied. Many of the early calculations were carried out on IBM 7090 and CDC 6600 class machines. Hardware improvements, that allowed the consideration of more realistic problems, came in the late 1960’s with the arrival of the CDC 7600 computer. The most significant hardware improvement came in the mid to late 1970’s, however, when vector processing supercomputers became available to the computational community. These machines included the CDC Star-100 and the Cray 1, followed in the early 1980’s by the Cyber 205 and the Cray X-MP which gave performance capabilities several orders of magnitude greater than the previous scalar machines.3 Until this time, the state of computer resources had resulted in a major barrier to advancing the state of the art in modeling supersonic reacting flows. With the Cyber 205 and Cray X-MP, however, the researcher was now in a position to begin dealing with the detailed physics contained in these complex flows. The burden now returned at least partially to the state of numerical algorithms used to model supersonic combustion. Later experience would show that an even greater challenge rested in the physical modeling used to describe the flow physics in high-speed propulsion systems.

II. NASP and Early Code Development Efforts

As previously described, only the NASA and JHU/APL hypersonic programs continued into the 1970’s.30 Both programs were limited to ground based experimental programs and modest theoretical and computational programs to guide and analyze the experimental efforts. A new national hypersonics program was needed to spur development and the need for more advanced theoretical and computational tools. The program to develop a single-stage to orbit hypersonic vehicle, the National AeroSpace Plane, or X-30, shown in Figure 1 began as a joint Air Force NASA program in 1985. That program had actually been underway since 1982 as a highly classified Defense Advanced Research Projects Agency (DARPA) project called Copper Canyon.31 Ronald Reagan, in his 1986 State of the Union Address, described the program as “a new Orient Express that could, by the end of the next decade, take off from Dulles Airport and accelerate up to twenty-five times the speed of sound, attaining low earth orbit or flying to Tokyo within two hours.” Unfortunately, the goals of the Orient Express and other uses of a single-stage to orbit vehicle were not achieved during the program. The related technology program for both an orbital and hypersonic cruise vehicle lasted for over 13 years, however, and other programs, albeit more modest or realistic, have continued to the present day.

The NASP technology program provided strong motivation for advancing the computational capabilities of the country in both the government and private sectors. Ground test facilities with sufficient test times were limited to around Mach 8, and higher Mach numbers, achievable in pulse facilities, could only be maintained for the order of milliseconds. In addition, the number of cycles available to parameterize a given engine flow path were limited, and the facilities were expensive to operate. Computational capabilities were needed to fill in the gaps. Short term efforts concentrated on extending existing capabilities for the simulation of high-subsonic and supersonic, turbulent reacting flows.

One of the first efforts in this new hypersonic program involved extension of the TWODLE code32 initially developed as a high-speed combustion research tool to include detailed models for finite-rate chemistry and kinetic-theory-based models for the molecular diffusion of momentum, heat, and species. This extended code evolved into the SPARK combustion program utilized in a number of early studies of the Copper Canyon and NASP flow paths. Carpenter33 extended the SPARK code to three dimensions and added generalized equilibrium chemistry and finite-rate chemistry models that allowed consideration of any fuel-air system with any number of reaction paths.34 Three-dimensional parabolized Navier-Stokes programs were also developed to model supersonic combustor flow fields. These programs provided a more efficient solution procedure if the flow field contained no subsonic regions. Chitsomboon developed a three-dimensional parabolized Navier-Stokes (PNS) program35 by extending a two dimensional PNS program that he had developed earlier.36,37 He solved the conventional parabolized Navier-Stokes equations together with a set of species continuity equations. A new three-dimensional explicit upwind PNS algorithm based on Roe’s flux-difference splitting was then developed by Korte.38 The method was second order accurate in the marching direction as well as the cross-stream directions. The algorithm was extended by White to include finite rate chemical reactions. In addition, the unsteady Riemann problem, rather than the steady Riemann problem used in the original formulation, was solved using the unsteady Riemann solver of Roe.39 During this same period, Gielda developed a non-reacting three-dimensional explicit PNS program40 using the MacCormack explicit algorithm.18 Gielda extended his code to multiple species by adding the parabolized species continuity equations to the governing equation system.41 He also incorporated both an equilibrium and a global one-step H2-air finite rate scheme into the program. Kamath then employed the Gielda algorithm to develop a parabolized version of the three-dimensional SPARK combustion code.33 He generalized the coordinate transformation to allow the streamwise coordinate to be orientated in the most supersonic direction. He also used the generalized equilibrium and finite rate chemistry schemes developed by Carpenter34 so any
multistep reaction scheme could be considered with the algorithm. All of these codes were vectorized to run efficiently on available vector supercomputers of the day including the Cray 2 and the Cyber 205.

In addition to the codes extended or sponsored by NASA, the codes developed by Spalding, Dash, MacCormack, and their colleagues continued to be popular tools for modeling supersonic reacting flows typical of those found in scramjet combustors. The Spalding three-dimensional parabolized Navier-Stokes code, SHIP, as modified by Evans, was still being used to carry out engineering design studies of scramjet configurations as well as basic high speed fuel-air mixing studies. The two-dimensional parabolized Navier-Stokes code, SCORCH, of Dash saw considerable use performing analyses of the NASP propulsion system. In addition, the code was also used to carry out several fundamental studies of experiments being used to design that propulsion system.

The development of a number of new algorithms was underway in the early or mid-1980s with the majority falling into the general class of monotone methods, that is, methods that employed flux-correcting or flux-limiting procedures to preserve high numerical resolution without the numerical oscillations associated with higher accuracy. Included in this class of algorithms were Flux Corrected Transport (FCT) methods, total variation diminishing (TVD) methods, and TVD-like methods that exhibit TVD behavior. These algorithms offered the modeler advantages over the previous methods when studying scramjet problems. Many of the codes utilizing these algorithms were developed to model supersonic or hypersonic flow with interacting air chemistry moving about configurations of interest.

The first monotone method applied to chemically reacting flows was the Flux Corrected Transport (FCT) algorithm developed by Boris and Book. Its development actually began in the 1970s and was revisited for propulsive flows in the late 1980s. In this method, a small amount of artificial diffusion was added to the governing equations in smooth regions of the flow to stabilize the solution. In regions where high gradients existed, larger amounts of diffusion were added to maintain monotonicity. The diffusion was added in such a manner that the overall dissipation was held below that of the earlier algorithms because most of the diffusion was subsequently removed. Zalesak later generalized the approach allowing the method to be readily incorporated into existing algorithms that did not provide monotone
behavior. In addition, the method could be more easily generalized to two and three spatial dimensions. A more recent discussion of the method was given by Oran.

Much of the new work was motivated by the need to model external flows about hypersonic vehicles including NASP as well as reentry vehicles. Therefore, the methods were developed to model high-speed strongly shocked flows undergoing air chemistry. To compute flows of this type, MacCormack and Candler developed an implicit flux split scheme, as an extension to MacCormack’s explicit predictor-corrector finite difference method, to solve the Navier-Stokes equations. MacCormack initially developed the implicit algorithm to consider only nonreacting flows. A finite volume approach was used to discretize the flux terms. In addition, Steger-Warming flux vector splitting was introduced to more properly account for the propagation of information through the flow field. A finite volume approach was used to discretize the flux terms. In addition, Steger-Warming flux vector splitting was introduced to more properly account for the propagation of information through the flow field. Following development of the basic algorithm, Candler and MacCormack extended the method to consider high-speed air flows that were ionized and in thermodynamic and chemical nonequilibrium. Subsequent successes modeling flows with air chemistry made it apparent that the algorithms could readily be modified to consider internal flows with combustion chemistry, and, therefore, serve as a means for modeling scramjet combustor flow fields.

Flux splitting methods were also employed by Grossman, Walters, and Cinnella to model high speed chemically reacting flow problems. Grossman and Walters initially developed their algorithm to solve the Euler equations for nonreacting flows, but included real gas effects. Three forms of flux splitting were considered, including Steger-Warming flux vector splitting, van Leer flux vector splitting, and Roe flux difference splitting. Each of these splitting methods was originally derived to be applied to ideal gas flows. They were rederived by Grossman to allow their application to problems with real gas effects. The flux split equations were solved using a two-step predictor-corrector method that was second-order accurate in space and time. Spatial differences were formed using the MUSCL differencing procedure and flux limiting by Anderson. Following the successful application of the algorithm to a one-dimensional shock tube problem, real gas splitting was incorporated into a two-dimensional implicit finite volume code that originally utilized van Leer splitting and Gauss-Seidel line relaxation to solve the equations governing ideal gas flows.

Grossman and Cinnella then extended the algorithms to include vibrational and chemical nonequilibrium by appending species continuity equations to account for each chemical species present in the reacting flow and vibrational energy conservation equations to account for those species in vibrational nonequilibrium. The authors then redeveloped the relationships described previously that were required to implement Steger-Warming, van Leer, and Roe flux splitting. Once these splitting approaches had been implemented, a finite volume scheme was used along with either an explicit Runge-Kutta time integration or an implicit Euler time integration to solve the governing equations. Nonequilibrium effects were modeled with a five species, five-reaction model that included $N_2$, $O_2$, $NO$, $N$, and $O$. Extensions of the algorithm to two- and three-dimensions were then carried out.

Additional interesting work using flux splitting was also conducted by Liou, van Leer, and Shuen. The authors again employed van Leer flux vector splitting or Roe flux difference splitting and derived real gas versions of these approaches. The derivations were begun by assuming a general equation of state for a real gas in equilibrium. Approaches similar to those discussed previously were then used to modify the splitting, but the number of assumptions employed were kept to a minimum. The modified splitting was then incorporated into an available TVD algorithm and used to model several problems described by the one-dimensional Euler equations. The algorithm was then extended to two- and three-dimensions.

A considerable amount of work was also undertaken to develop new TVD schemes for chemically reacting real gas flows. Beginning in 1985, Yee developed a symmetric TVD scheme that could be employed in the context of either explicit or implicit numerical integration procedures. The approach was later generalized to consider chemically reacting flows. Yee noted that her approach could readily be added to existing algorithms that did not exhibit TVD behavior, e.g. the 1969 MacCormack method, resulting in a more robust method with better shock capturing qualities. New explicit, semi-implicit, and implicit algorithms employing the symmetric TVD method were then developed and discussed. An explicit multistep TVD scheme was constructed using the 1969 MacCormack method for the first two (predictor-corrector) steps followed by the addition of a conservative dissipation term as a third step, such that the overall scheme was TVD. The dissipative term was made up of products of eigenvectors of Jacobians of the governing equation system and their associated eigenvalues, an entropy correction, and a limiter function. Details regarding the construction of the dissipative term and the determination of its magnitude is given in the reference. Finally, a fully implicit TVD method was developed including both implicit source and flux terms for situations where both chemistry and fluid scales were small and of the same order.

When implicit alternating-direction implicit (ADI) procedures were used, the factorization error that resulted when the implicit operator was spatially factored could not be neglected in some calculations. An alternate procedure developed by Gnoffo employed point implicit relaxation. Gnoffo used this procedure in his three-dimensional finite volume code with a symmetric TVD upwind discretization of the governing Navier-Stokes, species continuity, vibrational, and electron energy equations. Pseudo-time relaxation was used to drive the solution to a steady state. This procedure proved to be very efficient on vector computers. Two options for coupling the governing fluid and chemistry
equations, strong and weak implicit coupling, were also utilized. With strong implicit coupling, the complete equation set was solved as a unit, an approach typical of those described earlier. Weak implicit coupling involved splitting the fluid and chemistry equations into two groups, and applying the point-implicit method to each group separately during the relaxation process. The former approach was more physically exact, better accounting for complex wave interactions and fluid-kinetic coupling. The latter approach allowed for the relaxation strategy and time stepping to be tailored to the needs of the equation set.\textsuperscript{54} Air chemistry was modeled in the program using an eleven species scheme that included \( N, O, N_2, O_2, NO, N^+, O^+, N_2^+, O_2^+, NO^+ \), and \( e^- \). Further details on the chemistry model and other physical modeling are given in the reference.\textsuperscript{65}

Another attractive alternative to an ADI integration scheme for solving the spatially discretized governing equations was a lower-upper (LU) scheme that approximately splits the implicit operator into upper and lower operators that are independent of the dimensionality of the problem. Shuen and Yoon developed a scheme for solving the two-dimensional Navier-Stokes and species continuity equations governing chemically reacting flows that employed an implicit finite-volume time marching LU method.\textsuperscript{66} Details of the derivation of the LU scheme are given in by Shuen, et al.\textsuperscript{66} The approach was attractive because, even though the method was fully implicit, it required only scalar diagonal inversion for solution of the flow equations and diagonal block inversion of the species equations. The authors stated that as a result, the scheme exhibited a fast convergence rate while requiring only about the same amount of work as an explicit method.\textsuperscript{66} This advantage was particularly important when problems with a large number of chemical species were being solved. Following development of the LU code RPLUS using this technique, an eight species, fourteen-reaction chemistry model and an algebraic turbulence model were added to the program. Encouraged by their success, Yu and Shuen then extended the LU code to three-dimensions (RPLUS3D).\textsuperscript{67}

With the exception of Flux Corrected Transport, the methods described in the previous paragraphs have exhibited second-order numerical accuracy in both space and time. Two high-order accurate methods were also developed and applied to high-speed combustion problems. These methods offer improved accuracy and reduced phase error. One method was developed by Carpenter using a fourth-order compact finite-difference scheme.\textsuperscript{33} The scheme was initially developed by Abarbanel to accurately solve the Euler equations in two- and three-dimensions.\textsuperscript{68} Carpenter extended these ideas to the Navier-Stokes equations and used them to alter the 1969 MacCormack method, producing a fourth-order “compact MacCormack” scheme. The modifications did not change the basic structure of the MacCormack scheme, allowing it to be easily incorporated into existing codes using the 1969 algorithm. The modification significantly improved the accuracy of the algorithm, while markedly reducing the phase error. As a result, the improved scheme was able to crisply capture strong shocks with very little of the pre- and post-shock oscillations present in the old scheme. The algorithm in fact exhibited a TVD like behavior when capturing waves.

High-order accurate spectral methods were also applied to supersonic reacting flows. Drummond extended a Chebyshev spectral method developed for studying transitioning flows\textsuperscript{69,70} to include finite rate chemical reactions.\textsuperscript{71} To apply this method to the Navier-Stokes and species continuity equations, the flux terms in these equations were expanded in terms of Chebyshev series, and then the required spatial derivatives were taken. The resulting ordinary differential equations were then integrated with respect to time using a Runge-Kutta time stepping scheme. Drummond initially developed this technique for the one-dimensional Euler equations and species continuity equations.\textsuperscript{71} The method was then extended to multiple dimensions where a hybrid spectral-finite difference algorithm was used to model two-dimensional supersonic reacting flows.\textsuperscript{72}

Many of these high-speed code development activities reached some degree of maturity toward the end of the NASP era, but much work remained. In the late 1980s and early 1990s, the NASP program began to contract, although it was sustained for several years by a technology development program. This program allowed some of the more fundamental activities that we have discussed to continue, including computational and flow diagnostic development, and flow path research. Absent however was the all important flight program that either needed to be underway or at least planned for the near future. A flight program is the catalyst that drives technology development and synthesizes all of the efforts into a unified tool for development of the ultimate experiment, the flight of a hypersonic vehicle. Hypersonics research has gone through several cycles in the United States over the past 60 years. Fortunately the NASP program was followed in the next few years by another “cycle,” the Hyper-X flight program. The “run-up” to Hyper-X sustained the fundamental computational, diagnostic and experimental programs allowing them to mature to the supporting role that was required for a successful flight program.

III. Hyper-X and a New Generation of High-Speed Reacting Flow Codes for Scramjets

Following more than 40 years of ground-based scramjet research and testing, a strong consensus developed in the hypersonic propulsion community for moving air-breathing technology from ground facilities to flight. Even though much had been achieved in ground-based facilities, it was impossible to duplicate the complexities of hypersonic flight without flying in the atmosphere. From this recognition, the Hyper-X Project evolved in late 1995 as a joint effort of the NASA Langley and Dryden Research Centers.\textsuperscript{53,74} The program was planned to utilize a 12 foot hypersonic vehicle with a scramjet propulsion system to be launched from a B-52 aircraft and accelerated to hypersonic speeds by a Pegasus rocket. The stack (the Hyper-X aircraft and the rocket) was carried under the wing of the B-52 as shown in...
A layout of the Hyper-X vehicle is given in Figure 3. The vehicle was 148 in. long and 60 in. wide at the maximum extent between the tail fins. The scramjet propulsion system was 30 in. long and 19 in. wide. For flight, the vehicle was flown to around 40 thousand feet and then dropped from the carriage beneath the wing of the B-52. The Pegasus rocket was then ignited to boost the vehicle to around 95 thousand feet. At that altitude, the rocket and vehicle were separated, and the scramjet engine was ignited allowing the vehicle to cruise under its own power. Two successful Hyper-X flight tests at Mach 7 and Mach 10 were flown in March and November of 2004.

The Hyper-X Program brought a resurgence of effort in hypersonics including wind tunnel and flow path testing and more fundamental work in measurement diagnostics, chemical kinetics and non-reacting and reacting flow simulation and modeling. We will concentrate in this paper on the code development and modeling activities.
Much of the early work associated with the Hyper-X Program was fundamental in nature. As a consequence, the development of new combustion codes tended to focus on capabilities for detailed analyses of the engine flow field. Computer resources were still limited, but by constraining analyses to critical regions of the scramjet, reasonable analyses were possible. Codes were developed to study the fuel injection process and the mixing and combustion of fuel and air downstream of injectors. Detailed fuel injector design was also considered in order to enhance fuel-air mixing and enable the highest level of mixing and combustion efficiency.

Hyper-X was a flight program, however, and understanding critical regions of the engine flow field was extremely important, but only part of the problem facing researchers. The overall engine flow path had to be designed, and that design depended on both experimental research and computational analyses. Ground based facilities, where the experimental work was conducted, functioned in the lower Mach number range of the vehicle and were expensive to operate. Computational tools were needed to establish initial designs for testing and to fill in the regions between test points in the facilities. As a consequence, code development forked in two directions with one branch continuing along theoretical grounds and the other concentrating on the development of design codes. The development of these codes over a number of years produced many of the programs in use today for both fundamental studies and design codes. Some of the codes in fact served both purposes. We will trace the development of these codes for the remainder of this paper. Program development that was initiated to create codes for commercial use will not be considered in this paper. In addition, not every code capable of simulating high-speed reacting flows will be discussed, but the author will attempt to cover every class of code that is capable of performing these analyses.

One of the first efforts to develop a code for scramjet development began in 1987. The GASP code solved the steady and unsteady Euler, parabolized Navier-Stokes, thin-layer Navier-Stokes, and Navier-Stokes equations. It utilized as options preconditioning, approximate factorization, line Gauss Seidel, Generalized Minimal Residual, mesh sequencing and multi-grid. Inviscid flux definition in GASP utilized several options, including Roe’s and Van Leer’s upwind biased formulations and central differencing with artificial viscosity. Central differences were used to define viscous fluxes. Both algebraic and two-equation turbulence models with wall function options were used in the code. Generalized zonal-boundary interpolation was used across zonal intersections defined by a single logical boundary. Parallel processing was employed on shared memory computer architectures. A set of thermochemical kinetic models was provided for air chemistry, hydrogen-air combustion, and various hydrocarbon reactions in a database containing 455 reactions and 34 species. Thermal nonequilibrium was modeled using a separate vibrational temperature for each molecule or a lumped vibrational temperature common to all molecules. GASP was validated for a number of external and internal flow fields. The code was then employed to analyze the external flow fields about a number of hypersonic vehicles and high-speed engine flow paths.

Another initial effort to develop a new code for scramjet flow path design was undertaken at the NASA Langley Research Center. The LARCK code development project began in the early 1990s as a replacement for the SPARK combustion code. The program that evolved was a cell-centered, finite volume, multi-block, multi-grid, code to solve the full Reynolds averaged Navier-Stokes (RANS) equations for turbulent non-equilibrium chemically reacting flows. The code contained a generalized thermodynamics model for an arbitrary mixture of thermally perfect gases and an Arrhenius based finite-rate chemistry model with a generalized scheme that allowed for the specification of any chosen reaction model. Turbulence models included the Spalart-Allmaras model, the Wilcox high and low Reynolds number $k - \omega$ models, Wilcox’s compressible pressure gradient corrected wall matching procedure, Menters baseline and SST models, and the algebraic Reynolds stress models of Abid and Adumitroaie. Coupling between the turbulence and chemistry fields was also accounted for with Gaussian or beta assumed probability density functions to account for temperature variance effects on forward and backward kinetic rate coefficients in the chemistry model. Turbulence effects on the species production rates were also accounted for by modeling the sum of the species variances using a multivariate assumed probability density function. The LARCK code was validated against a number of 2-D and 3-D unit problems such as the flat plate flow, high Mach number compression ramp flow, and Mach 3 corner flow. It was then used to model individual scramjet component flows as well as the entire flow path in a scramjet engine.

The LARCK code served as a predecessor for another new analysis code for high-speed flows that has become a standard for simulating external and internal flows even to the present day. A program to develop the VULCAN code began in 1996 as a part of a ramjet-scramjet CFD code development effort at the Wright Patterson Air Force Base. The foundation program was developed at that time under an Air Force contract. The next year, the program development effort moved to the NASA Langley Research Center, and work has continued at the Center until the present day. Like its predecessor the program solved the equations governing two- and three-dimensional calorically perfect or thermally perfect non-equilibrium chemically reacting flows. The code used a structured grid, cell centered, finite volume, density based method. Inviscid fluxes were computed to second order accuracy using van Leer’s MUSCL scheme with either the flux difference split scheme of Roe or the low dissipation flux split scheme of Edwards. Viscous fluxes were computed to second order accuracy using either a thin layer gradient or full gradient construction. The full spatially elliptic Euler or full Navier-Stokes equations were solved by integrating the conservative form
of the unsteady equations in real or pseudo-time (where only a steady-state solution is desired). Time-derivative preconditioning allowed the code to be applied to low speed flows even though it had been primarily developed for high-speed regimes. In addition, the code could solve the spatially hyperbolic Euler or parabolized Navier-Stokes equations. By using a four level hierarchy of domain decomposition, grouping finite volume cells into blocks and blocks into regions, an entire physical domain could be discretized into a computational domain (the fourth level) for analysis.

Chemical reaction was modeled in the VULCAN code using a generalized Arrhenius based model. Any number of reactions in an overall reaction mechanism could be considered. Global reaction models were often considered where possible to reduce the number of chemical reactions and species being solved. Mean flow turbulence models used in the code included the $k - \epsilon$ and $k - \omega$ models previously used in the LARCK code as well improved turbulent kinetic energy models that were being developed in parallel with VULCAN. Interactions between the turbulence field and chemistry were modeled with an assumed beta probability density function (PDF) to account for the effects of temperature fluctuations on chemical reaction rates and a multivariate assumed beta PDF to account for the effect of species fluctuations on species production. However, the statistical dependence among the scalars was not accounted for by these models.

One of the first uses of the VULCAN code was the investigation of advanced fuel injection schemes for scramjet engines. The code was used to evaluate the cold flow mixing effectiveness of two fuel injection schemes, a ramp injector and a strut injector, being considered for new scramjet designs. The two injector designs are shown in Figures 4 and 5. Helium was used as the fuel simulant. Cold flow simulations were conducted for each design. The grid system for each configuration is shown in Figures 6 and 7. Mass fraction contours from the simulations for both configurations are shown in Figures 8 and 9. The authors note “the effect of streamwise vorticity generated along the sides of the ramps is clearly evident in the fuel plume at the 4-inch cross stream plane. A relatively strong oblique shock is formed in the next 4-inch segment of the combustor through the interaction of the incident ramp shocks and the underexpanded jets. This shock wave turns the fuel plume towards the center of the combustor. The fuel and air mixing from this point onward is primarily driven by turbulent diffusion. Streamwise vorticity for the ramp injectors is
generated by the “spillage” of flow from the high pressure region above the ramps to the low pressure region between the ramps. The situation is reversed for the strut injectors. A high pressure region exists between the struts due the
the swept leading edges driving the flow over the top of each strut creating a streamwise vortex. The interaction of this vortex with the uppermost fuel injectors is clearly evident in the cross stream planes. The lip shock generated near the top of the fuel injector interacts with the reattachment shock (a small rearward facing step exists at the strut injection plane) to produce an oblique shock wave just upstream of the 4-inch cross stream plane. These oblique shocks (one near the top wall of the combustor and one near the bottom wall) interact near the center of the combustor driving the fuel away from the combustor walls. As with the ramp configuration, the mixing from this point onward is rather slow and diffusion dominated. The shock structure for each configuration is illustrated in the pressure contours of Figures 10 and 11. As discussed above, the shock structure of each configuration is extremely complicated and strongly influences the fuel distribution throughout the combustor."

The total pressure recovery and mixing efficiency of the two configurations is given in Figure 12. The $x = 0$ station is the fuel injection plane. The authors note that in the total pressure recovery comparison, "the shock structure generated by the struts upstream of injection introduces a larger total pressure loss than does the shock structure of the ramp configuration. The blockage of the strut configuration is approximately 30% more than the ramp configuration which explains the larger total pressure loss initially. However, by the end of the combustor, the total pressure recovery is practically identical for both configurations. The mixing efficiency comparisons show the strut configuration significantly outperforms the ramp configuration with respect to mixing. Preliminary experimental values (reported in the paper) for the total pressure recovery at the 12 and 24 inch stations for the ramp injector configuration were measured as 0.44 and 0.38, respectively. The CFD results compare very well with these values."

Calculations of the type illustrated here are critically important to scramjet engine design, and they are representative of the many calculations conducted for Hyper-X. The calculations can be carried out relatively quickly and provide design data that can then be tested experimentally on the way to a final design. Arriving at the final configuration using only experimental research would be a much more costly and time consuming exercise.

Work on the VULCAN code for the past 10 years has focused on continuing algorithm improvements and the addition of large eddy simulation (LES) capabilities, also enabling LES/RANS simulations. Steady-state Reynolds-averaged Navier-Stokes simulations with VULCAN and a number of other combustion codes have been and are currently employed for scramjet engine development. Such an approach is not without significant limitations, however. The required turbulence and combustion models have not significantly advanced in the past 20 years, and modelers must rely on experimental data and intuition to validate these phenomenological models. An excellent review of the modeled equations that are typically solved and the models needed to close the equations was given by Baurle. The limitations introduced by the models have resulted in the move to higher-order modeling including LES and PDF methods.

Higher-order modeling allows the governing equations to be closed at a higher level, reducing or alleviating many of the limitations imposed by the lower order models used in RANS. LES attempts to resolve the large-scale structures in a flow while only modeling the smaller scales. On the order of 90 percent of the transport of mass, momentum and energy is accomplished by the large scale eddies, and modeling is only required for dissipative small scales. In addition, the dissipative scales are more universal in nature, and therefore, more readily modeled. But along with its stated advantages, LES is computationally expensive, particularly for regions of the flow field near walls. It is for these reasons that a hybrid method of analysis, utilizing LES in interior flow regions of a propulsion system and RANS near engine walls, appeared so attractive.

A LES/RANS capability was added to VULCAN around 10 years ago. LES/RANS analyses have been utilized many times since this addition was made. Major issues for the inclusion of the capability included the methods for blending the RANS and LES model equations, control of excess dissipation and the treatment of inflow and outflow boundary conditions in LES regions of the flow. Two methods were utilized to accomplish the blending of the evolving RANS and LES solutions. The first method used a strategy termed Limited Numerical Scales, introduced by Batten, et al. to blend the length-scale — velocity-scale product affecting turbulent viscosity levels and reduce the RANS stresses in LES regions of the flow. The second blending strategy utilized the method of detached eddy simulation proposed by Spalart where the RANS modeled equations are used near solid surfaces where the flow is attached, and the LES equations are used for separated or detached flow regimes. The original model was built around the Spalart — Almara's one-equation model with blending accomplished by altering the length scale in the destruction term of the turbulence transport equation. The detached eddy simulation approach for blending was later altered to utilize the two-equation $k − \omega$ model of Menter using a formulation by Strelets. Details regarding the blending strategy as well as the control of dissipation and the specification of boundary conditions in LES regions are given by Baurle.

Several publications have resulted from LES/RANS analyses utilizing the VULCAN code. A considerable amount of work to perform LES/RANS analyses has also been conducted with other codes. An interesting LES/RANS simulation of a supersonic coaxial jet experiment was performed using the VULCAN code. The results are typical of other LES/RANS simulations such as those cited above in the references. The experiment was designed to study compressible mixing flow phenomena under conditions that are representative of those encountered in scramjet combustors. In the study, a LES/RANS simulation was compared with a RANS simulation to gather insight into the deficiencies of the Reynolds-averaged closure models. We will examine only the LES/RANS solution in this paper and leave it to the reference if the reader is interested in the comparison of the LES/RANS and RANS
A schematic of the coaxial nozzle assembly is shown in Figure 13. The center jet flow was either a mixture of 95% helium and 5% oxygen (by volume) or pure argon. A small amount of oxygen was added to the helium to allow the streamwise component of velocity to be measured using the RELIEF technique. The internal diameter of the center jet nozzle is 10 mm at the nozzle exit. The centerbody that forms the internal nozzle is 0.25 mm thick at the nozzle exit, providing a small blunt base to anchor the shear layer formed between the two nozzle streams. The coflow air nozzle has an internal diameter of 60.47 mm, and the outer surface of this nozzle extends 12.66 mm downstream of the center-body. The 38.6 deg juncture between the internal surface of the coflow nozzle and the conical exterior surface is sharp. Hence, there is no appreciable base region to segregate the outer jet flow from the surrounding ambient air. Further details concerning the geometry of the rig, and the methodology used for its design and instrumentation can be found in the reference.

The flow conditions for the two experiments are given in Tables 1 and 2. The nozzle streams are matched at a Mach number of 1.8. The flow velocity differs significantly, however, with the helium jet velocity more than twice that of the coflow jet and the argon jet velocity around 16% lower. The convective Mach number is around 0.7 for the helium case and 0.16 for the argon case. Therefore compressibility effects are present for the helium case, and the argon case behaves more like an incompressible flow.

All computational results for the coaxial jet simulation were obtained with the VULCAN code. Details of the numerical method and physical modeling are described in the reference. An azimuthal slice of the three-dimensional grid generated for the hybrid LES/RANS cases is shown in Figure 14. Details of the highly resolved region around the jet exit are shown in the insert to the figure. A highly resolved grid containing in excess of 43 million cells is utilized.

Table 1: Case 1 - Helium-air test conditions

<table>
<thead>
<tr>
<th>Nominal conditions</th>
<th>Center jet</th>
<th>Coflow jet</th>
<th>Ambient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach number</td>
<td>1.8(a)</td>
<td>1.8(a)</td>
<td>0.025(b)</td>
</tr>
<tr>
<td>Total temperature, K</td>
<td>305.0 (±9)</td>
<td>300.0 (±6)</td>
<td>294.6 (±6)</td>
</tr>
<tr>
<td>Total pressure, kPa</td>
<td>614.93 (±6)</td>
<td>579.80 (±4)</td>
<td>101.325 (±1)</td>
</tr>
</tbody>
</table>

\(a\)Nozzle design Mach number  
\(b\)Value assumed for the entrained ambient flow
An instantaneous image of the flow field for the helium inner jet case is shown in Figure 16. The upper image shows the magnitude of the density gradient (numerical Schlieren) and the bottom image shows the instantaneous normalized helium mass fraction. Significant turbulent structure has been captured in the simulation. The recirculation zone at the base of the inner nozzle exhibits large-scale unsteadiness that triggers Kelvin-Helmholtz instabilities in the region between the coaxial jets. These instabilities transition downstream to a turbulent state. The turbulent structures provide stirring of the helium and air and result in enhanced mixing. The Schlieren image shows unsteady shock and expansion waves that reflect through the jet structure.

Averaged LES/RANS helium mass fraction profiles are compared with experimental measurements in Figure 17. Overall, the predictions indicate a shear layer growth rate that is more rapid than the data indicates. This may have been caused by too low a level of subgrid scale modeled viscosity resulting from model coefficients chosen to promote the onset of flow instabilities. Suggestions for improvements to this situation are given in the paper.

Averaged pitot pressure profiles are compared with the data in Figure 18. Comparisons of the predictions and data also indicate that the jet mixing has been overpredicted at downstream stations. The predictions and data still agree reasonably well, however.

An instantaneous image of the flow field for the argon inner jet case is shown in Figure 19. The upper image again shows the magnitude of the density gradient (numerical Schlieren) and the bottom image shows the instantaneous normalized argon mass fraction. Kelvin-Helmholtz instabilities are again present in the shear layer between the jets, but they persist longer downstream before beginning to break down. The significantly lower level of shear in the shear layer delays the breakdown. As a result the overall level of stirring and enhanced mixing is reduced in this case.

Averaged LES/RANS argon mass fraction profiles are compared with experimental measurements in Figure 20. Overall, the predictions indicate a shear layer growth rate that is less rapid than the data indicates. Averaged pitot pressure profiles shown in Figure 18 also indicate a reduced degree of jet mixing. Again, the predictions and data agree reasonably well.

LES/RANS simulations clearly provide an improvement over RANS simulations. Turbulent structure which is averaged out in RANS simulations can be resolved by LES/RANS. Resolution of this structure results in a better definition of turbulent mixing processes although this definition may not be as accurate as desired. There are several ways suggested by the paper that offer the possibility for improvement in the method and work is continuing to...
incorporate these ideas.

Another activity to develop a program that can be applied to high-speed combustor flows began in 1993. The WIND code is a structured or unstructured compressible Navier-Stokes solver for modeling reacting internal or external turbulent flows. Spatial differencing employs either the Roe scheme, HLLC, HLLE or the Rusanov scheme. These schemes are available with algorithms ranging from first order to fifth order upwind biased schemes for structured grids and first or second order for unstructured grids. For temporal discretization using structured grids, the code can be run in explicit mode using a set of Runge-Kutta methods or implicitly using approximate factorization, Jacobi, Gauss-Seidel and MacCormack’s first order approximate factorization method. For unstructured grids, point-implicit and line implicit methods are utilized. For unsteady time-accurate simulations with both structured and unstructured grids, global Newton time stepping or dual time stepping is used with the implicit second-order schemes. Turbulence is modeled in the WIND code with the well established one- and two-equation turbulent kinetic energy models as well as the Rumsey-Gatski algebraic Reynolds stress model. Chemical reactions are modeled for both structured and unstructured grids using a general finite rate scheme that can be applied to any defined kinetics mechanism. A summary of the development of the WIND code and its current capabilities is given by Nelson along with a number of additional references and applications.

B. PDF Methods

Probability density function (PDF) methods have been used successfully to simulate turbulent reacting flows since the development of the Lagrangian Monte Carlo method by Pope in the mid-1980’s. Many of the applications of the method were related to fundamental studies, but they were later successfully extended to turbomachinery and other practical flows. In the mid-1990s, Pope and his students extended the method to compressible flows by adding the pressure and the internal energy to the conventional velocity PDF formulation that had been applied to incompressible flows. In this approach, the joint PDF of velocity, turbulent frequency, pressure, specific internal energy (or enthalpy) and mixture fraction was solved using a Lagrangian Monte Carlo method. By adding thermodynamic variables as mentioned above to the PDF equation, full closure of the joint PDF transport equation was obtained. Details are given in that reference.

Other groups also began the development of compressible hybrid PDF methods for high-speed reacting flows. In one effort, Hsu, et al. solved the joint PDF of species mass fraction and enthalpy using a Monte Carlo scheme to solve the PDF evolution equation. The procedure was coupled with a compressible CFD flow solver that provided the velocity and pressure fields. The approach was later extended to three dimensions and used to model the flow in a
Finally, the hybrid PDF method was compared with a traditional moment closure method (utilizing laminar chemistry) for an air piloted turbulent diffusion flame near extinction. Comparisons of the hybrid PDF method with data showed the technique predicted a turbulent flame structure with peak mean radial temperatures agreeing with the data. The moment closure method predicted a laminar-like flame structure with peak mean radial temperatures in the wrong location and over predicted by 500 K. Further details are given in the references.

As an alternative to solving an evolution equation for the PDF, other researchers have chosen to assume the mathematical form of the PDF. In one approach discussed earlier with the VULCAN code, interactions between the turbulence field and chemistry were modeled with an assumed beta PDF to account for the effects of temperature fluctuations on chemical reaction rates and a multivariate assumed beta PDF to account for the effect of species fluctuations on species production. Issues associated with cross-correlations of temperature and species, not considered in the previous works, were accounted for using a new assumed PDF approach. The approach was shown to have significant potential as an engineering tool, but further work was also suggested to refine the approach.
Figure 17: Comparison of normalized helium mass fraction with measured values
Figure 18: Comparison of helium pitot pressure with measured values
In our discussion of LES/RANS and PDF methods, we considered the limitations imposed by conventional RANS modeling. PDF methods offer one approach for closing the terms that must be modeled in RANS. LES provides another means for closing these terms while also allowing the large scale features of the flow to be computed rather than modeled. The flow features in the propulsion system of a hypersonic vehicle require this level of analysis. Nik, et al.\textsuperscript{140} summarizes these issues quite well. He notes that “the physics of high speed combustion is rich with many complexities. From the modeling standpoint, some of the primary issues are the development of accurate descriptors for turbulence, chemistry, compressibility, and turbulence-chemistry interactions. The phenomenon of mixing at both micro- and macro-scales and its role and capability (or lack thereof) to provide a suitable environment for combustion and the subsequent effects of combustion on hydrodynamics, are at the heart of hypersonic (and supersonic) physics. From the computational viewpoint, novel strategies are needed to allow affordable simulation of complex flows with state-of-the art physical models. The power of parallel scientific computing now allows inclusion of more complex

C. LES/FDF Methods for High-Speed Reacting Flows

In our discussion of LES/RANS and PDF methods, we considered the limitations imposed by conventional RANS modeling. PDF methods offer one approach for closing the terms that must be modeled in RANS. LES provides another means for closing these terms while also allowing the large scale features of the flow to be computed rather than modeled. The flow features in the propulsion system of a hypersonic vehicle require this level of analysis. Nik, et al.\textsuperscript{140} summarizes these issues quite well. He notes that “the physics of high speed combustion is rich with many complexities. From the modeling standpoint, some of the primary issues are the development of accurate descriptors for turbulence, chemistry, compressibility, and turbulence-chemistry interactions. The phenomenon of mixing at both micro- and macro-scales and its role and capability (or lack thereof) to provide a suitable environment for combustion and the subsequent effects of combustion on hydrodynamics, are at the heart of hypersonic (and supersonic) physics. From the computational viewpoint, novel strategies are needed to allow affordable simulation of complex flows with state-of-the art physical models. The power of parallel scientific computing now allows inclusion of more complex
Figure 20: Comparison of normalized argon mass fraction with measured values
Figure 21: Comparison of argon pitot pressure with measured values
physical phenomena which in turn translates into greatly improved predictive capabilities. It is now widely accepted
that the optimum means of capturing the detailed, unsteady physics of turbulent combustion is via large eddy simula-
tion (LES).141,142 The extension of this approach to actual engine design will certainly require significant additional
development and further enhancements in computer resources. But the potential certainly justifies the effort.

The critical element in successful LES is the accurate modeling of the subgrid scale variables. The filtered density
function (FDF) methodology has been effective in providing this closure.140,143 The filtered density function (FDF)
is essentially the PDF of the subgrid scale (SGS) variables. The idea of utilizing the PDF in LES simulations was
advanced by Givi,144 but it was the formal definition of FDF by Pope145 which provided the mathematical founda-
tion of LES/FDF. Following this significant advancement, a number of successes occurred in the development of the
LES/FDF method.146–149 Analogous to the construction of a PDF of specific flow variables, the FDF can consider
different flow variables in the context of either incompressible or compressible flow. A sequence of steps were taken
beginning with the development of the joint velocity-scalar (temperature, species mass fractions) FDF, the filtered
mass density function (FMDF) and concluding with the most sophisticated closure to date, the frequency-velocity-
scalar FMDF (FVS-FMDF) for incompressible flows.150,151 Work is currently underway to develop the FDF method
to provide for the LES of high-speed compressible turbulent reacting flows by way of an energy-pressure-velocity-
scalar FMDF (EPVS-FMDF). A simple form of this FMDF, the scalar FMDF (SFMDF) has been developed and is
currently being used to model a high-speed mixing flow. Details of the formulation of the method and its application
are given by Nik, et al.140

Using the SFMDF methodology, the LES of the coaxial nozzle assembly of Cutler123 was carried out. A schematic
of the coaxial nozzle assembly is shown in Figure 13. Recall that this is the same case that was simulated by the
VULCAN LES/RANS code earlier in the paper. Only the helium-air case is considered. The flow conditions are
given in Table 1. Computations were performed on a domain spanning 121mm by 50mm by 50mm diameters in the
streamwise (x), cross-stream (y), and spanwise (z) directions, with a Cartesian grid with 158 by 65 by 65 nodes,
respectively. The flow field was initialized to the inlet averaged filtered values. Other details of the computation are
given in the reference.140

Results for the simulations are given in Figures 22 and 23 providing values of the averaged filtered axial velocity,
\( \langle u_L \rangle \) and the averaged mass fraction of the center jet, \( \langle \phi_{He-O_2} \rangle_L \). The over-bar denotes the ensemble average values. Simulation I uses fixed coefficients and simulation II uses a dynamic model as described in the reference.140 By
examining the figures, it is seen that the dynamic model provides better agreement for velocity while the average
helium mass fraction is better predicted using fixed coefficients. The authors indicated that they will revisit the coaxial
jet case with the more sophisticated closures as their development is completed.

![Averaged filtered velocity profiles. - Experiment, – Simulation I, -.- Simulation II](image)

Figure 22: Averaged filtered velocity profiles. - Experiment, – Simulation I, -.- Simulation II
A number of additional cases have been simulated with LES/FDF methods including high-speed mixing and combusting flows. One of these interesting cases considered the LES of turbulent non-reacting and reacting flow in an axisymmetric dump combustor. For the reacting cases, the fuel introduced into the dump combustor was propane at a fuel equivalence ratio of 0.5. Chemistry was modeled with a one-step global reaction mechanism. The LES/FMDF methodology was utilized along with a high-order, structured-grid multiblock with a compact finite-difference numerical scheme. Details are given in the references. The code was first validated against relevant data and then used to simulate a dump combustor. The results were then compared with available experimental data.

A schematic of the experimental setup, the dump combustor, and the computational grid, with an image of its cross-section, is given in Figure 24. The grid is clustered near the walls, in the shear layer that forms off the step and at the inflow location.

Results for the non-reacting case are given in Figures 25 through 27. Figure 25 shows the radial variations of the time-averaged filtered mean velocity at several axial locations obtained by LES with various SGS stress models. Comparisons of the results with data are also shown. $C_d$ in Figure 25 is the Smagorinsky model coefficient. Mean velocities obtained with the Smagorinsky model with the larger coefficient and the RNG model compare reasonably well with the experimental data. Close to the inflow, the dynamic Smagorinsky model gives slightly better results. Figure 26 shows the centerline velocity decay in the dump combustor. The centerline velocity decay was studied in this figure as a function of different grid resolutions and adjusted Smagorinsky model coefficients. Finally, Figure 27 diagrams the instantaneous axial velocity at the $z = 0$ plane and isosurfaces of vorticity magnitude. The turbulent structure that is present in the dump combustor can be readily appreciated in this figure.

Results for the reacting flow cases are given in Figures 28 through 31. The configuration differs somewhat from the non-reacting case due to the addition of an upstream nozzle to allow better definition of inflow boundary conditions. Figure 28 compares the computed radial variations of mean axial filtered velocity with experimental data at four downstream stations. Radial variations of mean filtered temperature are compared with data in Figure 29. The axial velocity compares quite well with the data until the last station where the computation shows more rapid mixing away from the centerline. The predicted temperature agrees fairly well with the data downstream, but overpredicts the upstream data away from the centerline. Two dimensional contour plots of instantaneous filtered temperature and fuel (propane) mass fraction are given in Figures 30 and 31. The temperature contours in Figure 30 indicate high temperatures at and downstream of the step as expected in dump combustor configurations. The turbulent nature of the combustion processes is also quite apparent. The fuel mass fraction contours in Figure 31 show nearly complete consumption of fuel behind the step until about one-third of the axial distance downstream and the turbulent mixing...
and combustion of fuel beyond that station. The mixing and combustion process also penetrates significantly into the fuel core when proceeding downstream from the same station. More comparisons of the simulation results with data and further discussions of the comparisons are given in the reference.  

### IV. Concluding Remarks

This paper discusses the evolution over the past 40 years of computational methods for modeling high-speed reacting flow fields, particularly the flow fields in scramjets and other high-speed propulsion systems. The discussion follows from several hypersonic programs and the flight vehicles that resulted from the programs. The NASP Program and the technology program that followed provided strong motivation for advancing the computational capabilities of the country in both the government and private sectors. While the NASP program was not successful in developing a hypersonic vehicle, it did spawn the development of new computational capabilities. The Hyper-X Program beginning in 1995 revived high-speed computational research and development. This program culminated with the successful
Figure 26: Axial variations of centerline velocity

Figure 27: a) Contours of instantaneous axial velocity at the $z = 0$ plane and b) isosurfaces of vorticity magnitude
Figure 28: Radial variations of mean axial filtered velocity compared with data for reacting case (●, experiment; solid lines, LES)

Figure 29: Radial variation of mean filtered temperature compared with data for reacting case (●, experiment; solid lines, LES)

Figure 30: Two-dimensional contours of instantaneous filtered temperature for reacting case

Figure 31: Two-dimensional contours of fuel mass fraction for reacting case
flight of two hypersonic vehicles in 2004. A flight program is the catalyst that drives technology development and synthesizes all of the efforts into a unified tool for development of the ultimate experiment, the flight of a hypersonic vehicle. The genesis of most of the current day state-of-the-art computational tools for scramjet research and development began with this program. This paper attempts to cover this story from NASP and Hyper-X to the present day. A number of computer programs evolved during this period of time. The programs fell into three classes, including Reynolds-averaged Navier Stokes codes, hybrid Reynolds-averaged—large-eddy simulation codes, and large-eddy simulation codes. RANS/LES codes are evolving into the workhorse codes for scramjet flow path development in this decade, and LES/FDF methodology appears to offer the most promise for work in the future.

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American Institute of Aeronautics and Astronautics


