41st AIAA/ASME/SAE/ASEE Joint Propulsion Conference
Tucson, AZ, July 10-13, 2005

AIAA 2005-4524

CFD Code Validation of Wall Heat Fluxes for a GO_2/GH_2 Single Element Combustor

Jeff Lin*, Jeff S. West†, Robert W. Williams‡ and P. Kevin Tucker§
NASA/Marshall Space Flight Center, Huntsville, AL 35812

James D. Chenoweth**
CRAFT-Tech, Huntsville, AL

This paper puts forth the case for the need for improved injector design tools to meet NASA's Vision for Space Exploration goals. Requirements for this improved tool are outlined and discussed. The potential for Computational Fluid Dynamics (CFD) to meet these requirements is noted along with its current shortcomings, especially relative to demonstrated solution accuracy. The concept of verification and validation is introduced as the primary process for building and quantifying the confidence necessary for CFD to be useful as an injector design tool. The verification and validation process is considered in the context of the Marshall Space Flight Center (MSFC) Combustion Devices CFD Simulation Capability Roadmap via the Simulation Readiness Level (SRL) concept.

The portion of the validation process which demonstrates the ability of a CFD code to simulate heat fluxes to a rocket engine combustor wall is the focus of the current effort. The FDNS and Loci-CHEM codes are used to simulate a shear coaxial single element GO_2/GH_2 injector experiment. The experiment was conducted at a chamber pressure of 750 psia using hot propellants from preburners. A measured wall temperature profile is used as a boundary condition to facilitate the calculations. Converged solutions, obtained from both codes by using wall functions with the κ–ε turbulence model and integrating to the wall using Mentor's baseline turbulence model, are compared to the experimental data. The initial solutions from both codes revealed significant issues with the wall function implementation associated with the recirculation zone between the shear coaxial jet and the chamber wall. The FDNS solution with a corrected implementation shows marked improvement in overall character and level of comparison to the data. With the FDNS code, integrating to the wall with Mentor's baseline turbulence model actually produce a degraded solution when compared to the wall function solution with the κ–ε model. The Loci-CHEM solution, produced by integrating to the wall with Mentor's baseline turbulence model, matches both the heat flux rise rate in the near injector region and the peak heat flux level very well. However, it moderately over predicts the heat fluxes downstream of the reattachment point. The Loci-CHEM solution achieved by integrating to the wall with Mentor's baseline turbulence model was clearly superior to the other solutions produced in this effort.

---

* Aerospace Engineer, ER43, NASA MSFC, AL, 35812.
† Aerospace Engineer, ER43, NASA MSFC, AL, 35812.
‡ Aerospace Engineer, ET12, NASA MSFC, AL, 35812.
§ Aerospace Engineer, ER43, NASA MSFC, AL, 35812.
** Research Scientist, CRAFT-Tech, Huntsville, AL 35754

I. Introduction

UPPER stage engines will be a key element in NASA's new Vision for Space Exploration. Likely candidate cycles for these engines include the expander cycle and tap-off cycle. Both of these cycles need accurate, detailed thermal environment information in the combustion chamber for designs to be produced that result in efficient operation while meeting the durability requirements. Combustor thermal environments are a direct consequence of injector design and operation. Current injector design tools are mostly one-dimensional and empirical. These tools typically focus on performance with the thermal effects included secondarily. The design tool shortcoming forces either component over-design or an extensive, costly test program to reveal and fix serious design issues. Almost 50 years of experience has proven that injector/combustor failures are typically three-dimensional and thus local. As an example, note the severe injector-induced blanching and cracking in a Space Shuttle Main Engine main combustion chamber wall as shown in Figure 1. Given what are sure to be aggressive schedules and tight budgets for Space Exploration engine development, new injector design tools are needed to help reduce both the development time and cost for the combustion devices.

It is well known in the aerospace propulsion community that small changes in either the injector element or the entire injector itself can have large effects on both performance and thermal environments.[1] Given this circumstance, what then are the key requirements for a new design tool that promises robust designs in a shorter time and at a lower cost than can be had with the empirical tools currently in use? First, the new tool must be able to calculate injector performance and environments as a function of the details of injector design and flow physics. This aspect of the tool requirement is designated as solution fidelity. Secondly, the tool must be robust enough to complete simulations of the required fidelity in large numbers during the early stages of the design phase. The third requirement is accuracy. The new tool must be quantitative and the accuracy level demonstrated to ultimately be useful.

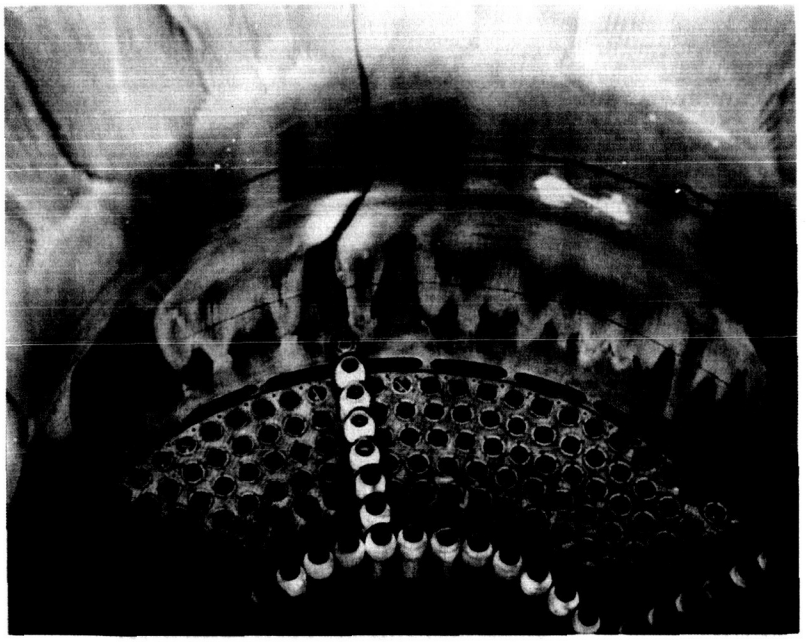

Figure 1. Blanching and cracking—evidence of multi-dimensional environments in a combustion chamber.

A. The Promise of Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) holds great, but to date largely unfilled, promise to be able to meet these requirements. In spite of the schedule and budget realities, injector designers hold to their legacy tools while rightly pointing out that the CFD solutions are too time consuming and are of questionable accuracy. NASA Marshall Space Flight Center (MSFC) has developed the Combustion Devices CFD Simulation Capability Roadmap for advancing CFD from the current state of occasional use in the design of combustion devices to the primary design tool.[2] Injector design is a key component of combustion device design and is thus the initial focus of the Roadmap execution. The MSFC Roadmap uses the notion of Simulation Readiness Level (SRL) to evaluate capability of CFD calculations on given model problems. The model problem concept, also from the MSFC Roadmap, represents the decomposition of a large complex system; here a rocket engine thrust chamber assembly, into smaller, simpler parts. Model problems for this system would include, but not be limited to, both single- and small multi-element injectors. The SRL is based on the three design tool requirements noted above. Quantified levels of solution fidelity, robustness and demonstrated accuracy which comprise the SRL are shown in Table 1. The three SRL components

are related and all require considerable attention in the task of readying CFD as an injector design tool. However, the validation focus of this paper limits the discussion to accuracy demonstration.

Table 1. Simulation readiness level component description.

Level	Fidelity	Robustness	Accuracy
0	Extremely simple physics, boundary conditions and geometry	Have not completed any simulations	Not evaluated except for historical accuracy of tool (verification)
1	One of reasonably precise geometry, boundary conditions or physics	Have complete some solutions	Qualitative agreement with existing results of related problems
2	Two of reasonably precise geometry, boundary conditions or physics	Simulations with proven convergence and conservation	Quantitative agreement with existing results of related problems
3	Reasonably precise physics, boundary conditions and geometry	Simulations with proven convergence, conservation and grid independence	Qualitative agreement of relevant measures over a parametric space of a representative model problem
4	Reasonably precise physics, completely precise boundary conditions and as-built geometry	Fire and Forget (95%+ success rate) simulations with convergence, conservation and grid independence	Quantitative agreement of relevant measures over a parametric space of model problems
5	Completely precise physics, completely precise boundary conditions and as-built geometry`	Fire and Forget (95%+ success rate) simulations with convergence, conservation and grid independence plus ability to complete 100 solutions in 3 weeks	Quantitative agreement of relevant measures over a parametric space for the actual problem

B. The Path to Confidence in the CFD Results—Verification and Validation

If CFD is to be used as an injector design tool, code developers and code users must deal with a critical issue: How should confidence in simulations and modeling for design be critically assessed, and, where necessary, improved? Oberkampf et al [3] provide an insightful discussion of the issue in a report that presents their view of the state of the art in verification and validation. They note that verification and validation of computational simulations are the primary methods for building and quantifying this confidence.

Two model definitions help to facilitate the discussion. The conceptual model is composed of the PDEs for conservation of mass, momentum and energy along with auxiliary equations such as turbulence models and all of the initial conditions and boundary conditions of the PDEs. The computerized model is the computer code which implements the conceptual model. Oberkampf et al employ formal definitions of verification and validation to help make their arguments. *Verification* is defined as the process of determining that a model implementation accurately represents the developer's conceptual description of the model and solution to the model. *Validation* is defined as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended use of the model.

Verification deals with the fidelity between the conceptual model and the computerized model. Validation deals with the fidelity between the computerized model and experimental measurements. Verification is the first step in the overall validation process. It effectively provides evidence that the conceptual model is solved correctly by the discrete-mathematics computer code. Validation provides evidence for how accurately the computerized model simulates reality. According to Roache, [4] verification deals with mathematics and validation deals with physics.

Verification is the process which identifies, quantifies, and reduces errors in the computational model and its numerical solution by comparing the code with various types of highly accurate solutions. Verification results in quantification of numerical accuracy by demonstration. In terms of the MSFC SRL noted earlier, verification results in an accuracy level of 0 for a particular model problem.

Validation is a more complex issue and is actually an ongoing process. According to Oberkampf et al, the goals of validation are to identify and quantify the error and uncertainty in the conceptual models, estimate the error in the computational solution, estimate the experimental uncertainty and the compare the computational results with the experimental data. Because true validation experiments are usually not feasible on complex systems such as a full-scale rocket engine thrust chamber assembly, a building block approach is recommended by Oberkampf et al. This approach divides complex systems into at least three progressively more complex tiers: unit physics problems, benchmark cases and subsystem cases.

The validation using unit physics problems is associated with demonstrated accuracy Levels 1 and 2 from the SRL table, with Level 1 representing qualitative agreement and Level 2 quantitative agreement. The validation using benchmark problems is associated with accuracy Levels 3 and 4 when the benchmark problems address the model problem to which the SRL refers. Validation to Level 5 is done on subsystems of the actual system.

II. Background

The portion of the injector design tool validation process discussed in this paper deals with a shear coaxial single element injector using GO_2/GH_2 propellants. This model problem is probably the simplest injector model problem in terms of geometry and physics. The shear coaxial injector geometry is comprised of two concentric tubes. The H_2/O_2 chemistry is relatively simple and well known. The fact that the propellants are gaseous allows for ideal gas assumptions rather than the much more complex situation with liquid propellants where multiple phases must be simulated. Also, the single element injector model problem allows easier, cheaper and more detailed data acquisition than multi-element injectors. Even though the upper stage cycles noted earlier would use LO_2 as the oxidant, this injector is a good step in the building block approach espoused by Oberkampf et al. There is a current effort directed by MSFC to acquire similar data on a range of injectors using the LO_2/GH_2 propellant system.[5]

The specific aspect of the shear coaxial single element injector with GO_2/GH_2 propellants dealt with in this paper is the heat flux generated from the injector by the burning propellants to the combustion chamber wall. The wall heat flux is an essential validation effort for Space Exploration upper stage engines—and most other engines. The wall heat flux profile also gives an indirect indication of the degree of mixing created by the injector.

It should be noted that this validation step at MSFC is out of sequence in the verification and validation process and thus potentially of less value than it might otherwise be. Little of the Levels 1 and 2 validations on the unit physics problems have been accomplished to provide the foundation for this work. Unfortunately, misconceptions about the importance of the verification and validation process have retarded validation efforts associated with accuracy Levels 1 and 2. Since validation work at the unit physics level is viewed by resource providers as too basic and not connected closely enough to the "real problem", resources are typically not provided for this type of effort. If the MSFC goal of advancing CFD into the forefront of injector design is to be realized, this perception must be changed.

III. Scope of the Current Effort

The current effort is focused on validating selected CFD codes for the prediction of wall heat fluxes. Two CFD codes, FDNS (version 500-CVS) and Loci-CHEM (version 2) are used to simulate a shear coaxial single element GO_2/GH_2 injector experiment. The experiment was conducted at a chamber pressure of 750 psia using hot propellants generated by oxidizer and fuel preburners. A measured wall temperature profile is used as a boundary condition to facilitate the heat flux calculations. Each code was used to calculate the wall heat fluxes by first using a wall function treatment and then by integrating the governing equations to the wall.

The effort presented here was motivated by a transition under way in the Thermal and Combustion Analysis Branch at MSFC. The FDNS code, in use at MSFC for over 15 years, has significant limitations regarding its use as a design tool and is thus being phased out of use at MSFC. FDNS is limited to modeling complex geometries with structured grids, often forcing restrictive geometry assumptions to enable solutions. There is a need to increase the geometric fidelity of calculations by less restrictive assumptions. FDNS also lacks the desired scalability to run efficiently on large numbers of CPUs. Solution robustness, that is the ability to produce many solutions during the design phase, requires efficient code scalability. These issues drive the requirement for modern, efficient, scalable codes. The Loci-CHEM code is one of the codes being developed by MSFC to replace FDNS. So, it is prudent to compare the accuracy of these codes during this transition period.

In the context of this transition, there is the need to evaluate the accuracy of both codes. The accuracy level currently achievable with FDNS must be maintained or improved upon during, and as a result of, the transition to Loci-CHEM. The current effort has three aspects. First, solutions were generated on the same grid using both codes

in the wall function mode. FDNS employed the standard κ–ε turbulence model and Loci-CHEM used Mentor's baseline model (BSL) with a wall function treatment. These results were compared to each other and to the experimental data.

The second aspect of this part of the overall validation process was to compare the accuracy of the two wall treatments. This evaluation was made by generating another solution using FDNS with a finer grid and integrating to the wall using Mentor's BSL turbulence model. Integrating to the wall is considerably more computationally intensive because of the grid spacing requirements in the near wall region, especially for structured grids. This issue, while not paramount for axisymmetric representations of a single element injector in this effort, has significant implications for the required three-dimensional simulations of multi-element injectors.

The third aspect was to evaluate the accuracy of both codes when integrating to the wall. Mentor's BSL turbulence model was chosen for the comparison. Loci-CHEM was used to generate such a solution to compare with the corresponding FDNS solution just noted.

IV. Details of Codes Used

The reasons for conducting this validation effort using both the FDNS and Loci-CHEM codes are outlined above. The FDNS code, with the above-noted limitations, does have some advantages. It has a state-of-the-art real fluids model that allows calculations with liquid propellants.[6] While this model is not used in the calculations in this paper, it will be an important capability for injector simulations for upper stage engines for the Exploration Vision. The Loci-CHEM code, while having many desirable features relating to simulation fidelity (for geometry) and robustness, is still under development. Pertinent code details are given below.

A. FDNS500-CVS

FDNS (version 500-CVS) is a general purpose, multidimensional, multi-species, viscous flow, pressure-based reacting flow solver. It was developed at Marshall Space Flight Center (MSFC) and is continually being improved by NASA/MSFC personnel and its supporting contractors. The code solves the Reynolds-averaged transport equations with a variety of options for physical models and boundary conditions. To solve the system of nonlinear partial differential equations, the code uses a finite-volume method to establish a system of linearized algebraic equations. Several difference schemes are available to approximate the convective terms of the momentum, energy and continuity equations, including central difference,[7] upwind and total-variation-diminishing (TVD) schemes of second and third spatial order.[8]

Viscous fluxes and source terms are discretized using a central-difference approximation. A pressure-based predictor plus multiple-corrector solution method is employed so that flow over a wide speed range (from low subsonic to supersonic) can be analyzed. The basic idea of this pressure-based method is to perform corrections for the pressure and velocity fields by solving a pressure correction equation so that velocity and pressure coupling is enforced, based on the continuity constraint at the end of each iteration.

A seven species, 9-reaction detailed reaction mechanism[9] is used to describe the finite rate, hydrogen oxygen chemistry. Several turbulence models are available to describe the turbulent flow; standard and extended[10] κ–ε turbulence models employing wall functions[11], a low Reynolds number (integrate to the wall) model[12] and three low Reynolds number κ–ω two equation models including the Mentor's baseline model used in this effort.[13]

FDNS is comprised of mostly FORTRAN-77 code and is supported on all popular UNIX variants and compilers. Serial and parallel versions are supported using either PVM or MPI parallel libraries. FDNS500-CVS is moderately scalable; it is able to effectively (with approximately 50% parallel efficiency) use up to 16 CPUs with axisymmetric models of up to approximately 250,000 cells.

B. Loci-CHEM

Loci-CHEM, version 2, is a finite-volume flow solver for generalized grids developed at Mississippi State University in part via NASA and NSF funded efforts. CHEM uses high resolution approximate Riemann solvers to solve finite-rate chemically reacting viscous turbulent flows. Details of the numerical formulation are presented in the CHEM user guide.[14]

As opposed to FDNS, Loci-CHEM is a density-based computational fluid dynamics algorithm. A preliminary implementation of preconditioning is available, yet has the limitation of not being robust for chemically reacting flows and is thus not used in the calculation presented here. Preconditioning methods for chemically reacting flows are being actively researched in the continuing development of Loci-CHEM.

Various chemical reaction mechanisms are available, including the model described in the previous section for FDNS500-CVS. Several turbulence models are available, including the Spalart-Allmaraas one equation model and a family of three $\kappa-\omega$ models corresponding to those mentioned in the previous section on FDNS500-CVS.

Loci-CHEM is comprised entirely of C and C++ code and is supported on all popular UNIX variants and compilers. Parallelism is supplied by the Loci[15] framework which exploits multi-threaded and MPI libraries to provide parallel capability. Loci-CHEM is quite scalable; it is able to very efficiently (with approximately 90% parallel efficiency) use up to 64 CPUs on axisymmetric models of up to 250,000 cells.

V. Experiment Modeled

The calculations presented in this paper are based on the experiments of Santoro and Pal[16] performed at the Pennsylvania State University's Cryogenic Combustion Laboratory (CCL). The purpose of the experimental effort was to characterize the chamber wall heat flux for a single element injector using gaseous oxygen and gaseous hydrogen as propellants with the focus on providing benchmark quality data for CFD code validation.

A chamber heavily instrumented for wall temperature and heat flux measurements was specifically designed and fabricated to achieve this goal. The instrumentation consisted of arrays of Gardon type heat flux gauges and coaxial thermocouples. A schematic of the injector configuration including instrumentation locations is shown in Figure 2. The main chamber has a diameter of 1.5 inches and is 11.25 inches long. The water cooled nozzle has a throat diameter of 0.322 inch. The reference for both the experiment and calculations is x=0 at the injector face.

Experiments were performed on a single element shear coaxial injector. Measurements were made at pressures of 300, 450, 600, and 750 psia for both ambient temperature propellants and hot propellants. For the hot propellant cases, the oxygen is run through an oxidizer-rich preburner (OPB), and the hydrogen is run through a fuel-rich preburner (FPB). A photograph of the test rig can be seen in Figure 3. For the present calculations the 750 psia, hot gas case was chosen for code comparison. A summary of the flow conditions for this case can be found in Table 2.

Table 2. Experimental conditions for the 750 psia case.

Pc = 750 psia	GO_2	GH_2
Temperature (K)	767.54	798.09
Mass Flow Rate (lb_m/sec)	0.1994	0.0730
O_2 Mass Fraction	0.9462	0.0
H_2 Mass Fraction	0.0	0.4130
H_2O mass Fraction	0.0538	0.5870

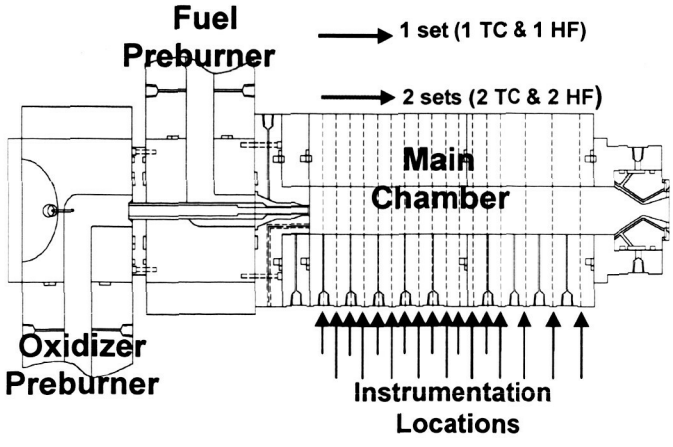

Figure 2. Schematic of experimental set-up.

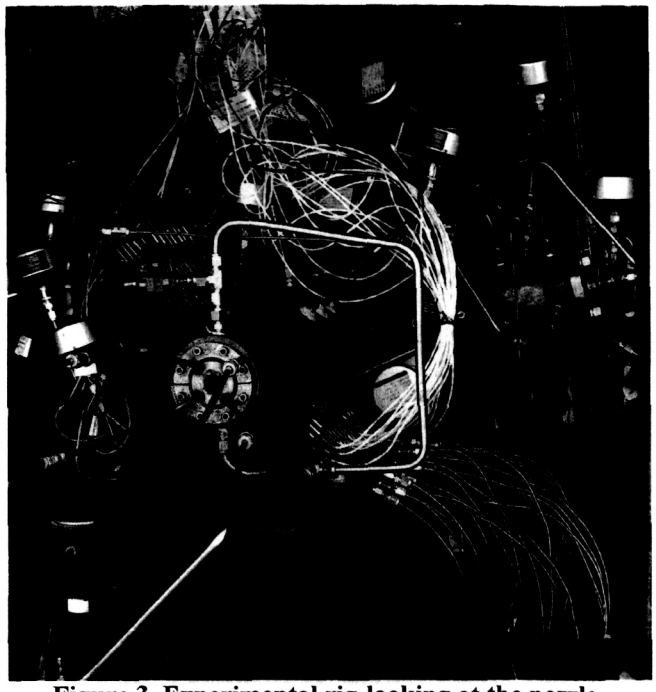

Figure 3. Experimental rig-looking at the nozzle

VI. Computational Models

An effort was made throughout the study to perform the calculations in such a way that the results would be directly comparable and solid conclusions could be drawn from those results. This ground rule was enforced as much as possible in the grid generation, boundary condition specification, flowfield initialization, code set up (including turbulence model selection), job execution and convergence criteria used. This section documents those details of the effort.

A. Grids, Boundary Conditions and Flowfield Initialization

Two grids were used in the effort; a coarse grid for the wall function simulations for both codes and a finer grid for the simulations in which both codes integrated the equations to the wall. The fine grid is shown in Figure 4 for illustration. Both grids were generated with GRIDGEN V15 from Pointwise Corporation.[17] the entire domain from injector inlet to nozzle exit, is shown on top, while a closer view of the injector is shown on the bottom. A comparison of the grid spacing in the nozzle inlet region of two grids is shown in Figure 5. The coarse grid, used for the simulations with wall functions has 61,243 grid points. The near-wall spacing between the chamber wall and the first point from the wall is 0.05 with an initial stretch rate ranging from 1.06 to 1.1. The fine grid, used for the simulations where the equations were integrated to the wall, has 117,648 grid points. The near-wall spacing between the chamber wall and the first point from the wall is 10^{-5} with an initial stretch rate ranging from 1.1 to 1.2. The final grids used in this effort were the result of an iterative effort to achieve certain y^+ values. The y^+ values for all solutions are noted in the Results and Discussion section.

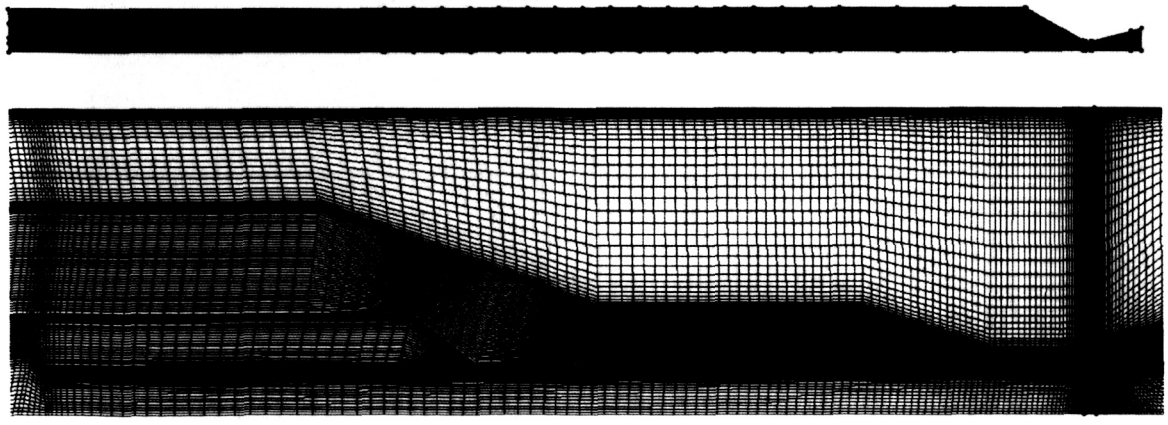

Figure 4. Grid illustration (top-entire domain, bottom-injector detail).

A sketch showing the boundary conditions for all solutions is shown in Figure 6. Both the oxygen and hydrogen inlets are fixed mass flow rate where the velocity is a specified (constant) value to yield the desired flow rate. The inlet walls and post tip are adiabatic, no-slip walls. A temperature profile obtained from the experimental data is

used on the no-slip, chamber wall and is plotted in Figure 7. For the faceplate and nozzle wall an isothermal, no-slip wall condition is imposed with the temperatures being set to the first and last data points from the profile, respectively. The centerline is a symmetry boundary, and the nozzle exit is specified as a supersonic outlet.

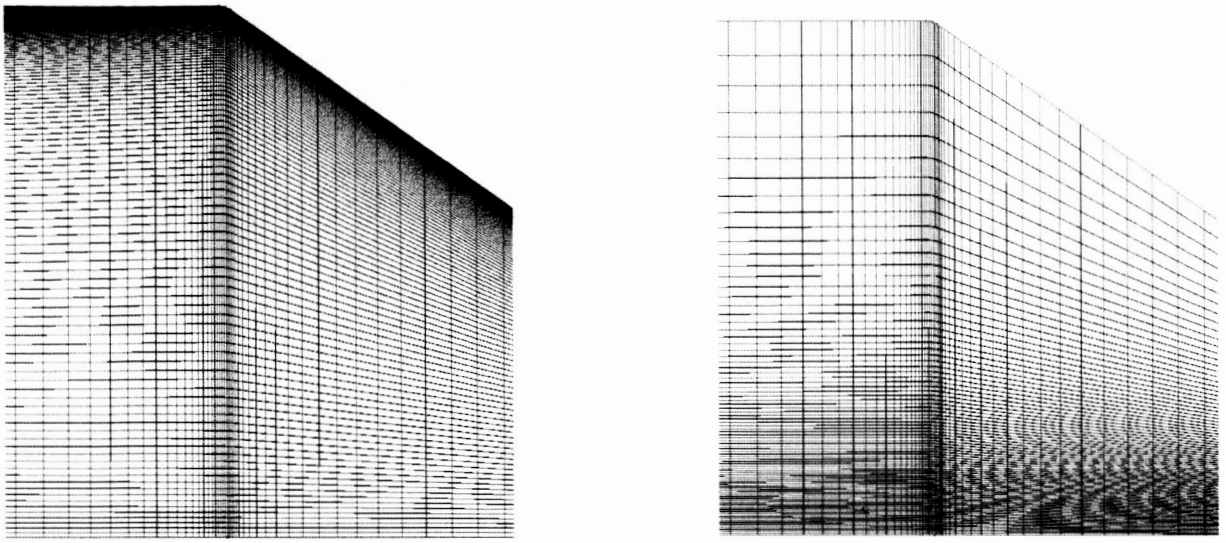

Figure 5. Grid spacing comparison (fine grid on left, coarse grid on right).

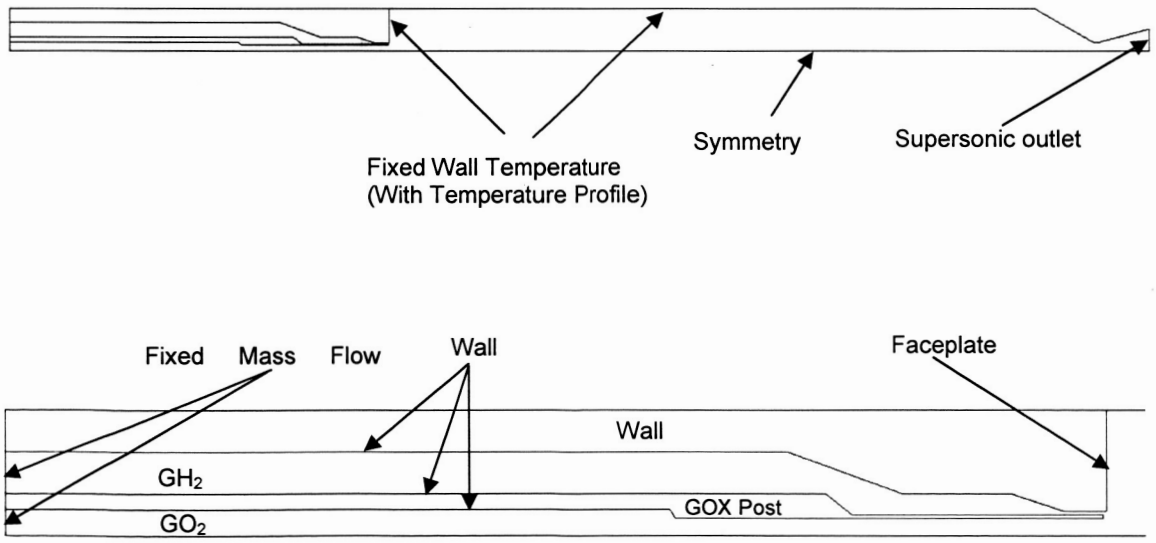

Figure 6. Boundary conditions used in calculations.

The flowfield was initialized similarly for both FDNS and Loci-CHEM. For both cases, the inlets (excluding the inflow plane), chamber and nozzle are filled with quiescent steam. FDNS used steam at 3000 K, and Loci-CHEM used steam at 783 K. For ignition, FDNS had a high enough temperature that self ignition occurred. For Loci-CHEM, a volumetric spark utility was used. This option was turned on for 1000 iterations and then turned off after a reasonably vigorous flame was established.

A third order upwind TVD scheme was used in the FDNS simulations. For stability purposes, FDNS has a parameter which can be varied to average in a percentage of first order differencing. This parameter was set at 10%

for the results shown in this document. For the Loci-CHEM code, a strictly second order, scheme was used with no averaging.

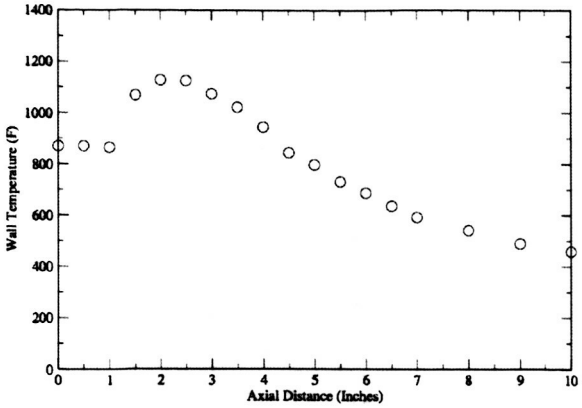

Figure 7. Measured chamber wall temperature profile.

B. Turbulence Models

We chose to restrict the turbulence models used in this study to those based upon the κ–ε model, with various wall treatments. Two models were used with FDNS, the standard κ–ε model in the wall function treatment[7] and Mentor's baseline model when integrating to the wall. Two models were used in Loci-CHEM, the Mentor's baseline model with wall function treatment[13] and Mentor's model with no wall function treatment for simulations where the equations were integrated to the wall. Mentor's baseline model is a blend of the κ–ε model away from the wall and Wilcox's κ–ω model near the wall. As such, the models exercised in both codes can be characterized as κ–ε models with different wall treatments.

C. Convergence Criteria

Solution convergence was evaluated by a combination of residual drop, mass flow convergence (integrated mass at inlet vs. integrated mass outlet), and temperature behavior as a function of solution iteration at selected probe point locations throughout the flowfield.

A sample residual plot from an FDNS solution is shown in Figure 8. While classical residual behavior in not necessarily observed, there is a residual drop of two to five orders of magnitude, with essentially no changes after slightly less than 60,000 iterations. Figure 9 shows the overall mass conservation as a function of iteration. The inlet mass flowrate, 0.2724 lb_m/sec is shown in red and the outlet mass flowrate is shown in green. Mass conservation is typically achieved to levels below 0.1%; here before 60,000 iterations. The temperature from a flowfield probe located near the flame just downstream of the injector post tip is plotted as a function of iteration number in Figure 10. The probe temperature is steady at about 2500K after less than 60,000 iterations. This solution is typical and is deemed to be well-converged.

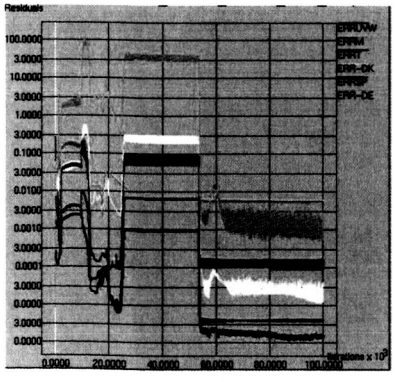

Figure 8. Residuals

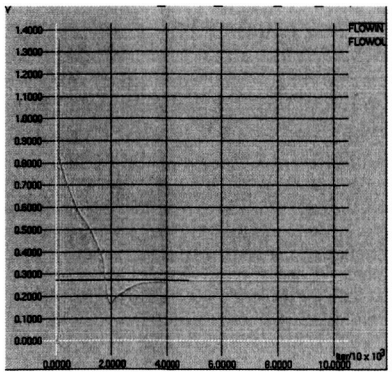

Figure 9. Mass conservation

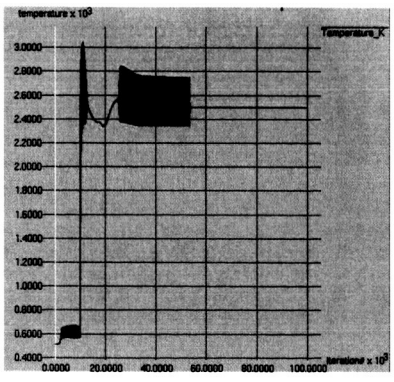

Figure 10. Temperature probe.

VII. Results and Discussion

Figures 11-14 show representative contour plots of the single element flowfield. They are made from the Loci-CHEM simulation accomplished by integrating to the chamber wall and are used here to illustrate the propellant combustion process. (Note only the portion of the chamber containing the flame development is shown.) The temperature field is shown in Figure 11. The 768 K oxygen-rich stream flows toward the chamber in the center tube, while the 798 K hydrogen-rich stream flows in the surrounding annulus. The streams are separated by the oxygen

post. The streams mix and begin to combust in the oxygen post tip wake where the flame holding occurs. The burning shear layer broadens and consumes more of the propellants, as seen in Figures 12 and 13, until all the oxygen is consumed and the flame closes off several inches downstream of the injector face. The resulting water vapor contour plot is shown in Figure 14. A significant feature of the flow is the large recirculation zone between the flame and the chamber wall. Shown in Figure 15, this recirculation zone is over 75% of the flame length. The size of the recirculation zone is a function of the chamber diameter, which at 1.5 inches, is actually too large for this single element injector. The space between the flame and the wall is larger than in actual multi-element combustion chambers. This oversized recirculation zone dominates the flowfield. Since it is not actually representative, its presence clouds to some degree the data interpretation and the calculation to data comparison.

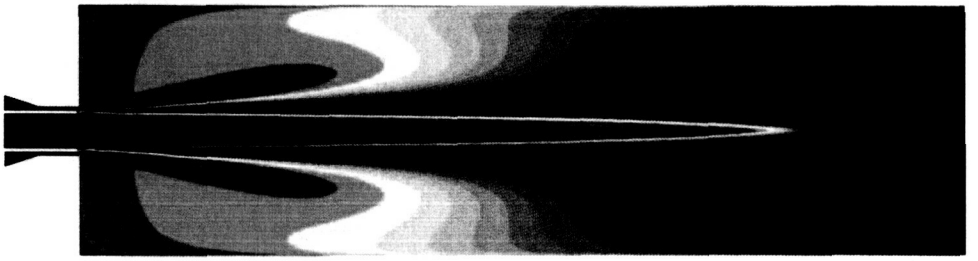

Figure 11. Single element temperature contours.

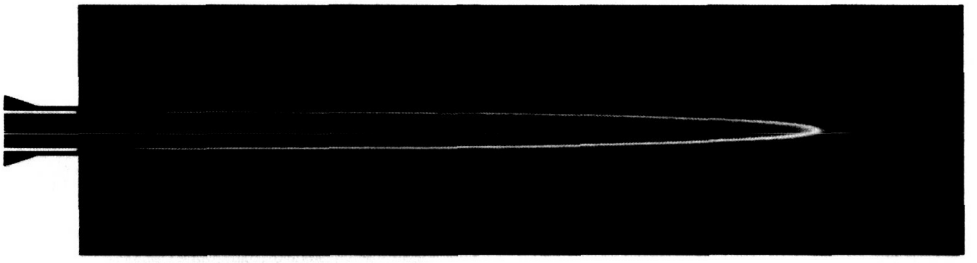

Figure 12. Single element oxygen contours.

Figure 13. Single element hydrogen contours.

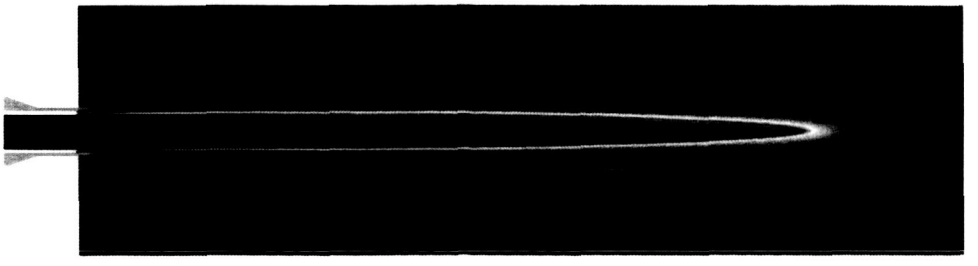

Figure 14. Single element water vapor contours.

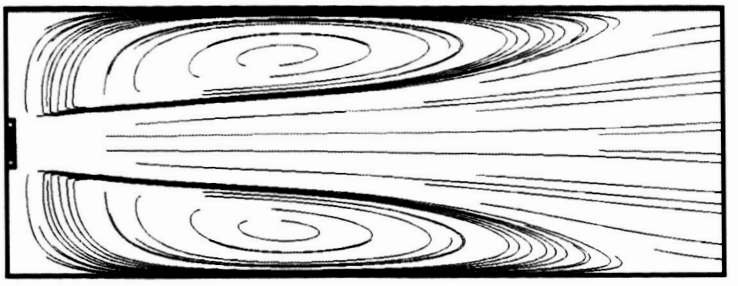

Figure 15. Streamline in the recirculation zone.

A. Results with Wall Functions for FDNS and Loci-CHEM

Initial calculations with the wall function treatment were accomplished with the original implementation of the wall functions, using the standard κ–ε turbulence model in FDNS and Mentor's baseline model in Loci-CHEM. The same grid was used for calculations with both codes. Figure 16 shows the resulting y^+ values plotted as a function of axial distance for both codes. For the wall function treatment in FDNS, the y^+ value should be above about 45 since there is no damping function in the near wall region. For FDNS, the y^+ requirement is generally met except in the regions with very low or no velocity; i.e. the corner between the injector face and chamber wall and at the reattachment point. The wall function implementation in Loci-CHEM is such that at y^+ values above 0.01, the wall function is used, while the code switches to a low Reynolds number turbulence model below this threshold. This presents no practical limitations for the Loci-CHEM code in terms of y^+ requirements. Results from the initial calculations are shown compared to the experimental data in Figure 17. The results are very similar for both codes. The predicted heat fluxes rise very slowly, under predict the experimental peak heat flux by about 70%, go to almost zero at the reattachment point and rise gradually to the level of the data by the 10 inch location where the last measurement is made.

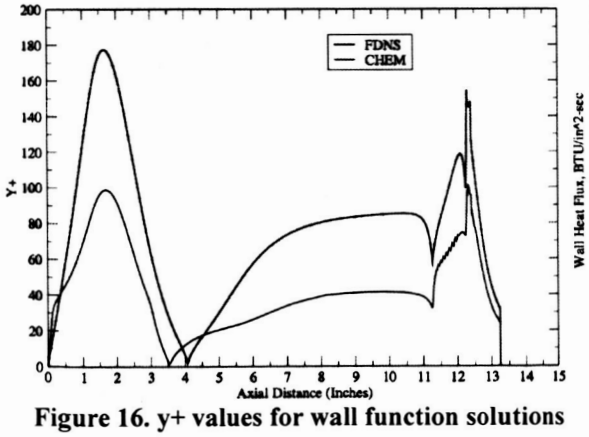

Figure 16. y+ values for wall function solutions

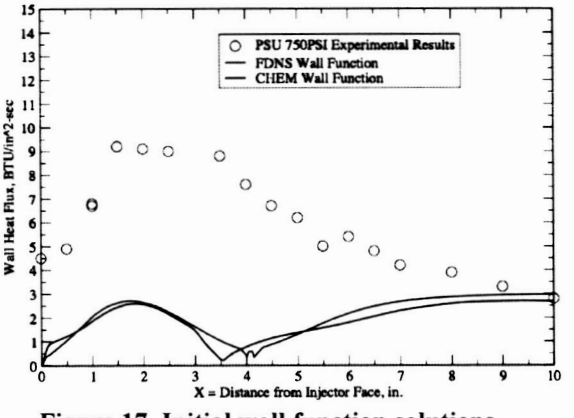

Figure 17. Initial wall function solutions.

A wall function modification was made in the FDNS code to account for the calculation of zero shear stress at the reattachment point. Results from the FDNS calculation made after the wall function modification are shown in shown in Figure 18 and are compared to both the results from the original wall function implementation and experimental data. After the modification, the results are considerably improved when compared to the data. First, the character of the calculated solution is more like the data. The heat flux rise rate is steeper, there is no dip to nearly zero at the reattachment point and the calculation matches the data well from about five inches downstream of the injector to the last data point taken at 10 inches from the injector. However, the peak heat flux level is under predicted by about 35% according to the data. The two pieces of information most useful to designers are the heat flux rise rate and the peak heat flux level. Clearly, the level of agreement with the data is not acceptable in either case.

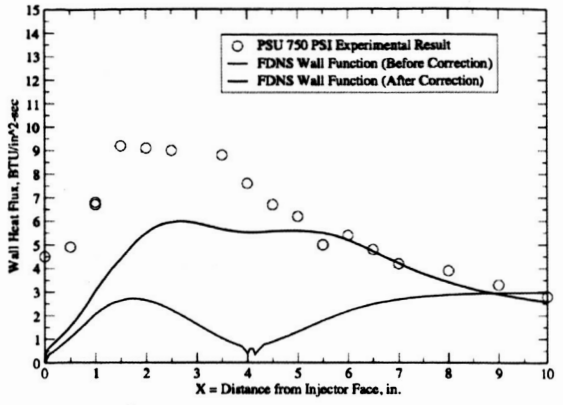

Figure 18. Wall function solution comparisons

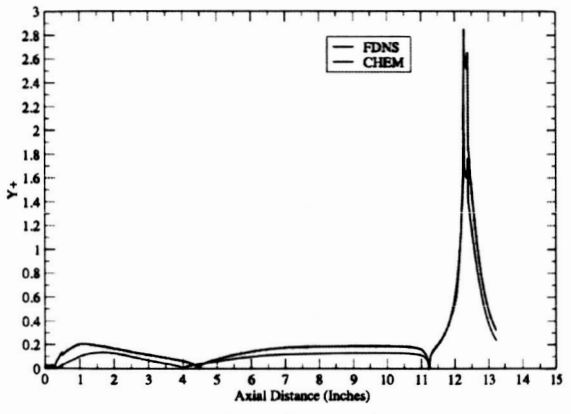

Figure 19. y+ values for the integrate to the wall solutions.

B. Results Obtained by Integrating to the Wall with FDNS and Loci-CHEM

Next, solutions were obtained from both codes by integrating to the wall. A new, finer grid was generated to accommodate the near wall grid spacing requirements. This grid, used to obtain solutions from both codes, was shown earlier in Figure 4. It has 117, 648 grid points with the first point off the chamber wall located at 10^{-5} inches from the wall. The y^+ values from both solutions are plotted in Figure 19 as a function of axial distance from the injector. In the straight, barrel portion of the chamber where the heat flux measurements are made, the y^+ values are all less than 0.25 easily meeting the requirement that they be less than one.

1. Comparison of FDNS Solutions—Wall Functions versus Integrate to the Wall

Temperature contours from FDNS solutions obtained by both using wall functions and integrating to the wall are shown in Figure 20. The flame length, where the relatively cold oxygen on the centerline is totally consumed, in the case with wall functions is about 25% shorter than in the case where the equations are integrated to the wall. The propellants are mixed and combusted much quicker in the wall function solution. The structure and temperature of the recirculation zone is also quite different for the two cases. This result is somewhat unexpected since the same turbulence model is used in these areas. As noted earlier, the κ–ε turbulence model is used in the wall function solution. The Mentor BSL model also uses the κ–ε model in the far field. Figure 21 shows the heat flux profile for both FDNS results compared to the experimental data. Again, the result is surprising. One would have expected the solution obtained by integrating to the wall to be improved over the wall function solution, but it is clearly not. It is essentially equivalent to the wall function solution in the recirculation zone. Downstream of the recirculation zone, from an axial distance of about six inches to the end of the chamber, it performs worse than the wall function solution. Neither solution offers the designer the required accuracy on either the heat flux rise rate or the peak heat flux level.

Figure 20. Temperature comparisons for FDNS (top-wall functions, bottom-integrate to the wall)

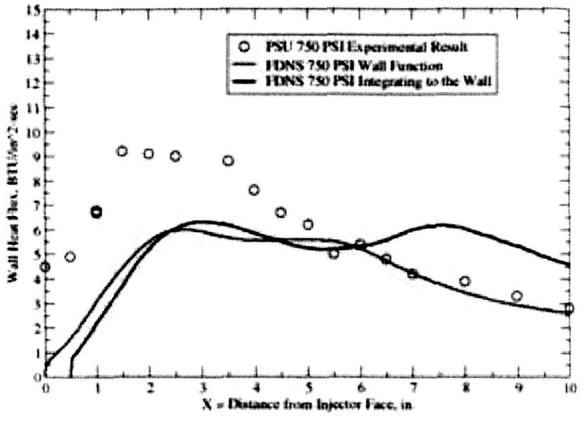

Figure 21. FDNS heat flux profiles obtained using wall functions and integrating to the wall.

2. Comparison of the Solutions Obtained by Integrating to the Wall—FDNS versus Loci-CHEM

Temperature contours obtained by integrating to the wall using both FDNS and Loci-CHEM are shown in Figure 22. Both codes employed the Mentor BSL turbulence model to achieve solutions. The flame in the Loci-CHEM solution is about 25% shorter than the flame from the FDNS solution. Considering the significant impact the turbulence model plays in simulating these mixing dominated flows, it was expected these two solutions would have been more similar. The flame length from the Loci-CHEM solution is approximately the same as the flame length from the FDNS solution using wall functions and the κ–ε turbulence model. Since these solutions employ the same turbulence model in the region away from the wall, these results are qualitatively consistent with intuition. The heat flux profiles from the two solutions where the equations were integrated to the wall are shown in Figure 23. The Loci-CHEM solution is clearly superior. It has a heat flux rise rate very close to that shown in the data, although shifted downstream slightly. The peak heat flux is matched very well, within about 5% of the data. Downstream of the reattachment point, the results are not as good. At the five inch axial location, the Loci-CHEM solution over predicts the data by approximately 40%. From the seven inch axial location to the end of the chamber, the heat flux prediction is about 25% high.

Figure 22. Heat flux contours by integrating to the wall (top-FDNS, bottom-Loci-CHEM)

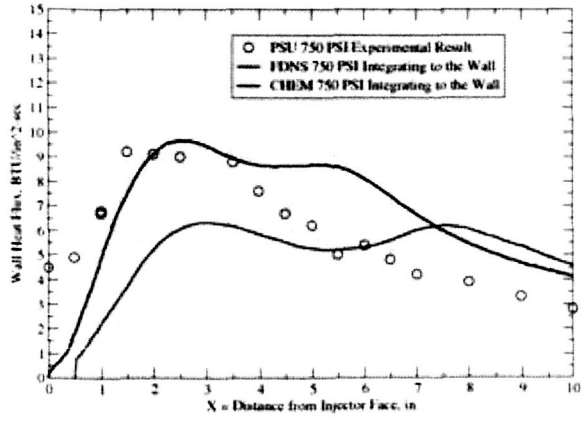

Figure 23. Heat flux profiles from FDNS and Loci-CHEM obtained by integrating to the wall.

3. Issues and Future Work

The comparisons just discussed bring to light two issues; one, specific to these calculations and the other more general. First, global comparisons of the flame structure were not consistent with intuition. Regardless of the wall treatment, all the solutions were derived using the same turbulence models in regions away from the combustor wall. Hence, the flame length from the FDNS solution with the BSL turbulence model should have been more in line with the other two solutions. These results point to the possibility of implementation issues, especially with the BSL model in the FDNS code. Concrete conclusions are difficult to reach when the details are not well understood. Closer examination of the implementation of these turbulence models is under way. This work clearly falls in the verification area.

The second issue is a more general, philosophical one that was alluded to earlier. The work conducted in this study is on the GO_2/GH_2 shear coaxial single element model problem. Since this effort examines a relevant

measure (i.e. heat flux) of a representative model problem, Table 1 indicates this is the beginning of an attempt to demonstrate accuracy to Level 3. However, the unit physics validation at Levels 1 and 2 has not been completed. So, the current work is really out of the proper verification and validation sequence. The main implication is that the heat flux comparison provides no feedback to the validation effort on how to improve the computational model performance. The more detailed information required to for guidance, such as mean and fluctuating velocity fields and species and temperature distributions typically are made at the unit physics level of experiment. Maximum benefit is derived form the verification and validation process only when the work is conducted in the proper sequence.

In terms of demonstrated accuracy level, it seems the wall function solutions are not adequate. At this point, neither is the integrate to the wall solution from FDNS. However, comparison of the flame length in the results leads to the question of implementation of the BSL model in FDNS. This potential inconsistency points out the need for verification before validation as being the proper and necessary order in the overall process. The Loci-CHEM solution obtained by integrating the equations to the wall merits an approximate demonstrated accuracy of somewhat less than Level 3 for heat flux calculation for this model problem. However, as noted earlier, there has been insufficient validation effort at Levels 1 and 2 to adequately underpin the Level 3 accuracy. Also, the code has not been exercised over the required parametric space to merit the Level 3 accuracy designation. Efforts to remove both of these deficiencies are under way.

VIII. Conclusions

Conclusions from this effort are drawn at two levels. The first level is general and somewhat philosophical. The point has been made that meeting the Exploration Vision schedule and budget will require a new design tool for combustion devices, especially injectors. From a technical standpoint, the need is based on the inability of the current, empirical design tools to account for the three-dimensional environments resulting from injector design and operation. CFD is noted as having the potential to meet the requirements for the new design tool. However, realizing that potential with CFD requires significant effort in the areas of solution fidelity, solution accuracy and demonstrated solution accuracy. The accuracy component of the design requirement was the focus of this effort. The case is made for verification and validation being the process by which confidence in simulations for design can be critically assessed and improved.

The second level of conclusions is specific to the calculations presented on validation of computational models for a GO_2/GH_2 shear coaxial single element injector. The effort examines the capability of the FDNS and Loci-CHEM CFD codes to predict experimentally determined combustor wall heat fluxes. Specifically, calculations used variants of the κ–ε turbulence model with different wall treatments.

Three groups of comparisons were made. First, the calculations from both codes using wall functions, even after a modification, fell short of a designer's requirements in terms of the initial heat flux rise rate and the peak heat flux level. Secondly, the results with FDNS integrating to the wall on a finer grid using Mentor's BSL turbulence model was actually somewhat worse than the FDNS wall function solution. Thirdly, the Loci-CHEM solution obtained on the same fine grid with Mentor's BSL turbulence model was clearly superior to the other simulation results. It did a very good job of capturing the initial heat flux rise rate, although it was shifted downstream somewhat, and the peak heat flux level. However, downstream of the reattachment point, the wall heat flux was over predicted by 25-40%. The Loci-CHEM solution obtained by integrating the equations to the wall merits an approximate demonstrated accuracy of somewhat less than Level 3 for heat flux calculation for this model problem. Validation steps to improve this rating were noted.

IX. References

[1]Gill, G.S., and Nurick, W.H., *Liquid Rocket Engine Injectors*, NASA SP-8089, 1976

[2]Tucker, K., West, J., Williams, R., Rocker, M., Canabal, F., Robles, B., Garcia, R., and Chenoweth, J., "Using CFD as a Rocket Injector Design Tool: Recent Progress at Marshall Space Flight Center," Fifth International Symposium on Liquid Space Propulsion (CD-ROM), Chattanooga, TN, 2003.

[3]Oberfampf, W. L., Trucano, T. G., and Hirsch, C., "Verification, Validation and predictive Capability in Computational Engineering and Physics," Sandia National Laboratories, Report SAND2003-3769, Albuquerque, NM, February, 2003.

[4]Roache, P. J., *Verification and Validation in Computational Science and Engineering*, Hermosa Publishers, Albuquerque, NM, 1998.

[5]Jones, G., Protz, C., Trinh, H., Tucker, K., Nesman, T. and Hulks, J., "Status of the Combustion Devices Injector Technology Program at the NASA MSFC," AIAA Paper 2005-4530, July, 2005.

[6]Cheng, G.C., and Farmer, R.C., "Development of Linearized Real-Fluid Model in Simulating Spray Combustion Flows," AIAA-2005-735, January, 2005.

[7]Wang, T.-S. and Chen, Y.-S., "Unified Navier-Stokes Flowfield and Performance Analysis of Liquid Rocket Engines," *Journal of Propulsion and Power*, Vol. 9, No. 5, Sept-Oct 1993, pp.678-685.

[8]Chen, Y.-S., Liaw, P., Shang, H.-M. and Chen, C.P., "Numerical Analysis of Complex Internal and External Viscous Flows with a Second-Order Pressure-Based Method," AIAA Paper 93-2966, July 1993.

[9]Wang, T.-S., McConnaughey, P., Warsi, S., and Chen, Y.-S., "Computational Pollutant Environment Assessment from Propulsion System Testing," *Journal of Spacecraft and Rockets*, Vol. 33, No. 3, May-June 1996, pp.386-392.

[10]Chen, Y.-S. and Kim, S.W., "Computation of Turbulent Flows Using an Extended κ-ε Turbulence Closure Model," NASA CR-179204, Oct. 1987.

[11]Chen, Y.-S., Cheng, G.C. and Farmer, R.C., "Reacting and Non-Reacting Flow Simulation for Film Cooling in 2-D Supersonic Flows," AIAA Paper 92-3602, July 1992

[12]Chen, Y-S, and Lee, C., P.,"Application of Advanced CFD Method for SLI Support", Final Report contract Number NAS8-02126, NASA MSFC December, 2004.

[13]Chen, Y-S., and Lee, C., P., "Combustor Heat Verification and Validation" Final Report, Contract Number NNM04AB54C, NASA MSFC, December, 2004.

[14]E. A. Luke and X-L. Tong and J. Wu and P. Cinnella "CHEM 2: A Finite-Rate Viscous Chemistry Solver -- The User Guide" MSSU-COE-ERC-04-07 Mississippi State University, September, 2004.

[15]Luke, E. A., "A Rule-Based Specification System for Computational Fluid Dynamics", Ph.D. Dissertation, Mississippi State University, Starkville, MS, 1999

[16]Marshall, W., Pal, S. and Santoro, R., "Benchmark Wall Heat Flux Data for a GO_2/GH^2 Single Element Combustor," AIAA-2005-3572, July, 2005.

[17]Gridgen, Software package, Version 15, Pointwise, Inc., Bedford, Texas, 2005.