Use, Assessment, and Improvement of the Loci-CHEM CFD Code for Simulation of Combustion in a Single Element GO_2/GH_2 Injector and Chamber

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This paper documents a continuing effort at Marshall Space Flight Center (MSFC) to use, assess, and continually improve CFD codes to the point of material utility in the design of rocket engine combustion devices. This paper describes how the code is presently being used to simulate combustion in a single element combustion chamber with shear coaxial injectors using gaseous oxygen and gaseous hydrogen propellants. The ultimate purpose of the efforts documented is to assess and further improve the Loci-CHEM code and the implementation of it. Single element shear coaxial injectors were tested as part of the Staged Combustion Injector Technology (SCIT) program, where detailed chamber wall heat fluxes were measured. Data was taken over a range of chamber pressures for propellants injected at both ambient and elevated temperatures. Several test cases are simulated as part of the effort to demonstrate use of the Loci-CHEM CFD code and to enable us to make improvements in the code as needed. The simulations presented also inlcude a grid independence study on hybrid grids. Several two-equation eddy viscosity low Reynolds number turbulence models are also evaluated as part of the study. All calculations are presented with a comparison to the experimental data. Weaknesses of the code relative to test data are discussed and continuing efforts to improve the code are presented.

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University of Maryland

Overview

- Summary
- Background
- Scope of the Current Effort
- Computational Tools (CFD Codes)
- Application to Vision for Space Exploration (VSE)
- Test Description
- CFD Simulations
- Results
- Conclusions
- Recommendations for Future Work

Summary Statement

- This presentation documents a continuing effort at Marshall Space Flight Center (MSFC) to use, assess, and continually improve CFD codes to the point of material utility in the design of rocket engine combustion devices.

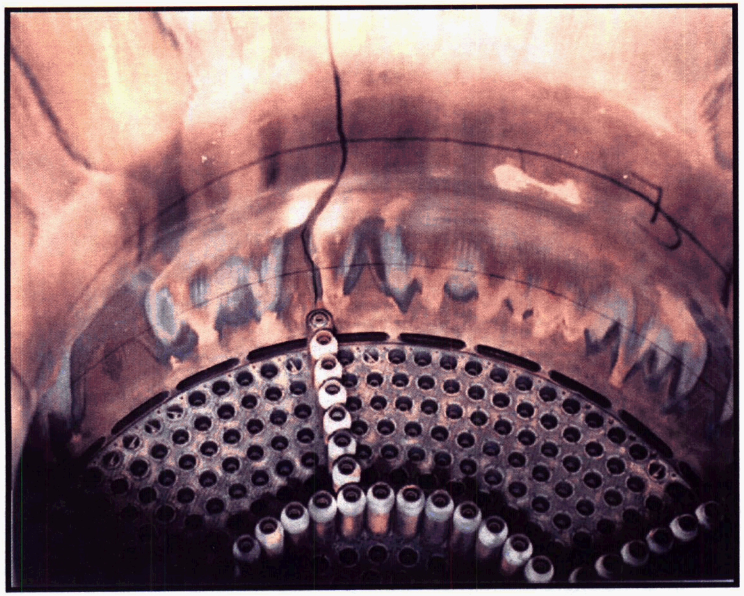
- CIRCLE FROM DEV. TO USE BACK TO DEV.

- TEST IS VERY CRITICAL

Background

The Need for Improved Injector Design Tools

- Issues with current injector design tools
  - 1-D, empirical
  - Result in costly, time consuming test, fail, fix development program



Environments are 3 dimensional

- Requirements for new injector design tools
  - Fidelity-must be able to calculate performance & 3-D environments as a function of injector design details and flow physics
  - Robustness-must be able to produce large numbers of solutions over a parametric space during the design phase
  - Accuracy- must be demonstrated to yield quantitative results

Background

The combustion CFD technology effort at NASA/Marshall Space Flight Center is guided by a Combustion Devices CFD Simulation Capability Roadmap. The Roadmap objective is:

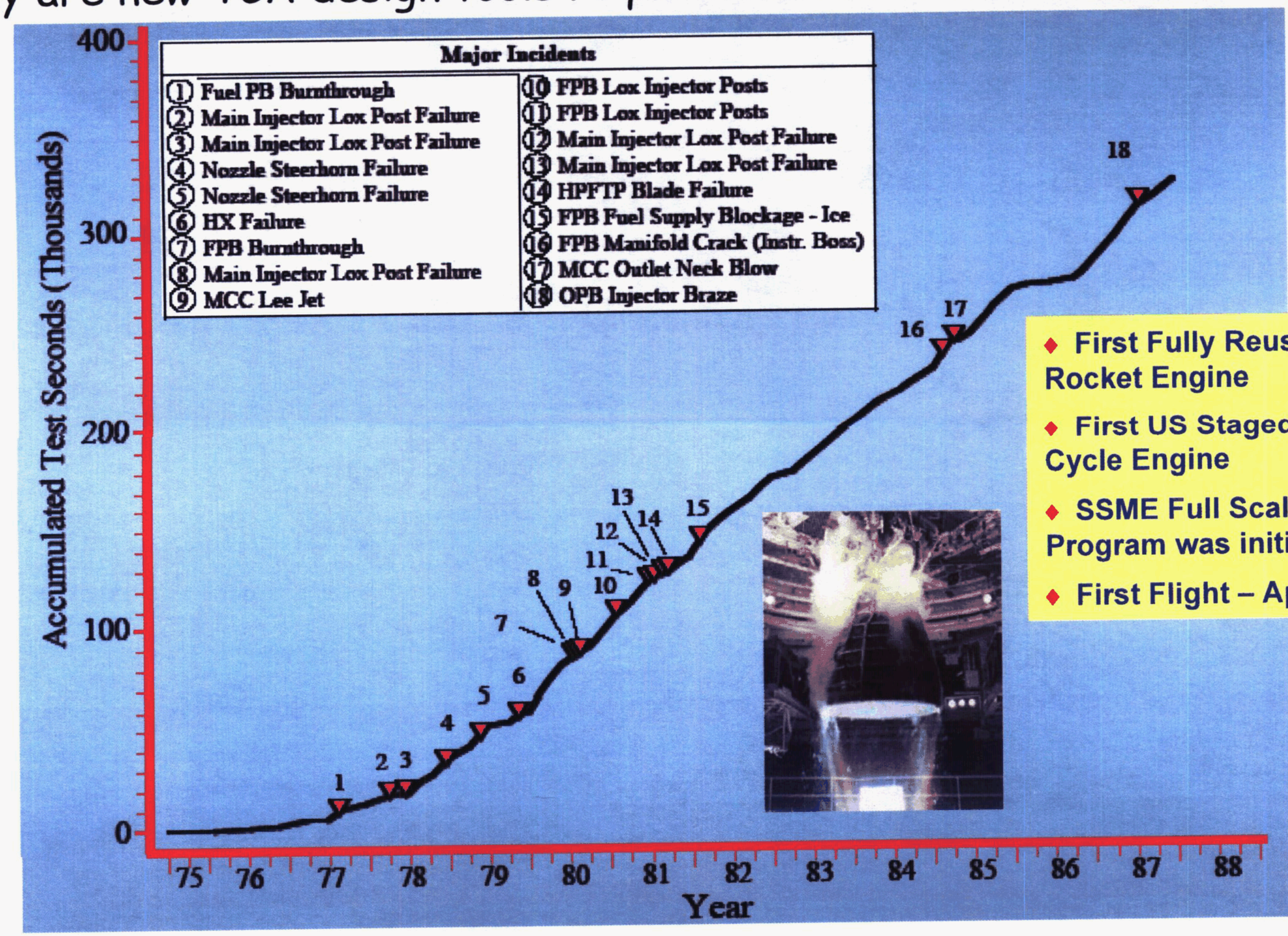
To enable the use of CFD as a tool for the Simulation of Preburners, Ducting, Thrust Chamber Assemblies and Supporting Infrastructure in terms of Performance, Life, and Stability so as to affect the design process in a timely fashion

- If CFD is to be used as an injector design tool, code developers & code users must address this key issue:

  How should confidence (i.e. demonstrated accuracy capability) in simulations and modeling for design be critically addressed, and where necessary, improved?

- Verification & Validation of computational solutions are the primary means to quantify and build this confidence

Why are new TCA design tools required? Look at the SSME development--



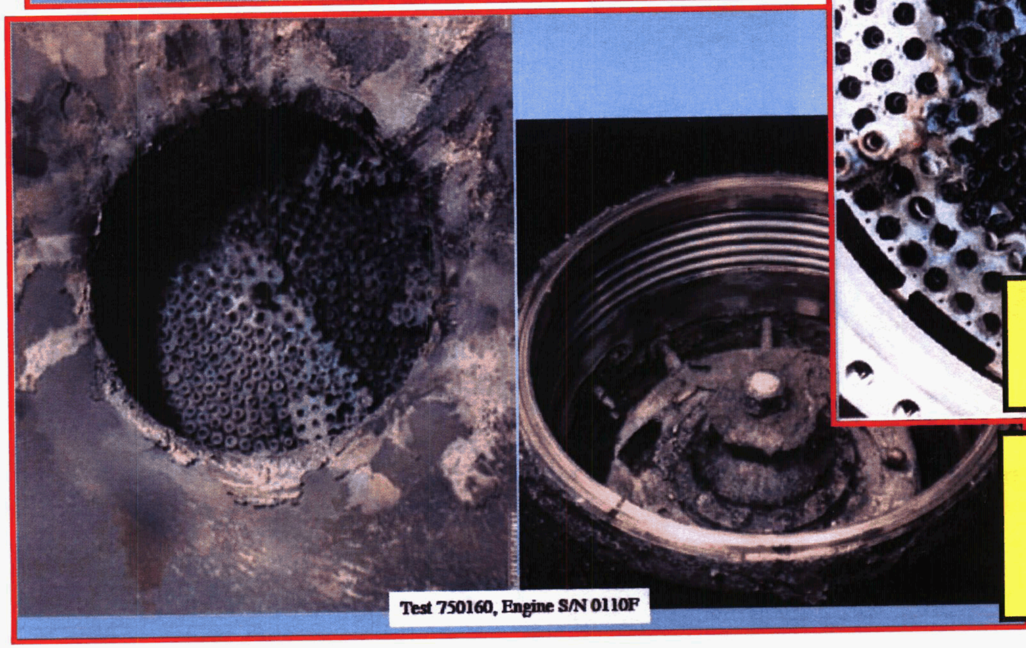
- First Fully Reusable Cryogenic Rocket Engine
- First US Staged Combustion Cycle Engine
- SSME Full Scale Development Program was initiated in April 1972
- First Flight – April 1981

Note: All SSME information from—
"Combustion Devices Failures During Space Shuttle Main Engine Development," Goetz, O. K., Monk, J. C., 5th International Symposium on Liquid Space Propulsion Long Life Combustion Devices Technology, Chattanooga, TN, 2003.

Background - Constellation University Institutes Project
TCA Virtual Institute Vision-Objective

Oxidizer Preburner
Failure at 188 sec.
July 1, 1987

Main Injector Failure at 233 sec.
July 15, 1981

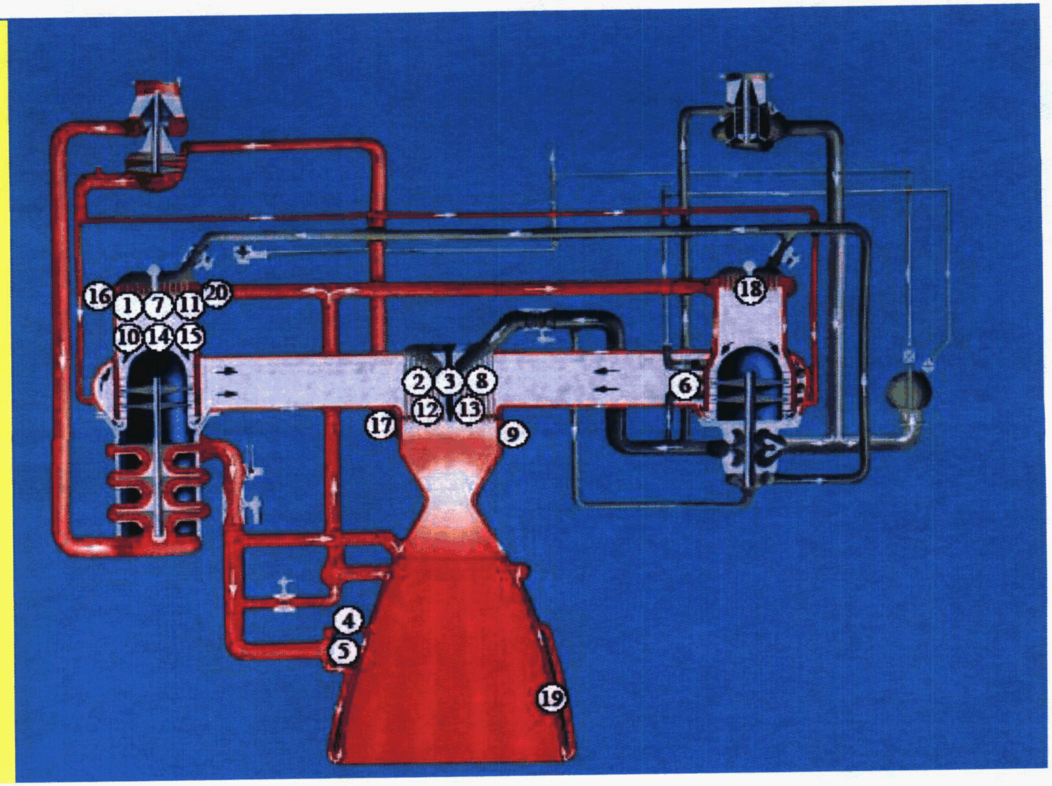


Fuel Preburner
Failure at 3.6 sec.
February 12, 1982

Background - Constellation University Institutes Project
TCA Virtual Institute Vision-Objective

Injector design is the heart of this overall vision

- **The large majority (~80%) of Combustion Devices failures occur in the injector**
- **Injector design details and physical processes occurring here govern:**
  - Ignition
  - Performance
  - Environments in the entire combustor or TCA
  - Stability



The design space that contains an injector with reliable ignition characteristics, high performance and stable operation with sufficiently benign environments has historically been located only after several time consuming and costly design, test, fail cycles. *This is a direct consequence of modeling very complex flow phenomena with relatively simple, empirical tools.*

CFD Codes being Developed for MSFC Injector Devices Design Efforts

Two codes are being developed in parallel, but <u>independently</u> from each other

- These two codes are used, and continually improved in the design of rocket engine combustion devices
  - <u>Loci-CHEM, version 3: Density-based</u>
  - Loci-Stream: Pressure-based (not discussed here)
  - Replacing FDNS (Finite Difference, Navier-Stokes), solver that has been used at MSFC for 15 years
- Loci-Chem:
  - 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 are presented in the CHEM user guide, Ref.4)
  - Density-based computational fluid dynamics (CFD) algorithm
    - Preliminary implementation of pre-conditioning is available and is used extensively here
    - Preconditioning methods for a chemically reacting flows are presently in beta mod
      - very important component in the continuing development of Loci-CHEM.
  - Several turbulence models are available: Three Two-Equation Models and a One-Equation Model
    - Menter's Shear Stress Transport Model (SST)
      - general purpose model that is reasonably effective at predicting flow separations
    - Menter's Baseline Model (BSL)
      - Blended model: k-ω near the wall, k-ε away from the wall
    - Wilcox's k-ω model (KW)
      - non-physical sensitivity to the free-steam k and ω values
    - Spalart-Allmaraas one equation model
      - Loci-CHEM is comprised entirely of C and C++ code and is supported on all popular UNIX variants and compile
    - Typically require first cell from wall y+ values from 1 to 0.1.
  - Parallelism is supplied by the Loci framework (Ref. 5)
    - exploits multi-threaded and MPI libraries to provide parallel capability
  - Loci-CHEM is quite scalable
    - approximately 90% parallel efficiency on to 64 CPUs on the axisymmetric simulations that were part of this effort.

Application to Vision for Space Exploration

- The ultimate purpose of the efforts documented is to assess and further improve the Loci-CHEM code and the implementation of it, to make it a viable tool for the design of Liquid Propellant Engines used in the Vision for Space Exploration
  - J-2x LOX/Hydrogen engine (starting now)
    - ARES I (Crew Launch Vehicle) 2nd Stage
    - ARES V (Cargo Launch Vehicle) 2nd Stage
  - RS-68 X 5
    - ARES V 1st Stage
  - Lunar Lander / Lunar Take-off Engine
    - LOX / Methane
  - Thrust Vector / Roll Control Engines
  - Igniters

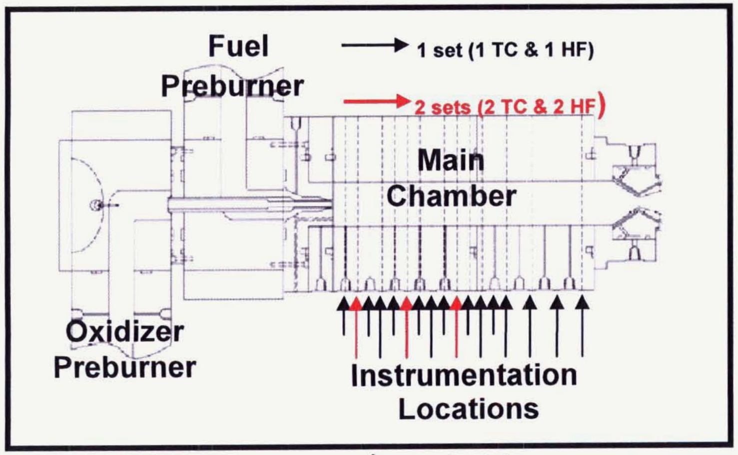
Test Effort

Experiment Program to lead toward better understanding of heat flux unit physics problem

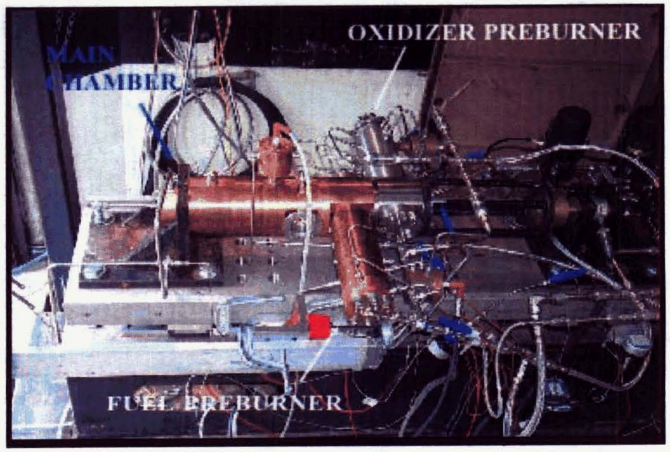
- Single element shear coaxial injectors were tested as part of the Staged Combustion Injector Technology (SCIT) program
  - performed at the Pennsylvania State University's (PSU) Cryogenic Combustion Laboratory (CCL) (Santoro and Pal[8])
    - Main purpose of experimental effort was to characterize the chamber wall heat flux for a single element injector using gaseous oxygen and gaseous hydrogen as propellants
      - focus on providing benchmark quality data for CFD code validation
  - Chamber is heavily instrumented for wall temperature and heat flux measurements
    - Allows several types of experiments to be conducted
      - Hot propellants (approximately 700 – 800 K)
        - » oxidizer-rich preburner (OPB), and a fuel-rich preburner (FPB)
        - » Ambient temperature propellants via operation without the pre-burners
        - » Instrumentation stations can be moved around from one test to another; allowing different sections of the combusting gases to be instrumented in more detail
- Data was taken over a range of chamber pressures for propellants injected at both ambient and elevated temperatures (8 cases)
  - 300, 450, 600, 750 psia
  - Propellant Temperatures of
    - ~300 K
    - ~700-800 K (via oxygen and fuel Pre-burners)

Test Effort

Experiment Modeled—Penn State University



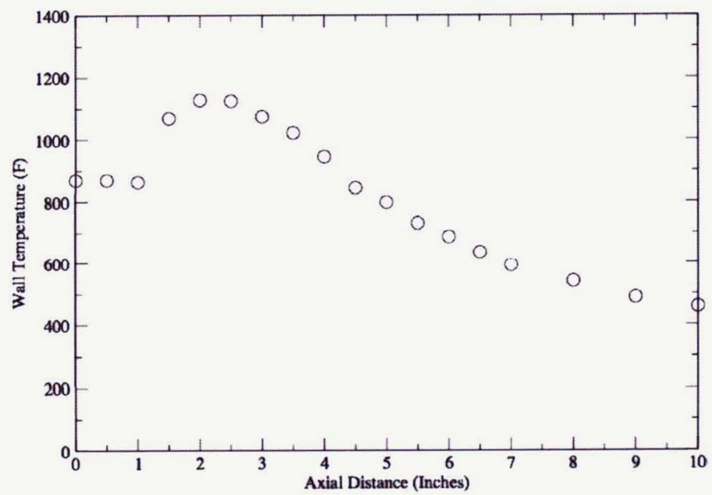
Test Rig Schematic



Test Rig Photo

750PSI	GO_2	GH_2
Temperature (K)	711.11	800.00
Mass Flow Rate (Lbm/sec)	0.1994	0.0730
O_2 Mass Fraction	0.9449	0.0
H_2 Mass Fraction	0.0	0.4018
H_2O Mass Fraction	0.0551	0.5982

750 psi Test Conditions

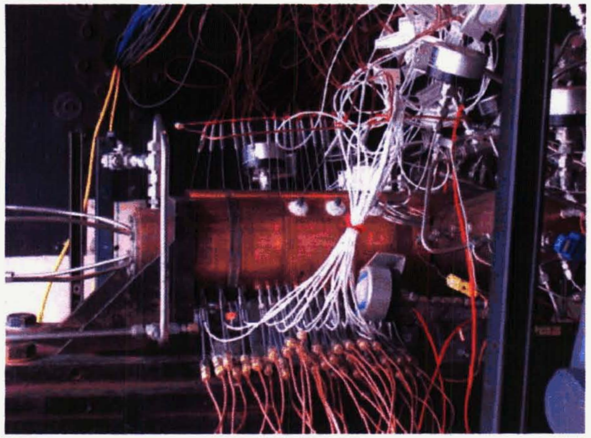


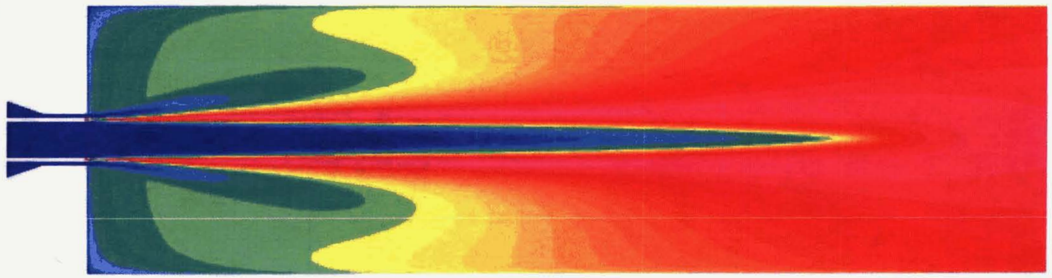
Measured Wall Temperatures at 750 psi

Test Effort – Relation to CFD Analysis

Code Validation for Chamber Wall Heat Flux

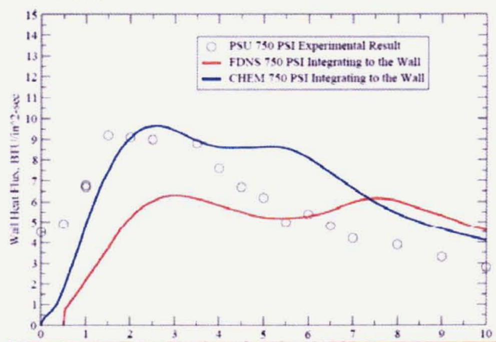
- Model Problem-Single element, shear coaxial injector with hot GO_2/GH_2 propellants
- Model Problem Aspect-Chamber wall heat flux
- Initial Demonstrated Accuracy Level-0 (minimal verification with flat plate)





CFD Analysis

Test Data



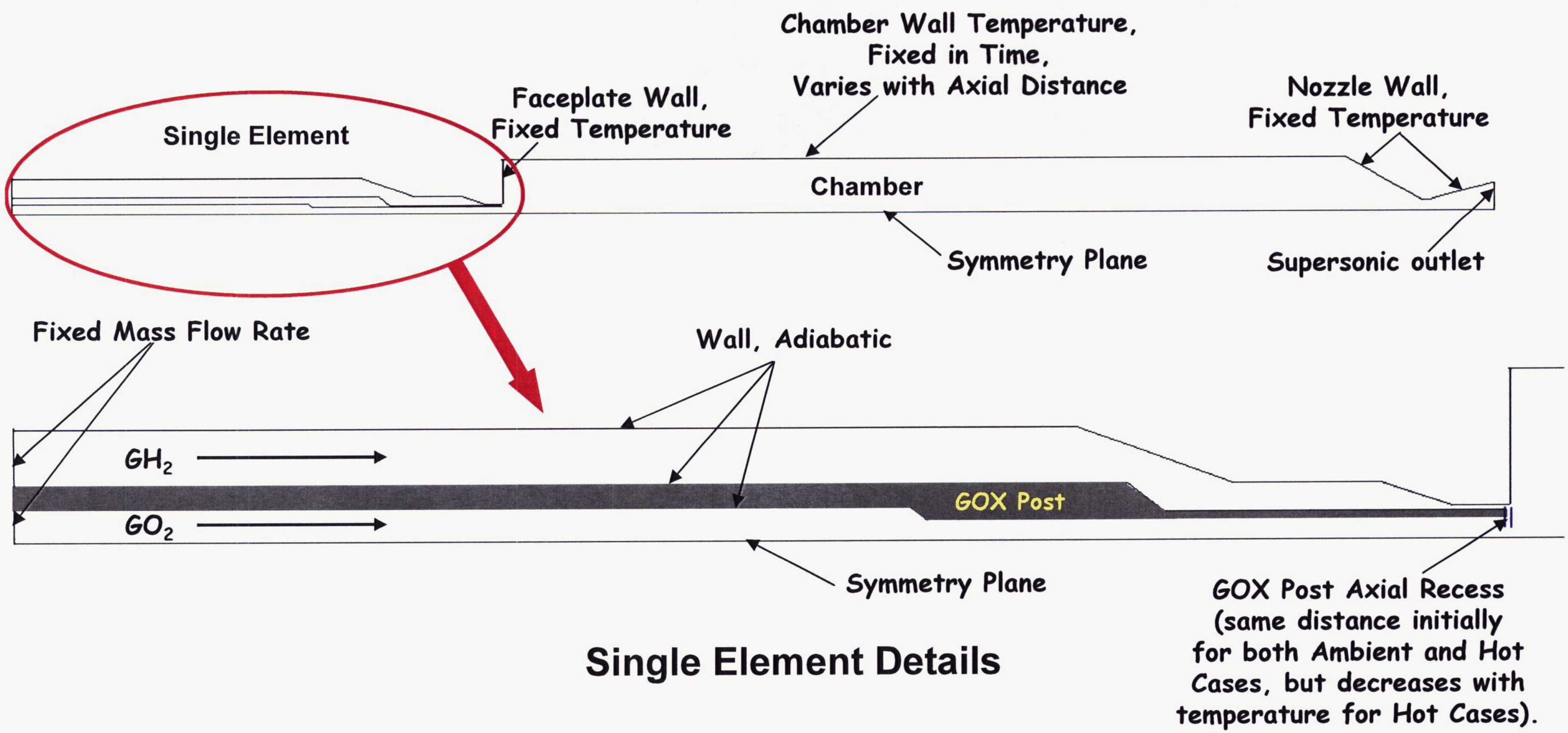
Accuracy Quantification

CFD Simulations

- CFD Simulation Summary
  - All 8 experiment types modeled
    - 4 Chamber pressures: 300, 450, 600, 750
    - 2 sets of Propellant Temperatures: Ambient (~300K) and Hot with Pre-burner (~700-800K)
  - The full set of simulations were conducted after an extensive set of simulations on one case (750 psia, hot propellants)
    - grid independence study on hybrid grids (with and without local refinement)
    - Several two-equation eddy viscosity low Reynolds number turbulence models were also evaluated as part of the study
    - Effect of Pre-Conditioning was also assessed
- All calculations are presented with a comparison to the experimental data

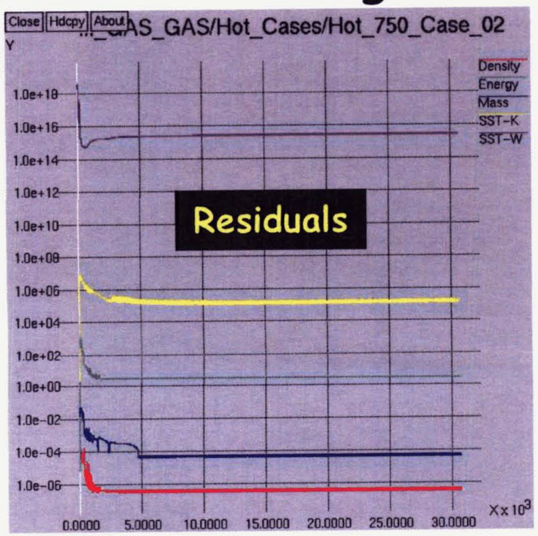
CFD Simulations - Boundary Conditions

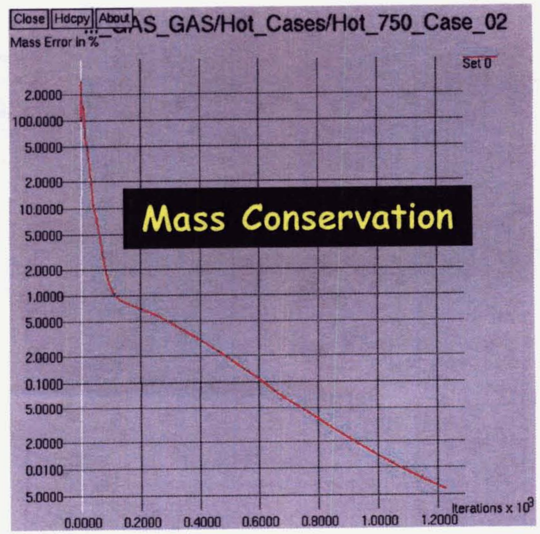
Computational Boundary Conditions

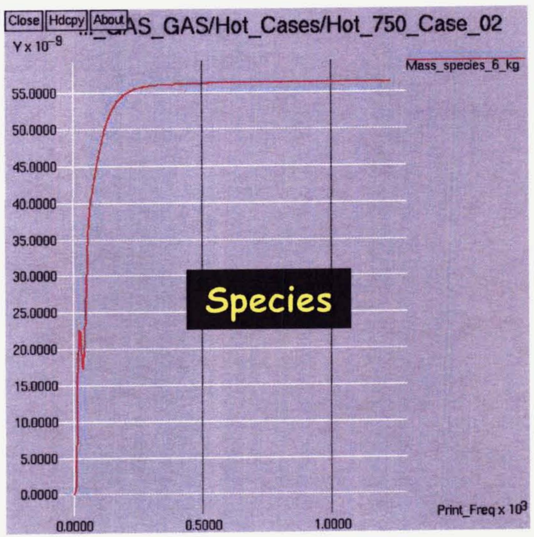


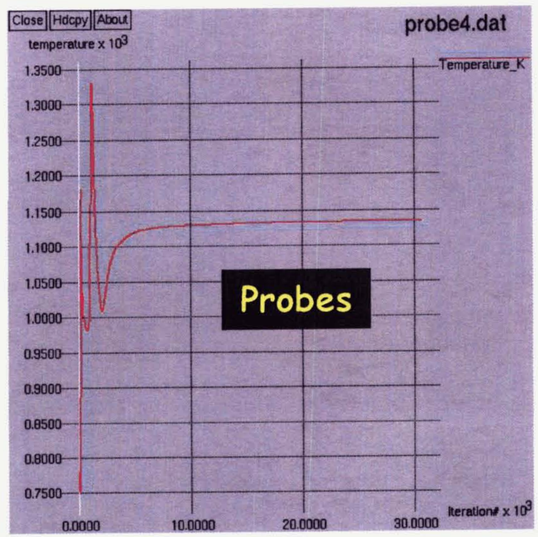
Computational Model - Typical Results

- Iteration Convergence



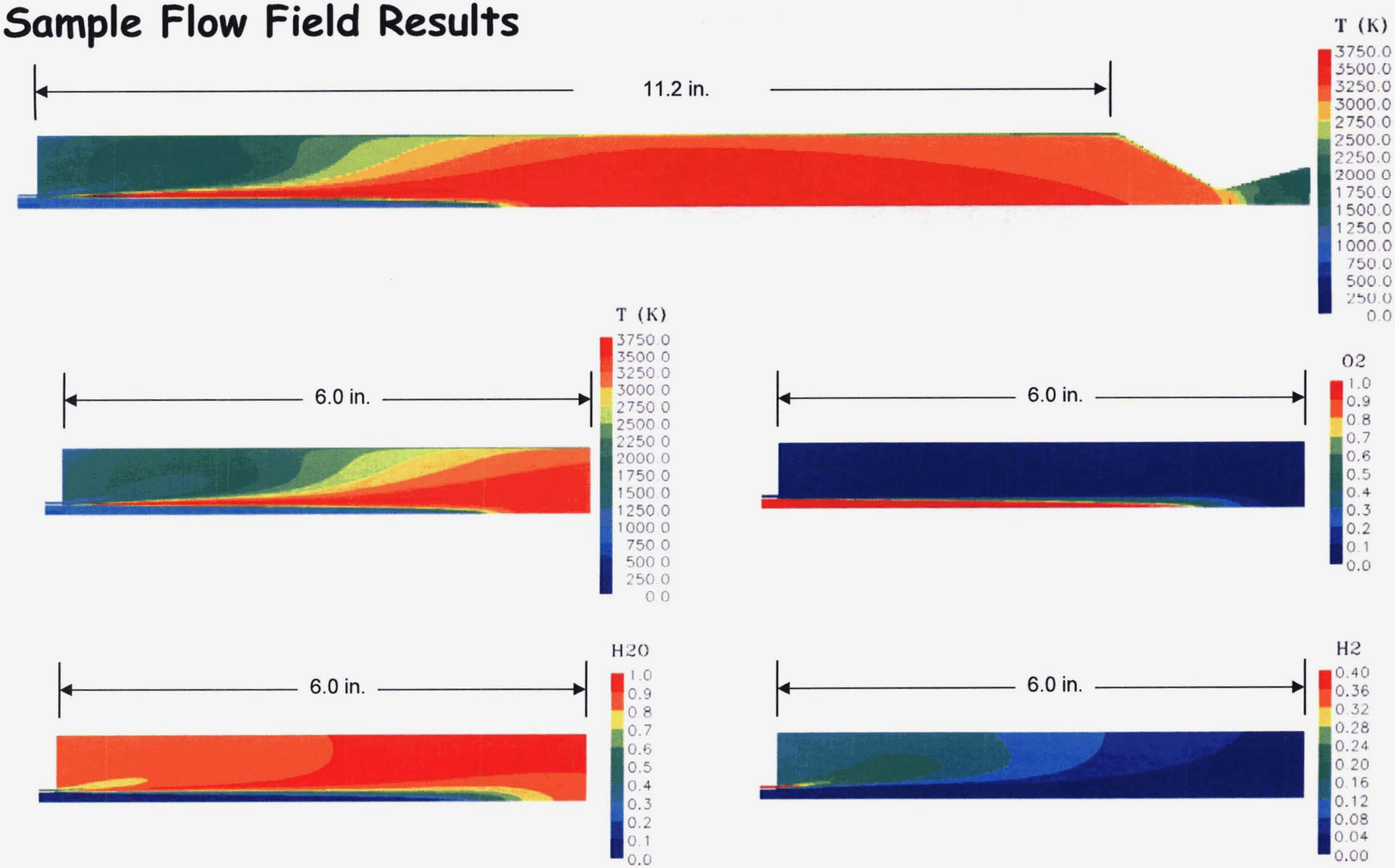




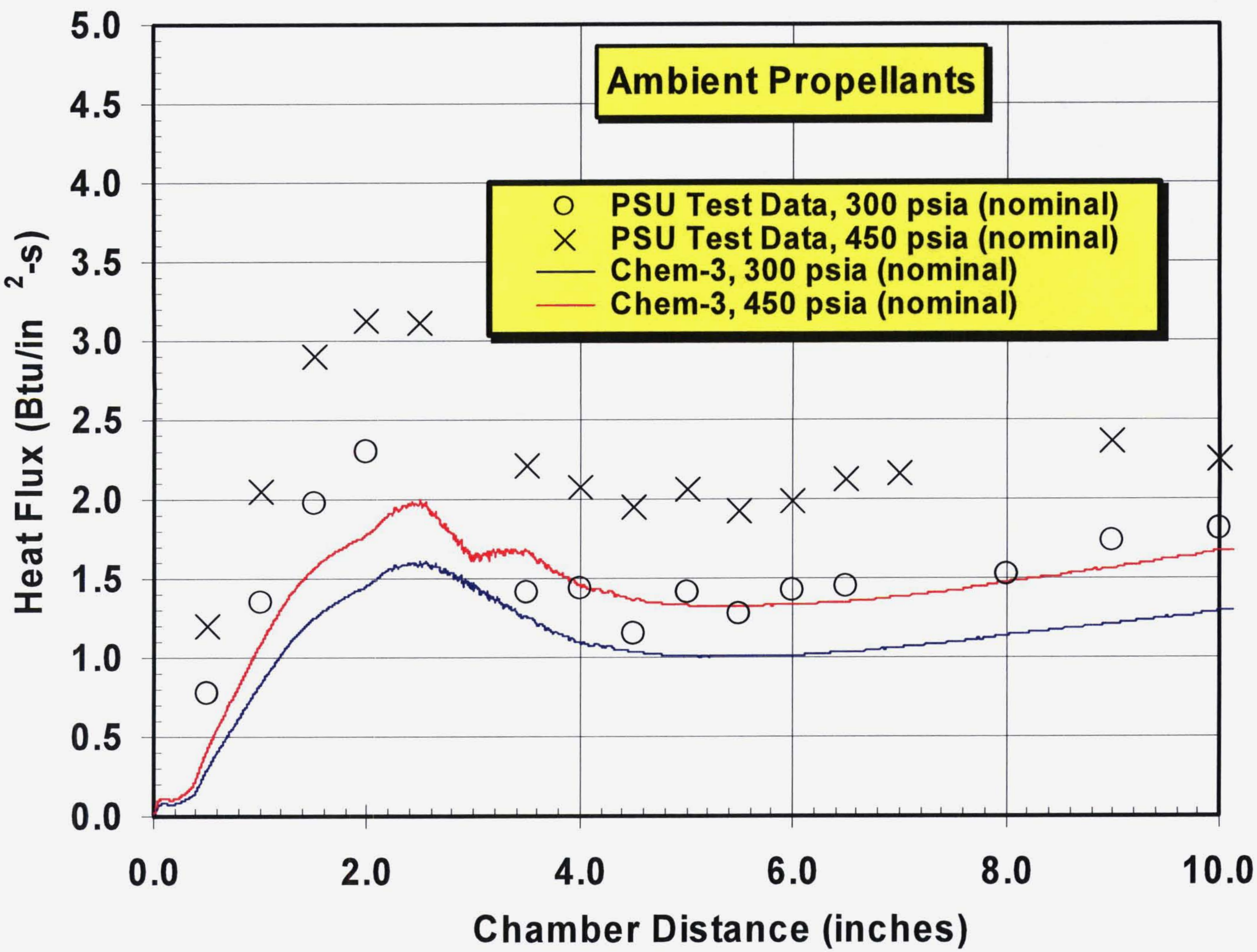


Computational Model - Typical Results

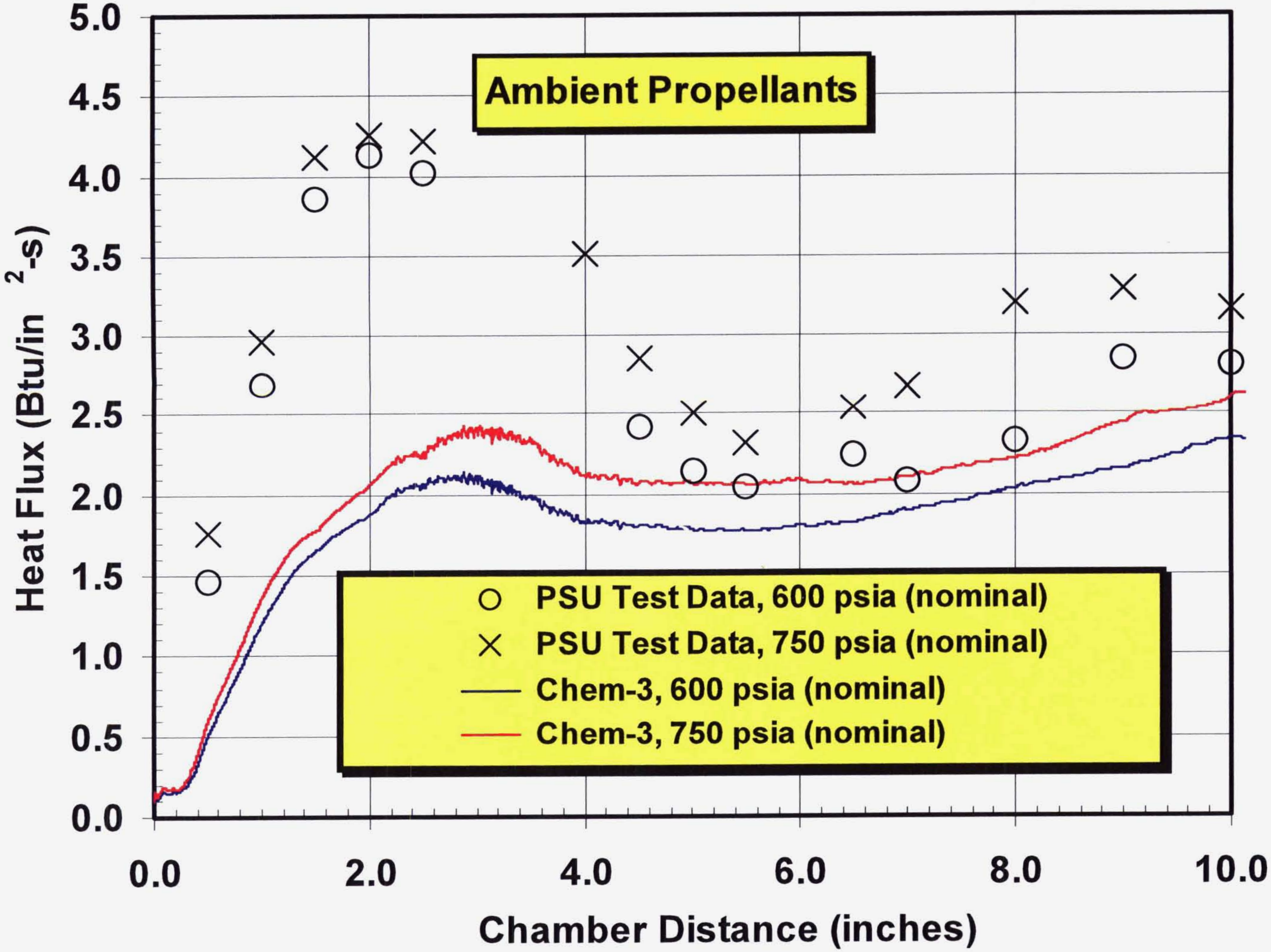
Sample Flow Field Results



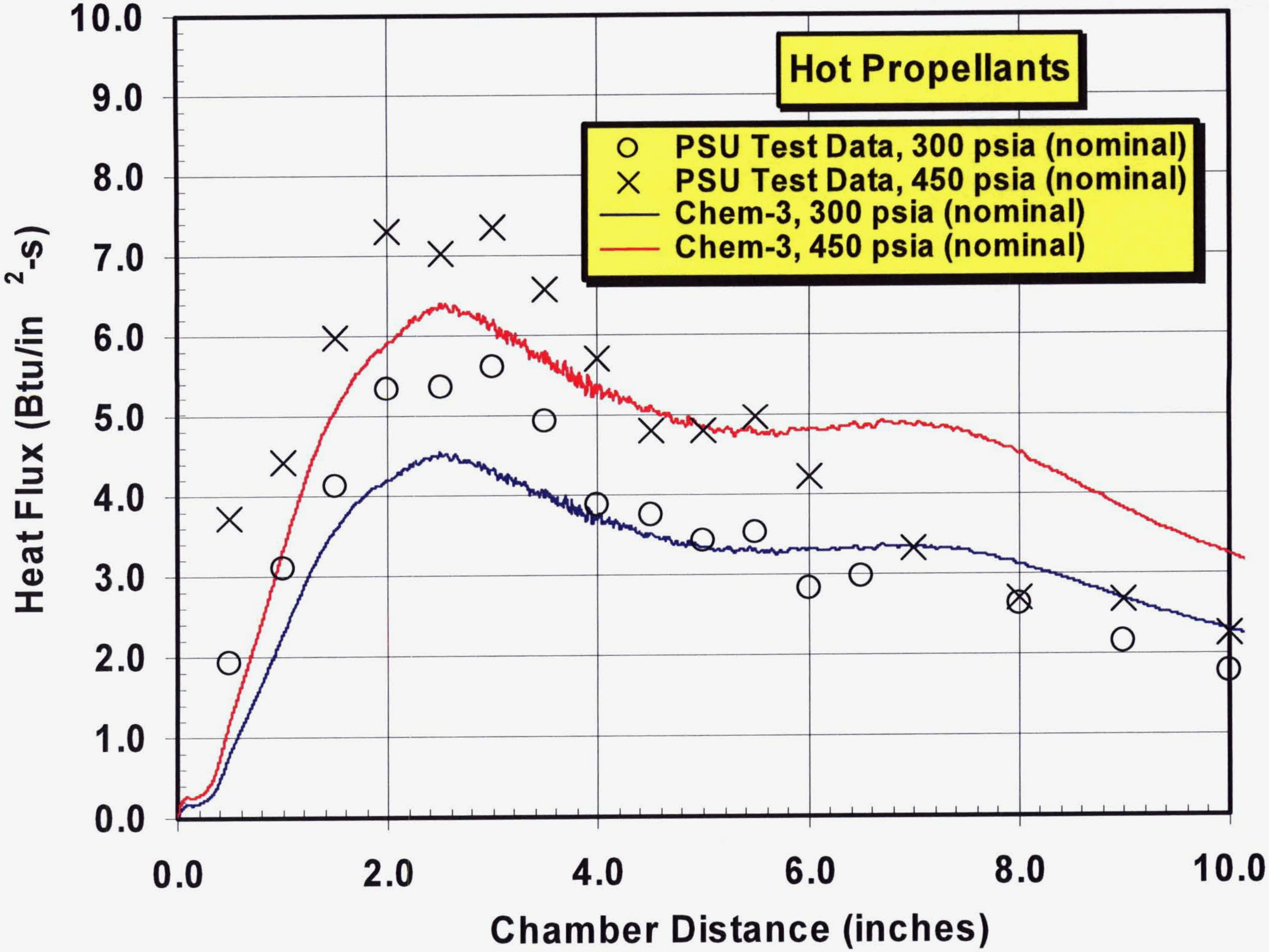
Ambient Propellant Results - 300 & 450 psia



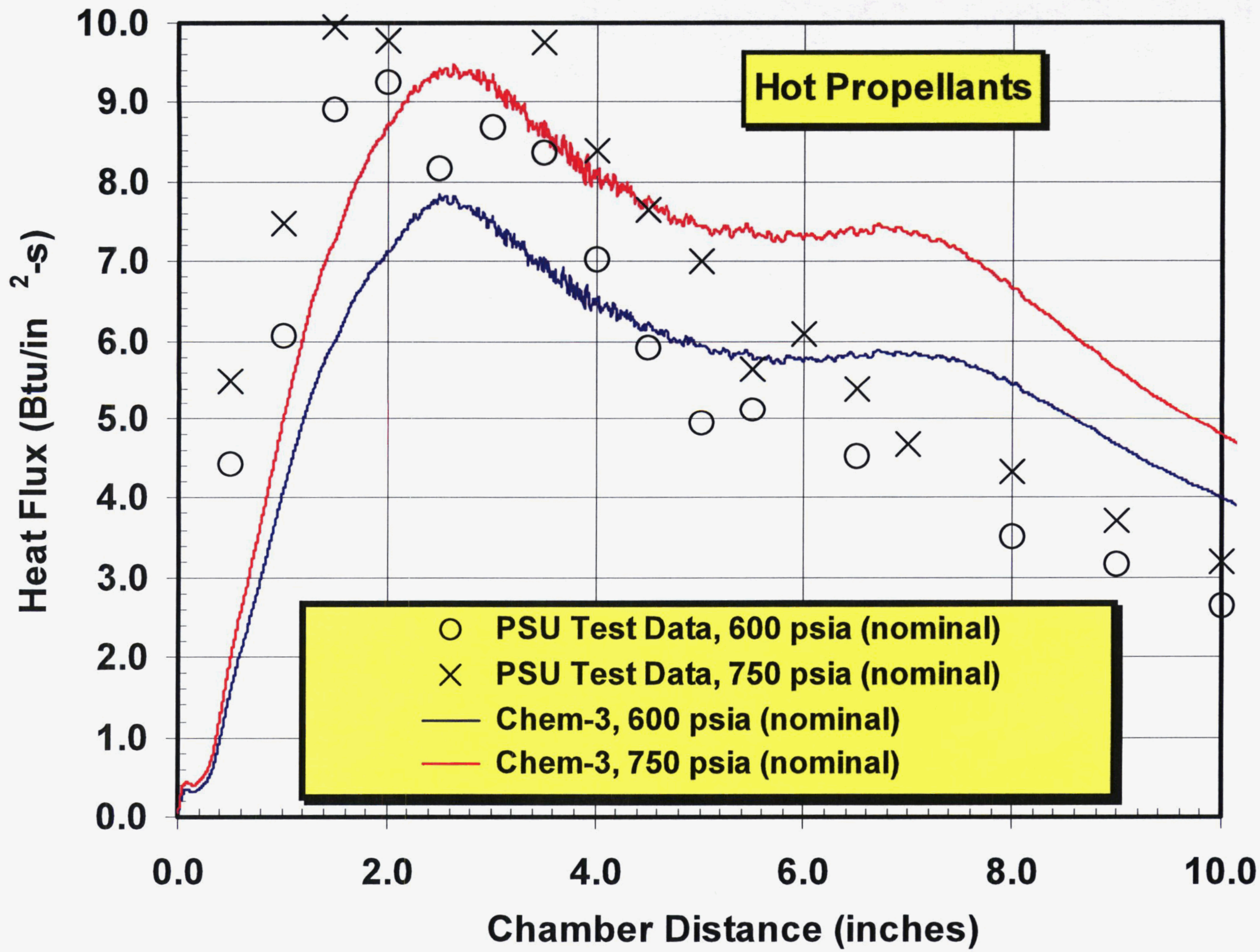
Ambient Propellant Results - 600 & 750 psia



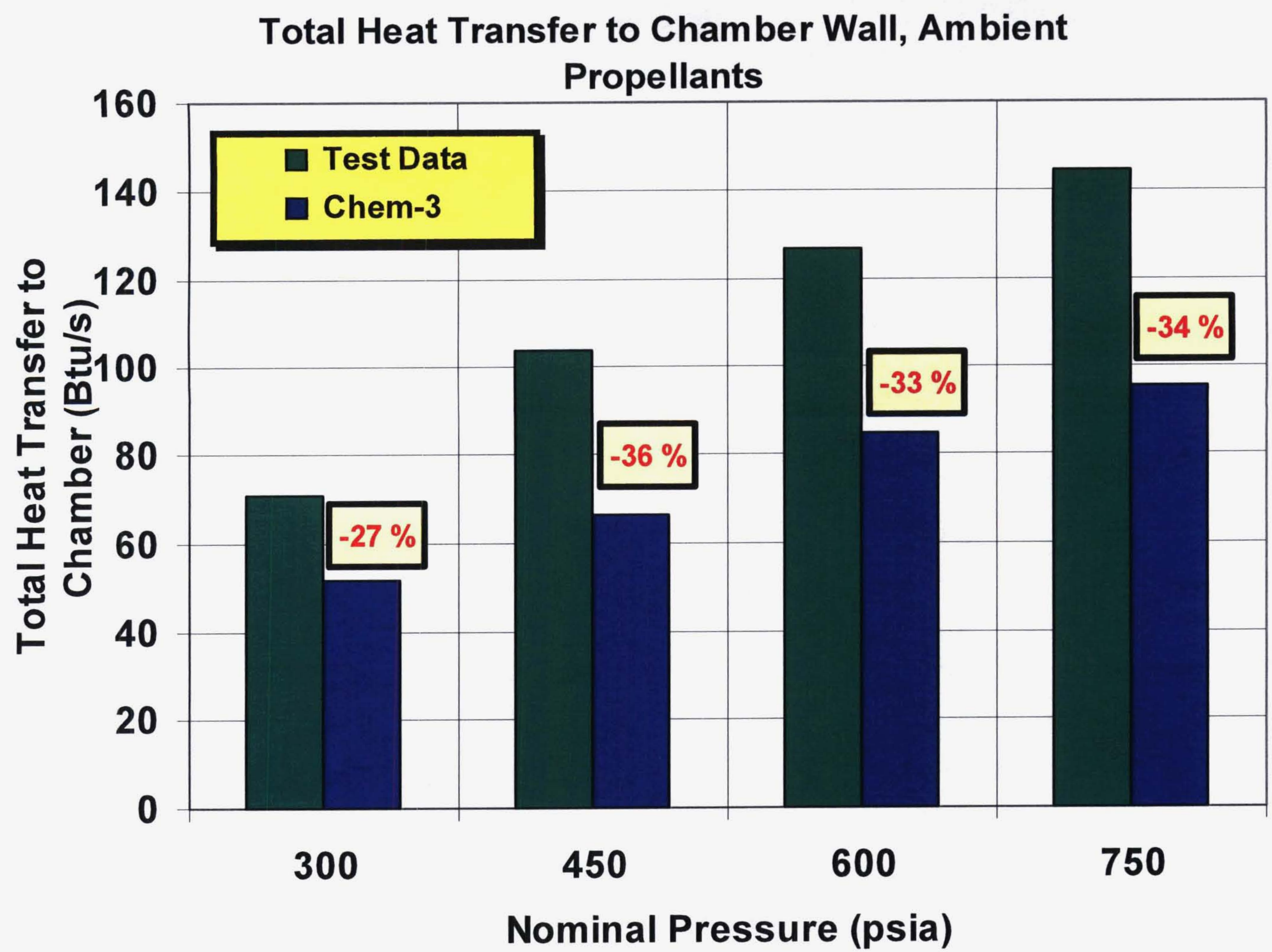
Hot Propellant (Pre-Burner) Results - 300 & 450 psia



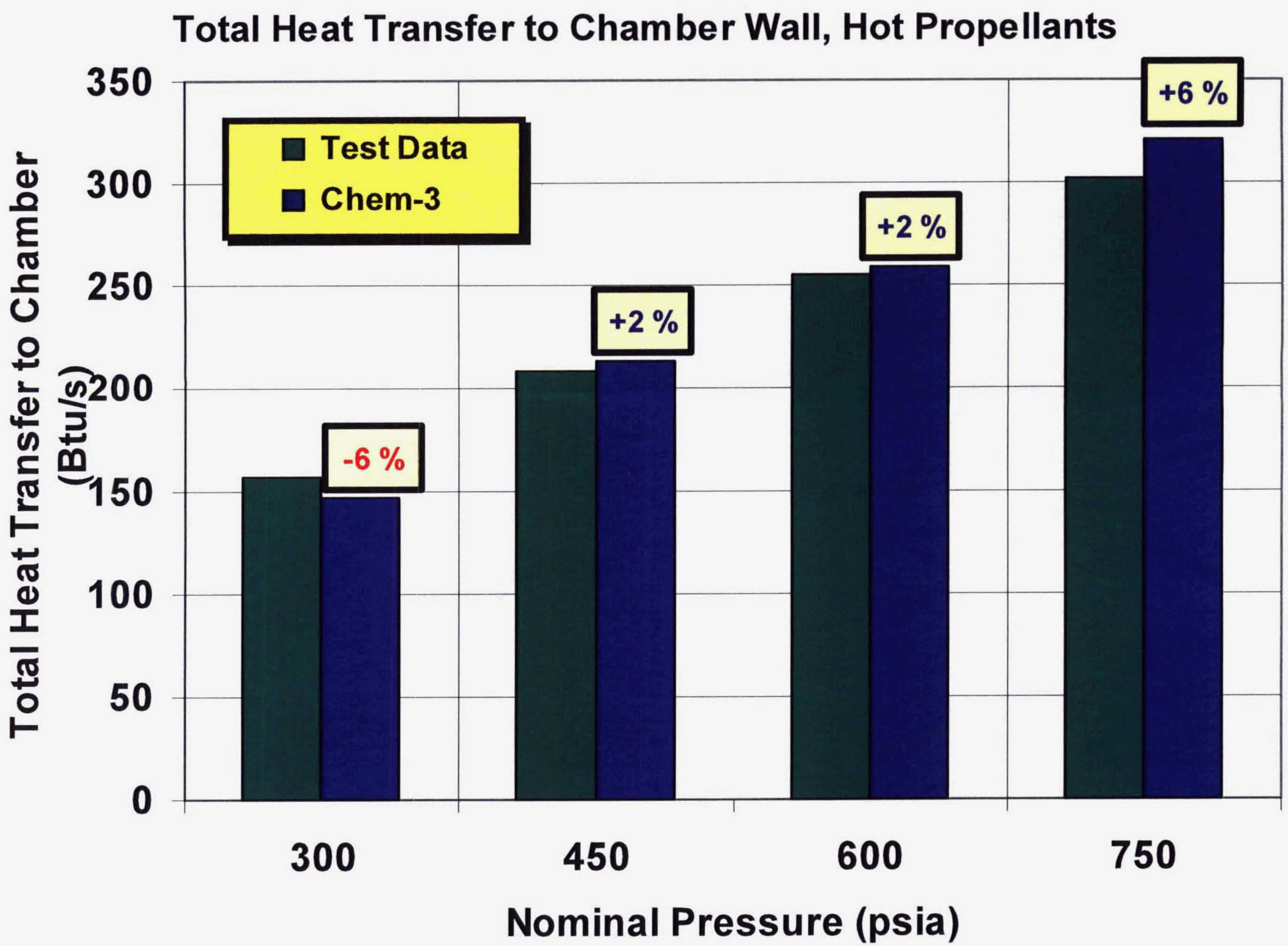
Hot Propellant (Pre-Burner) Results - 600 & 750 psia



Total Heat Transfer Rate to Chamber - Ambient Cases



Total Heat Transfer Rate to Chamber - Hot Cases



Conclusions of Pre-Conditioning, Turbulence Model Study and Mesh Studies

- All solutions with Loci-CHEM achieved demonstrated steady state and mesh convergence
- Overall, Loci-CHEM….
  - For the hot propellant (Pre-Burner) Cases
    - Satisfactorily predicts heat flux rise rate and peak heat flux
    - Significantly over-predicts the downstream heat flux
    - Predicts total heat transfer to the chamber wall (heat flux integrated over chamber length) within about 6%
  - For the ambient propellant Cases
    - Significantly under-predicts peak heat flux and downstream heat flux for the ambient cases
    - Significantly under-predicts total heat transfer to the chamber wall for the ambient cases
    - <u>Does not predict consumption of all oxygen in the fuel-rich combustion chamber</u>

Recommendations for Future Work

- Further decomposition of the problem into unit physics problems
  - Series of simple, representative jet problems
  - Series of simple, representative heat transfer problems
- Further Investigation of Mixing Phenomena and Turbulence Models
  - Suspect Inadequate Mixing caused Ambient Cases to not fully consume O_2
- Extensive Comparison to Well-understood and Trusted 1-D models
- Uncertainty and Sensitivity Analysis of test data
- Continue mesh studies in the direction of coarser grids
- Determine the cause of the over-prediction of the downstream heat flux
- Run the problem in the unsteady mode

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