Use, Assessment, and Improvement of the Loci-CHEM CFD Code for Simulation of Combustion in a Single Element \( \text{GO}_2/\text{GH}_2 \) Injector and Chamber

Douglas G. Westra, Ph.D.*, Jeff Lin*, Jeffrey S. West, Ph.D.*, Paul K. Tucker*

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 include 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.

* NASA/Marshall Space Flight Center
Mail Code ER43
MSFC, AL 35812
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

Doug Westra, Jeff Lin, Jeff West and Kevin Tucker
National Aeronautics and Space Administration
Marshall Space Flight Center
Huntsville, AL 35812
USA

Thermal & Fluids Analysis Workshop 2006
August 7-11, 2006
Goddard Space Flight Center
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

- 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

Environments are 3 dimensional
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.
Background - Constellation University Institutes Project
Thrust Chamber Assembly (TCA) Virtual Institute Vision-Objective

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

Note: All SSME information from—
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
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 independently from each other

- These two codes are used, and continually improved in the design of rocket engine combustion devices
  - Loci-CHEM, version 3: Density-based
  - 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: \( k-\omega \) near the wall, \( k-\varepsilon \) away from the wall
    - Wilcox's \( k-\omega \) model (KW)
      - non-physical sensitivity to the free-stream \( K \) and \( \omega \) values
    - Spalart-Allmaras 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.
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) 2\textsuperscript{nd} Stage
  - ARES V (Cargo Launch Vehicle) 2\textsuperscript{nd} Stage
- RS-68 X 5
  - ARES V 1\textsuperscript{st} 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®)
    - 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

<table>
<thead>
<tr>
<th>750PSI</th>
<th>$G_O_2$</th>
<th>$G_H_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (K)</td>
<td>711.11</td>
<td>800.00</td>
</tr>
<tr>
<td>Mass Flow Rate (Lbm/sec)</td>
<td>0.1994</td>
<td>0.0730</td>
</tr>
<tr>
<td>$O_2$ Mass Fraction</td>
<td>0.9449</td>
<td>0.0</td>
</tr>
<tr>
<td>$H_2$ Mass Fraction</td>
<td>0.0</td>
<td>0.4018</td>
</tr>
<tr>
<td>$H_2O$ Mass Fraction</td>
<td>0.0551</td>
<td>0.5982</td>
</tr>
</tbody>
</table>

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)

![Test Data](image1.png)

![CFD Analysis](image2.png)

![Accuracy Quantification](image3.png)
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
Computational Boundary Conditions

Single Element Details

- Chamber Wall Temperature, Fixed in Time, Varies with Axial Distance
- Faceplate Wall, Fixed Temperature
- Nozzle Wall, Fixed Temperature
- Supersonic outlet
- Fixed Mass Flow Rate
- Wall, Adiabatic
- $\text{GO}_2$
- $\text{GH}_2$
- GOX Post Axial Recess (same distance initially for both Ambient and Hot Cases, but decreases with temperature for Hot Cases)
Computational Model - Typical Results

- Iteration Convergence

![Residuals](image1)
![Mass Conservation](image2)
![Species](image3)
![Probes](image4)
Computational Model - Typical Results

Sample Flow Field Results

- 11.2 in.
- 6.0 in.
- 6.0 in.
- 6.0 in.

$T (K)$

- 3750.0
- 3500.0
- 3250.0
- 3000.0
- 2750.0
- 3500.0
- 2250.0
- 2000.0
- 1750.0
- 1500.0
- 1250.0
- 1000.0
- 750.0
- 500.0
- 250.0
- 125.0
- 0.0

$O_2$

- 1.0
- 0.9
- 0.8
- 0.7
- 0.6
- 0.5
- 0.4
- 0.3
- 0.2
- 0.1
- 0.0

$H_2O$

- 1.0
- 0.9
- 0.8
- 0.7
- 0.6
- 0.5
- 0.4
- 0.3
- 0.2
- 0.1
- 0.0

$H_2$

- 0.40
- 0.36
- 0.32
- 0.28
- 0.24
- 0.20
- 0.16
- 0.12
- 0.08
- 0.04
- 0.00
Ambient Propellant Results - 300 & 450 psia

![Graph showing ambient propellant results for 300 and 450 psia](image)

- PSU Test Data, 300 psia (nominal)
- PSU Test Data, 450 psia (nominal)
- Chem-3, 300 psia (nominal)
- Chem-3, 450 psia (nominal)
Ambient Propellant Results - 600 & 750 psia

![Graph showing heat flux vs. chamber distance for ambient propellants at 600 and 750 psia.](image)

- PSU Test Data, 600 psia (nominal)
- PSU Test Data, 750 psia (nominal)
- Chem-3, 600 psia (nominal)
- Chem-3, 750 psia (nominal)
Hot Propellant (Pre-Burner) Results - 300 & 450 psia

![Graph showing heat flux vs. chamber distance for hot propellants at 300 and 450 psia.](image)

- **Hot Propellants**
  - PSU Test Data, 300 psia (nominal)
  - PSU Test Data, 450 psia (nominal)
  - Chem-3, 300 psia (nominal)
  - Chem-3, 450 psia (nominal)
Hot Propellant (Pre-Burner) Results - 600 & 750 psia

- **PSU Test Data, 600 psia (nominal)**
- **PSU Test Data, 750 psia (nominal)**
- **Chem-3, 600 psia (nominal)**
- **Chem-3, 750 psia (nominal)**
Total Heat Transfer Rate to Chamber - Ambient Cases

Total Heat Transfer to Chamber Wall, Ambient Propellants

Nominal Pressure (psia)

Test Data
Chem-3

-27%
-36%
-33%
-34%
Total Heat Transfer Rate to Chamber - Hot Cases

Total Heat Transfer to Chamber Wall, Hot Propellants

- Test Data
- Chem-3

Nominal Pressure (psia)

<table>
<thead>
<tr>
<th>Pressure (psia)</th>
<th>Heat Transfer (Btu/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>-6%</td>
</tr>
<tr>
<td>450</td>
<td>+2%</td>
</tr>
<tr>
<td>600</td>
<td>+2%</td>
</tr>
<tr>
<td>750</td>
<td>+6%</td>
</tr>
</tbody>
</table>
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
    - Does not predict consumption of all oxygen in the fuel-rich combustion chamber
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
References


