Large Eddy Simulation of Shear Coaxial Rocket Injector: Real Fluid Effects

Jean-Pierre Hickey, Peter Ma and Matthias Ihme
Center for Turbulence Research, Stanford University
and
Siddharth Thakur
Streamline Numerics Inc.

49th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit
Research Program Objectives

- Develop high fidelity predictive capabilities for identifying the onset of thermo-acoustic instabilities in liquid rocket engines
- We aim to account for:
  - Real fluid effects
  - Wall heat transfer
  - Accurate modeling of topologically complex flames
  - Multi-injector and complex geometry systems
  - Cryogenic injection

Fluid Dynamics
- gas/liquid injection
- hydrodynamic instability
- turbulence

Acoustics
- eigenmodes
- injection coupling

Combustion
- chemical kinetics
- variable heat release
- flame wrinkling
## Topics of Discussion

### Modeling Real Fluid Effects
- Selection of the equation of state
- Determining primitive thermodynamic quantities
- Estimating transport properties

### Numerical Stability
- Numerical methods and stabilization techniques
- Canonical numerical problems

### Validation Cases
- Pure nitrogen mixing case
- Hydrogen/Oxygen injector
State of Real Fluid Research:
Report on work presented at the AIAA JPC
Work by Sandia

Presented:

- *Modeling of High Density Gradient Flows at Supercritical Pressure* (Lacaze & Oefelein, 2013)

Details about the numerics:

- Preconditioning to solve the low-Mach number flow
- Stability guaranteed by flux splitting and flux correction
- The flux correction uses a hybrid third-order scheme with a first-order unwinding
- Classical van Leer and van Albada flux limiters used (errors observed)
- Proposed a new switch based on the convective limiter
Idea behind the convective limiter:

\[
\phi^L = \phi^L_{i-1/2} = \frac{1}{2} (\phi_i + \phi_{i-1}) - \frac{1 - \nu_{i-1/2}(\phi)}{8} (\phi_i - 2\phi_{i-1} + \phi_{i-2}) - \frac{\nu_{i-1/2}(\phi)}{2} (\phi_i - \phi_{i-1}),
\]

\[
\phi^R = \phi^R_{i-1/2} = \frac{1}{2} (\phi_i + \phi_{i-1}) - \frac{1 - \nu_{i-1/2}(\phi)}{8} (\phi_{i+1} - 2\phi_i + \phi_{i-1}) - \frac{\nu_{i-1/2}(\phi)}{2} (\phi_i - \phi_{i-1}).
\]

\[
\nu_{i-1/2}(\phi) = \min \left(1, \max \left(0, \frac{\nu_i(\phi) + \nu_{i-1}(\phi)}{2}\right)\right)
\]

\[
\nu_{CL} = \max \left((A - B_1), (A - B_2)\right) \frac{1}{A + \alpha^{CL} A^{-1} + \varepsilon},
\]
Work by Sandia

Van Albada

Current Limiter
Work by Sandia
Goal: understand the theoretical thermodynamics of multi-species supercritical mixing
Work by Sandia
Developed a theoretical model to parameterize the injection between a diffusion dominated mixing and an atomization/spray regime.
Work by DLR

Presented:

- Continuous Phase Propellant Injection Model for Liquid Rocket Engines (Banuti & Hannemann, 2013)

Objectives:

- RANS based simulation with flamelet-like thermodynamic tabulation
- Tabulated a mixing model for efficient computations
Work by TUM

Presented:

*Large-Eddy Simulation of Turbulent Trans- and Supercritical Mixing*  
(Niedermeier et al., 2013)

Objectives:

- Implementation of the real fluid effects in INCA and OpenFoam
- Modified PISO scheme for pressure correction
Modeling Real Fluid Effects in Rocket Combustors
Real Fluid Effects

Real fluid characteristics:
- Repulsive intermolecular forces
- Sharp gradients
- Strong non-linearities
- High molecular diffusivities
- Localized buoyancy effects
- Reduction of surface tension
- Modification of transport properties

Need to accurately account for real fluid effects
Real Fluid Modeling: Equation of State

- Computationally efficient evaluation of thermodynamic variables
- Validity over large temperature and pressure ranges
- Appropriate mixing rules
- Thermodynamically consistent implementation

Systematic evaluation of various equations of state:
Real Fluid Modeling: Implementation

Implementation of the cubic Peng-Robinson equation of state:

\[
\begin{align*}
    p &= \frac{RT}{v - B_m} - \frac{A_m(T)}{v(v + B_m) + B_m(v - B_m)} \\
    A_m &= 0.457236 \left( RT_{c,\alpha\beta} \right)^2 \left[ 1 + C_{\alpha\beta} \left( 1 - \sqrt{T/T_{c,\alpha\beta}} \right) \right]^2 / p_{c,\alpha\beta,} \\
    B_m &= 0.077796 RT_{c,\alpha\alpha} / p_{c,\alpha\alpha}
\end{align*}
\]

Mixing rules are used for the evaluation of the critical properties (Miller et al., 2001, JFM).
Computation of Thermodynamic Quantities

Transported variables: internal energy $e$ and volume $v$

Initial approximation of temperature $T^0$

Iterate temperature and pressure until $e^n(v, T^n) = e$

Set thermodynamic EOS variables given $T^n$

$A_m, B_m, dp/dT|_{V,X}, dp/dv|_{T,X}$

Compute estimated $P^n$ given $T^n$, $v$, $A_m$ and $B_m$ using the EOS

$P^n$

Compute specific heat departure functions

$c_p, c_v$

Compute the internal energy, $e^n$

$e^n$

Compute the difference in energy $de = e^n - e$

Correct $T^{n+1} = T^n + dT$

Converged? No

$dT = de / C_v$

Converged? Yes

$p^n, T^n$
Transport Properties: Viscosity

Viscosity:

- **increases** with temperature for a gas;
- **decreases** with temperature for a liquid.

![Diagram showing the relationship between viscosity and temperature for liquids and gases.](image-url)
Estimation of the Gaseous Viscosity

Chung’s model (Chung et al., 1984, 1988):

\[ \mu = 36.344 \mu_m^* \frac{\sqrt{M_m T_{cm}}}{V_{cm}^{2/3}} \]

- Excellent estimation in the supercritical phase
- Inadequate estimation in the liquid phase
- Discontinuity for multispecies mixtures with differing signs of acentricity (e.g. H2/O2)
Estimation of the Liquid Viscosity

A simple Andrade model is used to account for liquid viscosity as a function of both pressure and temperature:

\[ \log \mu_l = A_1(p, T) + \frac{A_2(p, T)}{T} \]

The pressure is accounted for in the coefficients of the equation.
Handling Numerical Oscillations
Numerical Methods

Details about the numerics:

- Finite-volume based
- High-order polynomial flux reconstruction at the faces (Ham & Iaccarino, 2004; Khalighi et al., 2010)
- Large eddy simulation with subgrid scale model (Vreman, 2004, PoF)
- Third-order time explicit advancement
- Fully compressible solution of the Navier-Stokes equations

Solution of the Navier-Stokes equations. We solve for:

- density ($\rho$)
- momentum ($\rho u_i$)
- total energy ($\rho E$ where $E = e + \frac{1}{2}u_iu_i$)

The equations are closed with the Peng-Robinson equation of state.
Approach to Handling Numerical Oscillations

- The non-linearity of the EOS leads to highly unstable numerics
- Identification of regions of high sensitivity: \( \left. \frac{p}{\delta p} \frac{\delta v}{v} \right|_T \approx \left. \frac{p}{v} \frac{\partial v}{\partial p} \right|_T \).
Numerical Oscillations

- Dissipation is needed to remove the spurious oscillations
- Dissipation can come from:
  - Artificial viscosity (Terashima et al., 2011; Terashima & Koshi, 2012)
  - Lower-order numerics
- Implementation of a hybrid scheme
- Low-order schemes: first-order upwinding and essentially non-oscillatory (ENO) schemes
- A dual density-based sensor is used locally apply the lower-order numerics
Test Case: Propagating Transcritical Hot Spot

Nitrogen at the following initial conditions:

\[
U = 50 \text{ m/s}
\]
\[
p = 5.0 \text{ MPa}
\]
\[
T(x) = \begin{cases} 
163.8K & \text{if } x \text{ is in } [0.25, 0.75] \text{ m} \\
332.2K & \text{otherwise}
\end{cases}
\]
Test Case: Modified Shu-Osher Problem

Nitrogen at the following initial conditions (Terashima & Koshi, 2012):

if $x$ in $[-5, -4] \text{ m} =$

\[
\begin{aligned}
  p &= 41.32 \text{MPa} \\
  U &= 842.459 \text{m/s} \\
  T &= 596.6 \text{K},
\end{aligned}
\]

if $x$ in $[-4, +5] \text{ m} =$

\[
\begin{aligned}
  p &= 4.00 \text{MPa}, \\
  U &= 0 \text{m/s}, \\
  T &= 272.0 (1 + \sin(5x)) \text{K},
\end{aligned}
\]
Pure Mixing Validation Cases
Transcritical Nitrogen Mixing

- Nitrogen is injected into a pressurized vessel at 4 MPa
- Vessel temperature is 298.0 K
- Injection temperature is 126.9 K
Transcritical Nitrogen Mixing: 2D results (RCM1-case 3)

- Two resolutions: 66,000 and 225,000 control volumes
- Corresponds to 50 grid points within the injector
Transcritical Nitrogen Mixing: 3D results (RCMI1-case 4)

- Two resolutions: 3.5 million control volumes
- 80 control volumes in azimuthal direction
- Minimum spacing 0.005D (inlet diameter)
- Injection temperature is 137 K
Hydrogen/Oxygen Mixing: Setup

- **Outer-stream:**
  - Outer-diameter: 5.6 mm
  - Hydrogen at 275K and 254.9 m/s

- **Inner-stream:**
  - Inner-diameter: 3.6 mm
  - Oxygen at 150K and 8.27 m/s

- Base pressure is 6.0 MPa
- Vessel temperature 275 K
- Adiabatic walls
Hydrogen/Oxygen Mixing: Results
Hydrogen/Oxygen Mixing: Mass Fraction

(Loading Video...)
Conclusions and Future Progress

Conclusions:

- Implementation of a real fluid model for rocket combustors
- Numerical treatment to avoid spurious oscillations
- Validation on experimental test cases

Future work:

- Integrate flamelet-based combustion modeling
- Investigate influence of surface tension in cryogenic jets
- Modeling impedance boundary conditions for real fluids
- Multi-injector and complex geometry real fluid modeling
Thank you, questions?
References


