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14. ABSTRACT Predicting instabilities in liquid rocket engines requires the ability to simulate unsteady reacting flows at high pressures. Intake manifolds, injector design and placement, addition of baffles and acoustic cavities add to the complexity and size of the computational problem at hand. The current effort is focused on the improvement of the basic building blocks which make up the simulation tool. The ability of the toll to track acoustic waves in a low Mach number, unsteady flow with chemical reactions was demonstrated.					
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Combustion Stability Innovations for Liquid Rocket**

**Liquid Rocket Engine Combustion Instability
FA9550-08-C-0014**

Flow instabilities in rocket engines are triggered by the coupling between turbulence, flame fronts and acoustic waves. The ability to resolve scales of turbulence which affect the instability, tracking acoustic wave motions, capturing flame fronts and their interaction with turbulent eddies are required to numerically predict the onset of the instability and its limit-cycle amplitude and frequency. This report summarizes the developments at Metacomp Technologies geared towards rocket engine flow simulation. The focus of the current effort and how it fits in the overall goal of developing an accurate unsteady flow simulation capability is discussed below. Summary of the effort at Metacomp is followed by the research at Penn State and Georgia Tech.

Efforts and Accomplishments at Metacomp Technologies, Inc.

Resolution of acoustic waves in low-speed flows

Modern CFD methods are built on upwinding the inertia terms in the equations. Upwinding provides a systematic way of adding just enough numerical diffusion to prevent oscillations in the flow variables. Upwinding requires knowledge of the local wave speeds. When all the waves in the system are accounted for, numerical diffusion couples all the variables. This is also referred to as matrix diffusion. The main advantage of this strategy is the lack of tuning parameters. However two undesirable effects show up in low speed flow simulation. Firstly, the acoustic speed which is much larger than the flow speed dictates the size of the time step that can be taken within an explicit time update. Since the flow velocity is much smaller, a large number of much smaller time steps will have to be computed before any significant changes in the flow field can be detected. It is possible to overcome this with an implicit time update procedure. The second more detrimental effect arises from matrix diffusion proportional to the acoustic speed which dwarfs the flow speed on some components of the flow. The overwhelming diffusion contaminates the momentum equations. This translates to a fourth order smoothing proportional to the acoustic speed on the velocity field.

Preconditioning methods were developed to alleviate these two difficulties. Artificially lowering the speed of sound in the medium allows for a larger time step while simultaneously reducing the numerical diffusion that affects low speed flow simulation with the conservation form of the equations. While preconditioning works well for steady flow simulation, a dual time stepping scheme is necessary for transient flow simulation where tracking acoustic waves in time is critical to estimating flow dynamics as in a rocket engine. In the dual time stepping scheme, the conservation equations

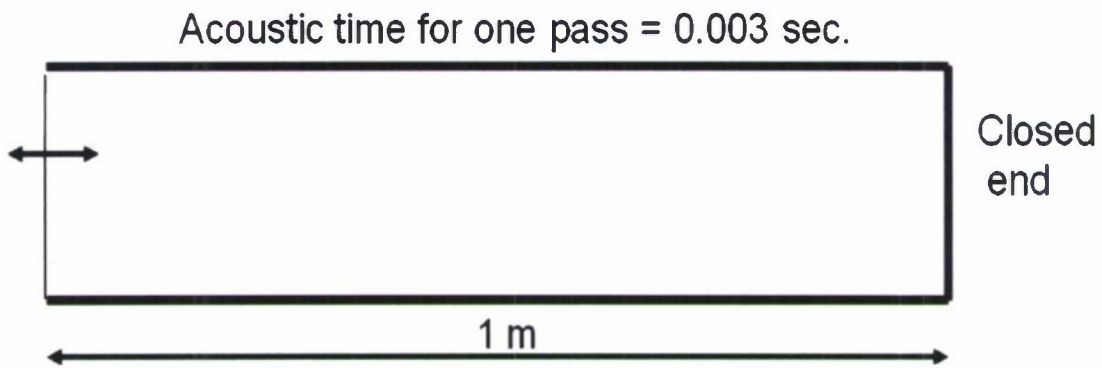
$$\Gamma \frac{\partial P}{\partial \tau} = - \left\{ \frac{\partial Q}{\partial t} + \nabla \cdot F \right\}$$

Q and P refer to the conservation and primitive variables, respectively. Γ is the preconditioning matrix. Convergence in pseudo time τ satisfies the unsteady form of the

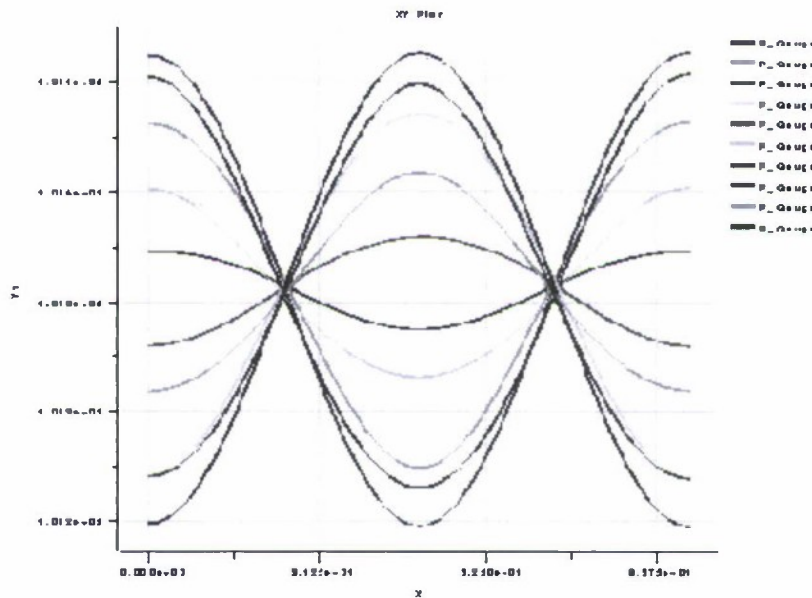
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conservation equations. This approach is consistent with acoustic propagation. However in practice the acoustic waves are heavily damped even with the dual time stepping strategy. A new limiter was developed to control pressure damping which is based on local mesh sizing. If the local mesh size is too large for a given time step size the preconditioning parameter is limited to prevent excessive smoothing of pressure waves.

The following figure shows the geometry of the test case used to assess the ability of the methodology to predict acoustic modes in a pipe open at the left end. An oscillating boundary at the open end generates standing waves within the pipe.



The following figure shows the second harmonic of the quarter wave mode at different time instances. Excellent agreement is obtained with analytical solutions.



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Acoustic Modes in AFRL Combustion Stability Test Rig

Simulations were also conducted to study the acoustic modes in the AFRL Combustion Stability test rig. The acoustic modes in the waveguides were estimated. The following figure shows the pressure wave at 130 Hz.

AFRL Actuator – Mode 1



The mode shape at 2970 Hz is shown below.

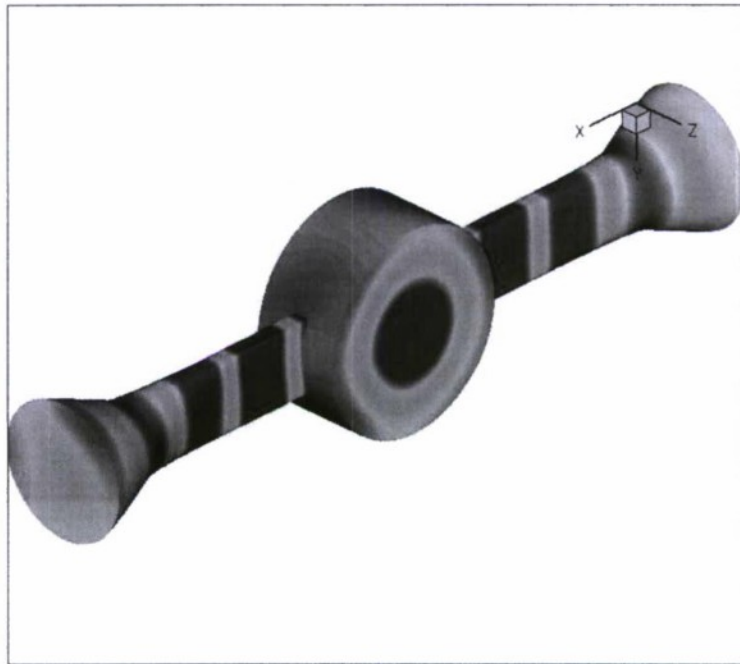


In the two cases shown above, the optical windows remained in place. The acoustic pathway is modeled as a continuous channel. The optical windows mesh seamlessly with

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the walls of the waveguides at the center of the test section. The two drivers at either end can operate at syne or at a specified phase difference.

The effect of close proximity of the optical windows to the combustion zone was addressed before hot firing the rig. Avoiding the optical sections of the wave guides would be advantageous from the point of view of thermal management. Removing the optical section all together would be desirable but its impact on flow evolution was of concern. The changes in mode shapes without the optical sections were investigated by modeling the entire volume of the test section.



The above figure shows pressure waves at a frequency of 2500 Hz. Modes from 130 Hz to 3000 Hz were obtained to study the chambers response. Quiescent condition at room temperature was assumed in evaluating these modes.

Hybrid RANS/LES (LNS) Methodology for Unsteady Flows

The LNS methodology developed at Metacomp Technologies provides a systematic way of LES. The LNS approach minimizes sub-grid dissipation when the computational mesh gets coarser. The LNS model takes mean flow quantities such turbulence kinetic energy and its dissipation and converts them into a fluctuating field of appropriate frequency when the computation grid is sufficient to resolve these scales. It does not need additional quantities which are difficult to measure at the boundaries to start the calculation. When the grid is sufficiently fine all fluctuation generated by the velocity field are resolved. They are converted to mean flow turbulence quantities only when the mesh is coarse.

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Temporal integration

Preconditioning is coupled to a dual time stepping scheme to preserve conservation in real time. The preconditioner operates on the inner loop driving the solution to the next time level. Sufficient number of inner iterations (< 10) is used to maintain second-order time accuracy.

Application to a gas-gas combustor

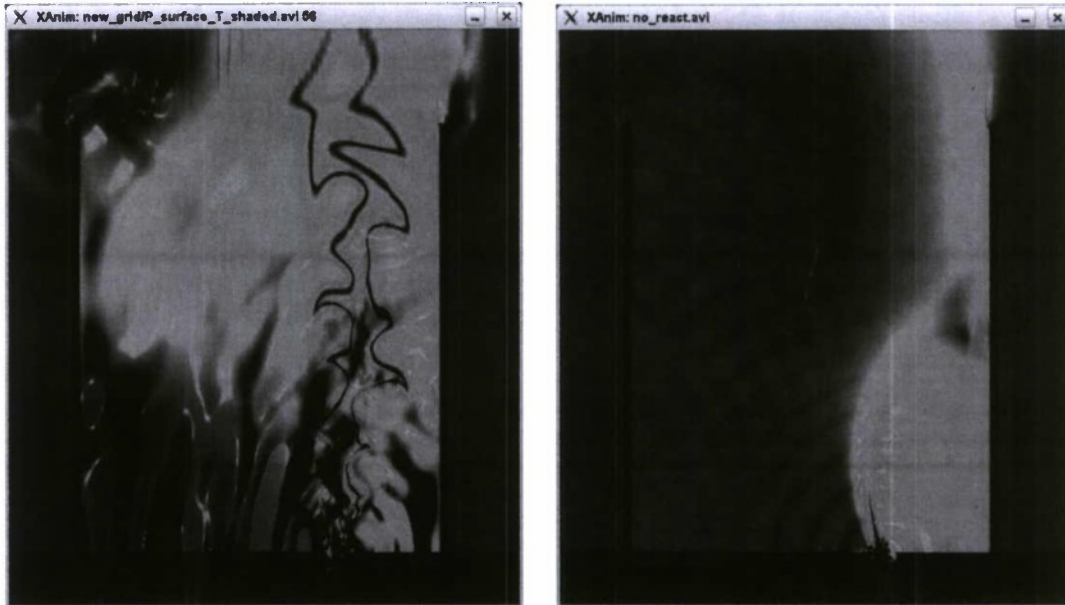
Under a separate effort funded by AFRL, the newly developed algorithm discussed above, was applied to a 2D cross-section of a $\text{CH}_4\text{-O}_2$ gas-gas atmospheric pressure test rig¹ to demonstrate the ability to capture combustion drive pressure oscillations. The results obtained are related to the methods described above and are presented here for completeness. They demonstrate the application of the methodology to simulate unsteady reacting flows.

The inlet geometry was truncated to retain geometric simplicity. A simple one step chemical kinetic mechanism was used in the simulation since the goal was to estimate whether the recent developments to CFD++ could overcome excessive pressure damping of preconditioned systems.

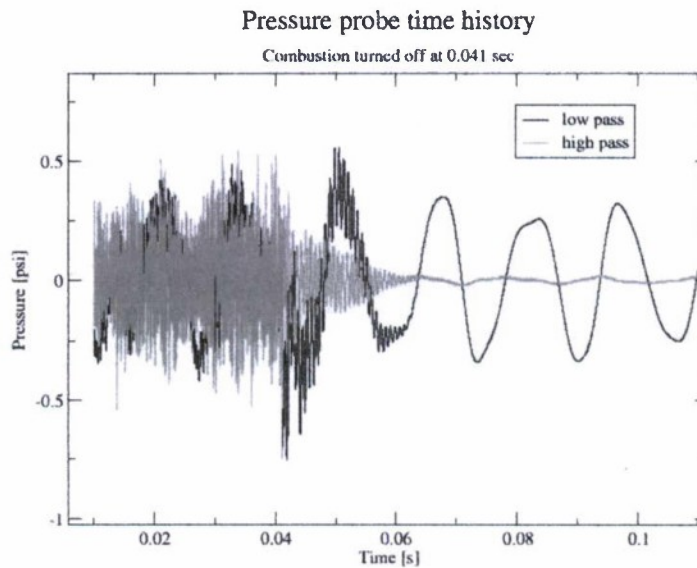
The following figures showing the flow field in the $\text{CH}_4\text{-O}_2$ burner. The figure on the left is with combustion on and shows temperature contours at an instant of time. These contours are raised to display pressure waves. When the reaction was turned off, the pressure oscillations get quieter as shown on the figure to the right. With the combustion off nearly circular pressure waves emanate from the injector corresponding to the frequency at which vortices are shed off. CH_4 contours are used in this figure since combustion is off and temperature remains uniform unlike the reacting flow shown on the left.

¹ Cavitt, R.C. et. al., "On The Laboratory Scale Survey of Pentad Injector Stability Characteristics", AIAA 2007-5587

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The output from pressure probe inside the combustor is shown below.

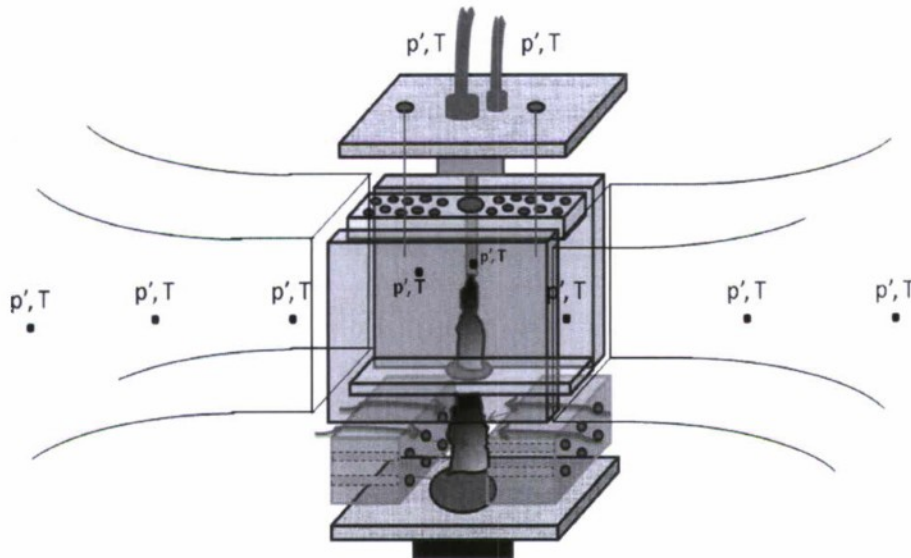


Combustion was turned off at about 0.041 seconds and the green curve in the above figure shows the high frequency content of the pressure tap decay in magnitude without the heat release driving the oscillations. The low frequency oscillations (shown in red) mark bulk sloshing within the chamber at about 70 Hz after the reaction was turned off. Vortex shedding frequency is around 20,000 Hz with significant amplitude of oscillation when reaction was on. The reaction also drives lower frequencies as shown by the red curve prior to 0.041 seconds.

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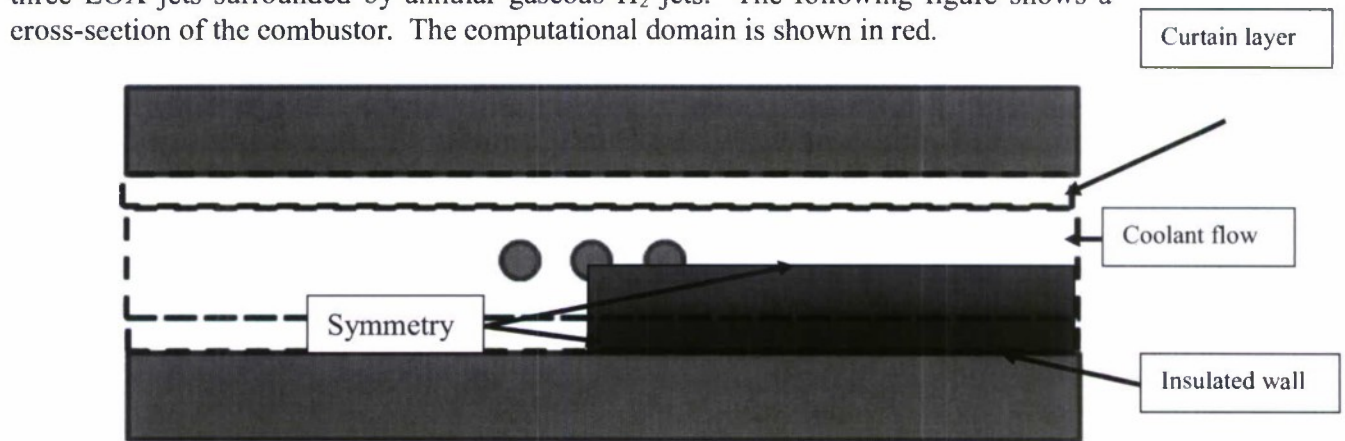
Heat Load on Wave Guides

The combustor stability test rig at AFRL uses acoustic waves to perturb the fuel jet and study its response to acoustic excitation. Wave guides are used to channel the acoustic energy on to the shear layers formed between the fuel and oxidizer jets. Flow diagnostics is facilitated by using optical windows for the waveguide at the center of the test section. A schematic of the facility is shown below.



CFD++ was used to study to simulate the flow through the test section. A top view of the flow chamber is shown in the figure below. Only one quarter of the domain shown in red was modeled for computational efficiency since the steady temperature distribution on the wall marked “insulated” in the figure would be a reasonable estimate for the heat load on the optical windows.

CFD++ was used to simulate steady flow in the AFRL test rig. The test facility contains three LOX jets surrounded by annular gaseous H_2 jets. The following figure shows a cross-section of the combustor. The computational domain is shown in red.



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The mass flow rate was specified for the LOX and gaseous H₂ jets. This was run at stoichiometric conditions. Coolant flow and curtain layer are both employed as the inlet boundary conditions with N₂ streaming at 4.5 m/sec at room temperature. In the computational model only three quarters of the fuel and oxidizer jets were simulated. LOX mass flow rate was 1.44 gm/sec at 100K. Gaseous Hydrogen streams in from the annular jets at 0.18 gm/sec. Temperature of H₂ at inlet was 200K. The LOX jet was modeled using EDP (Eulerian Dispersed Phase) mode in CFD++.

Information Set Type:	Equation set definition
This is information set number 1	
The title tag for this information set is eqnset_define	
Base Type:	Preconditioned Compressible RG NS/Euler
Equation of State:	Ideal Gas
Advection Terms:	Non-Linear
Viscous Terms:	yes
Turbulence Simulation:	◆ RANS ◆ LES
Turbulence Model:	2-equation Realizable k-eps More Models
Number of Color Tracers:	0
Number of Species Eqns. (n-1):	3
Eulerian Dispersed Phase (EDP):	◆ yes ◆ no
Number of Dispersed Species:	1
Energy & Melting Fraction for EDP:	◆ No ◆ Energy Only ◆ Energy + Melting Frac.
Turn on Diffusivity for EDP:	◆ yes ◆ no
Dispersed Phase Model Type:	General EDP mode
Activate Level-Sets:	◆ yes ◆ no
Activate P1 Radiation Model:	◆ yes ◆ no
Conjugate Heat Transfer:	◆ yes ◆ no
<p>Turbulence model recommendations: for transonic flows the R1 model or the cubic k-e closure should be used. For hypersonic flows the R1 model should be invoked. For external aero (where the body is far from the inflow boundary) and for internal flows the k-e-R model should be used. For all other flows, incl. free shear and free convection flows, the k-e or cubic k-e closure should be invoked. FOR UNSTEADY FLOWS USE EITHER THE CUBIC k-e OR THE LNS MODEL.</p>	
<input type="button" value="Accept and Exit"/>	

The figure shown above lists the equations chosen to simulate the flow. The two-equation k-epsilon model (RANS) was used. The carrier phase equations were solved using preconditioning to minimize numerical diffusion. The settings used in preconditioning the equation are shown in the following figure.

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Riemann Solvers: Help

Minimum dissipation on: LHS only LHS and RHS

Activate pressure acceleration: yes no Acceleration factor:

Precond. Lower bound based on: Fraction of max. velocity Specific given velocity

Transient-Case precon. limiting: Acoustic CFL-based limiting No limiting

Precond. turned off initially: yes (give steps below) no

Preconditioning Viscous Limit (Set to zero for Stokes' type flow)

Precond. lower bound velocity: m/s

[Click Here For Help With Preconditioning](#)

Use the "LHS and RHS" minimum dissipation controls for problems in which severe transients exist (e.g. strong shocks and expansions). Make sure that for your final solution, you have ramped DOWN the minimum dissipation to 0.0. Use the "Help set Courant # " button located in the time integration window to get recommended values for "LHS and RHS" parameters and to set them.

A simple one-step chemistry as shown below in the reactions window was employed.

Reaction number ← 1 →

Reaction forward rates are calculated as follows:

$$\text{Rate} = A \cdot \text{pow}(T, N) \cdot \text{pow}(P, K) \cdot \exp(-B / (R \cdot T))$$

A = Freq. Fac. N = Temper. Exp. B = Act. Ener.
P = Pressure/101325.000000 K = Pressure Exp. Unless you are "modifying" the reactions, the coefficient and exponent entries in the reactions below MUST be the same. In thermal non-equilibrium mode, the temperature, T is defined as:

$$T = \text{pow}(Tt, a) \cdot \text{pow}(Tv, b)$$

Tt = Translational Temperature
Tv = Vibrational Temperature
a = Trans. temp. expon.
b = Vib. temp. expon.

This is reaction number 1 Check reaction mass balance

Reactants				Products			
Coef.	Expon.			Coef.	Expon.		
<input type="text" value="2.0"/>	<input type="text" value="2.0"/>	H2	↓	<input type="text" value="2.0"/>	<input type="text" value="2.0"/>	H2O	↓
<input type="text" value="1.0"/>	<input type="text" value="1.0"/>	O2	↓				

Frequency factor: s⁻¹(m³/kmol)^{step_reactants-1} (always SI)

Temperature exponent:

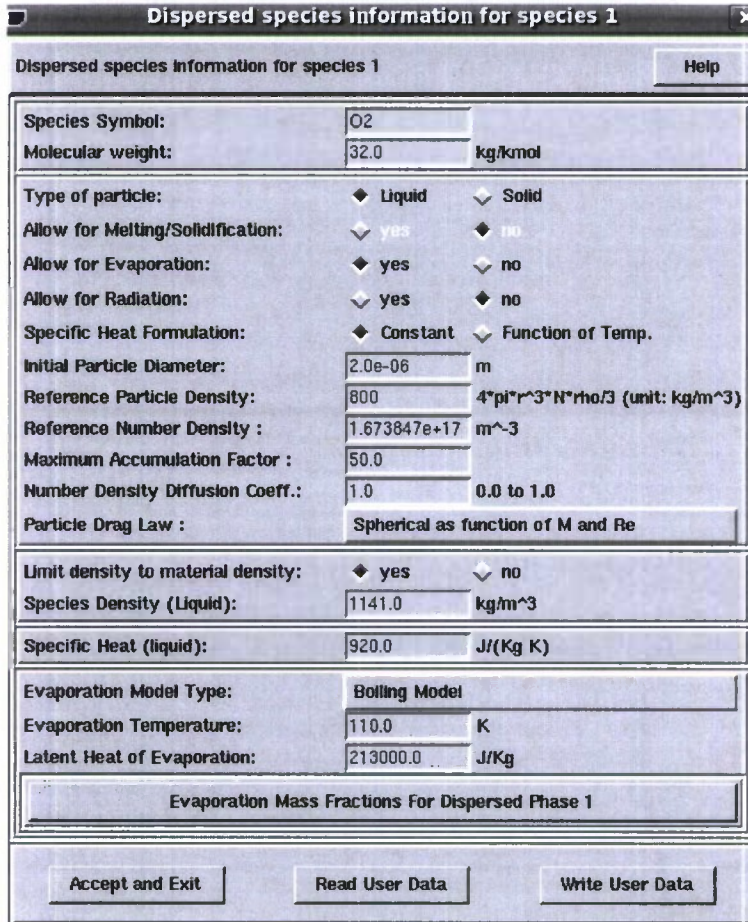
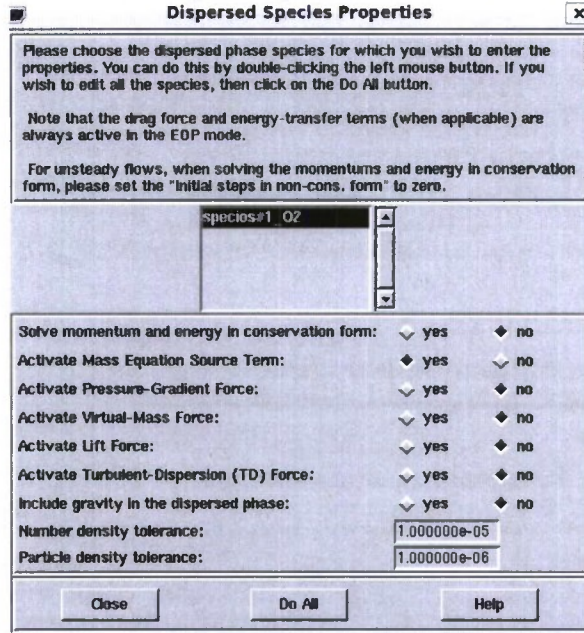
Pressure exponent:

Activation energy: J/kmol or N m/kmol (always SI)

Third Body Efficiencies for Reaction 1

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The options chosen to model the dispersed phase are shown in the following figures.



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The following figure lists the boundary conditions used in the simulation.

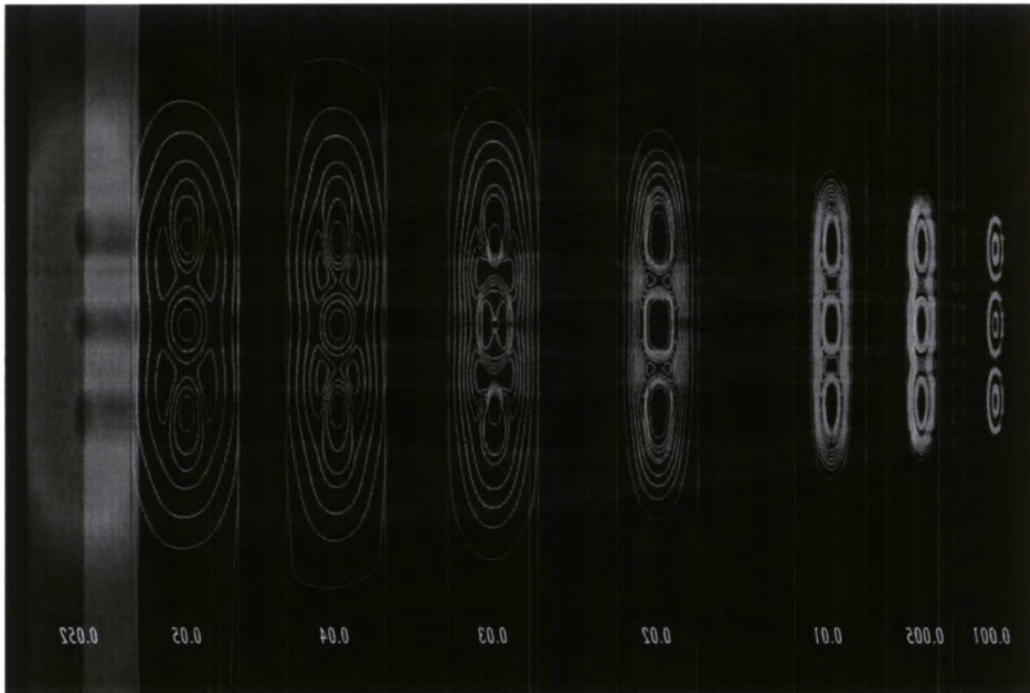
1	Characteristics-based inflow/outflow	CURTAIN_LAYER
2	Characteristics-based inflow/outflow	FILM_COOL_LAYER
3	Symmetry	SYMMETRY1
4	Simple back pressure	OUTLET
5	Symmetry	SYMMETRY2
6	Multi-species inviscid surface tangency	INVISCID
7	Multi-species adiabatic wall function	WALL
8	Mass flow rate and temperature inflow	INNER_JET
9	Multi-species adiabatic wall function	INNER_JET_WALL
10	Multi-species adiabatic wall function	OUTER_JET_WALL
11	Mass flow rate and temperature inflow	ANNULUS_JET

The frozen flow field was initially setup. A heat source was then applied to the near-neighborhood of the injectors to establish the flame. The heater was removed after the flame anchored itself. The time integration mode was switched to unsteady as shown in the following window and calculations were continued until residuals reached a plateau. The overall flux balance at this stage was within 1% of the inflow.

Time Integration:		Help	
Implicit scheme type:	Point-Implicit		
Global time step based on Courant #:	<input checked="" type="checkbox"/> yes <input type="checkbox"/> no		
Spatially Varying local time step:	<input checked="" type="checkbox"/> yes <input type="checkbox"/> no		
At restart, use Courant # for local time step from:	<input checked="" type="checkbox"/> Values Below <input type="checkbox"/> Restart File		
Courant # for local time step ramped from:	1.000000e+00	to:	1.000000e+01
Local Courant # ramped from global step number:	62734	to:	62934
Local Max. Courant # adjustment factor:	0.950000		
Terminate run if adjusted local Courant # is <	1.000000e-04		
Global time step size:	2.000000e-04 s		
Max. # of Internal (local) iter. per global step:	1		
Global step internal iter. termination criterion:	0.100000		
Order of global time stepping:	<input type="checkbox"/> 2nd <input checked="" type="checkbox"/> 1st		
Extrapolate using old dq/dt (1st iteration):	<input checked="" type="checkbox"/> no <input type="checkbox"/> 0th-order		
Local iteration convergence acceler.:	<input checked="" type="checkbox"/> Multigrid (new) <input type="checkbox"/> Multigrid (old) <input type="checkbox"/> Relaxation		Advanced Options
Turn on temporal-smoothing:	<input checked="" type="checkbox"/> yes <input type="checkbox"/> no	Smoothing factor:	0.500000
Turn on time-step spatial-smoothing:	<input type="checkbox"/> yes <input checked="" type="checkbox"/> no		
Turn on extra temp-smoothing for energy:	<input checked="" type="checkbox"/> yes <input type="checkbox"/> no	Smoothing factor:	1.000000e-01
Turn off transient dp/dt term:	<input type="checkbox"/> yes <input checked="" type="checkbox"/> no		
Turn on mass-balance acceleration:	<input type="checkbox"/> yes <input checked="" type="checkbox"/> no	Options	
Accept and Exit		Defaults	
Help Set Numerics		Cancel	

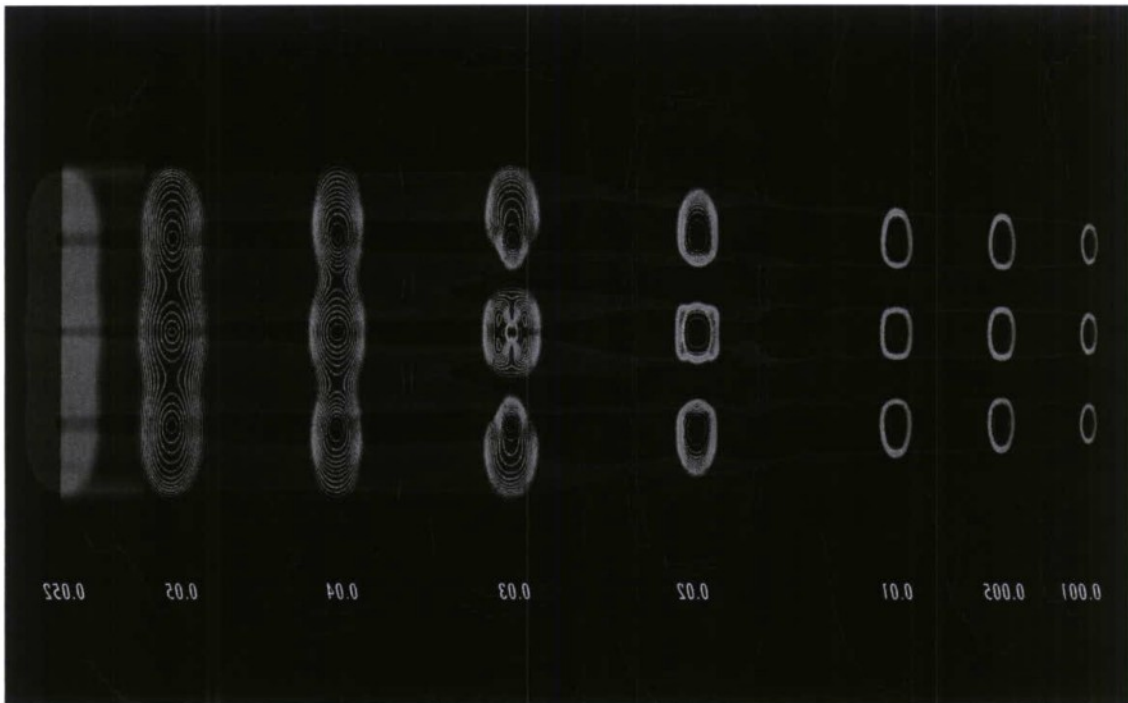
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The next set of figures show the flow field at different streamwise locations. The labels on the contour slices are x locations in meters. The streamwise velocity distribution below shows the development of the shear layer between the fuel and oxidizer streams.

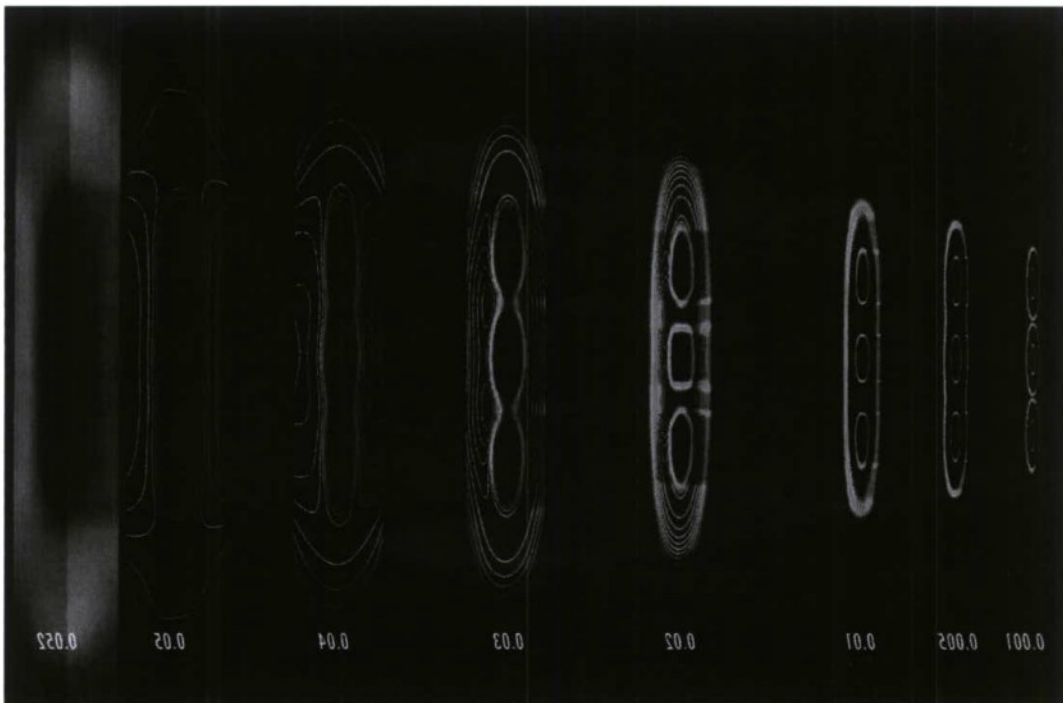


Gaseous O_2 at the corresponding planes can be seen in the next figure. Almost 50 % of the O_2 fluxes out of the domain due to lack of gaseous fuel. The last plane in the following figure shows the amount of O_2 leaving the test section. Lack of complete combustion may be attributed to mixing of the fuel stream with the inert coolant stream.

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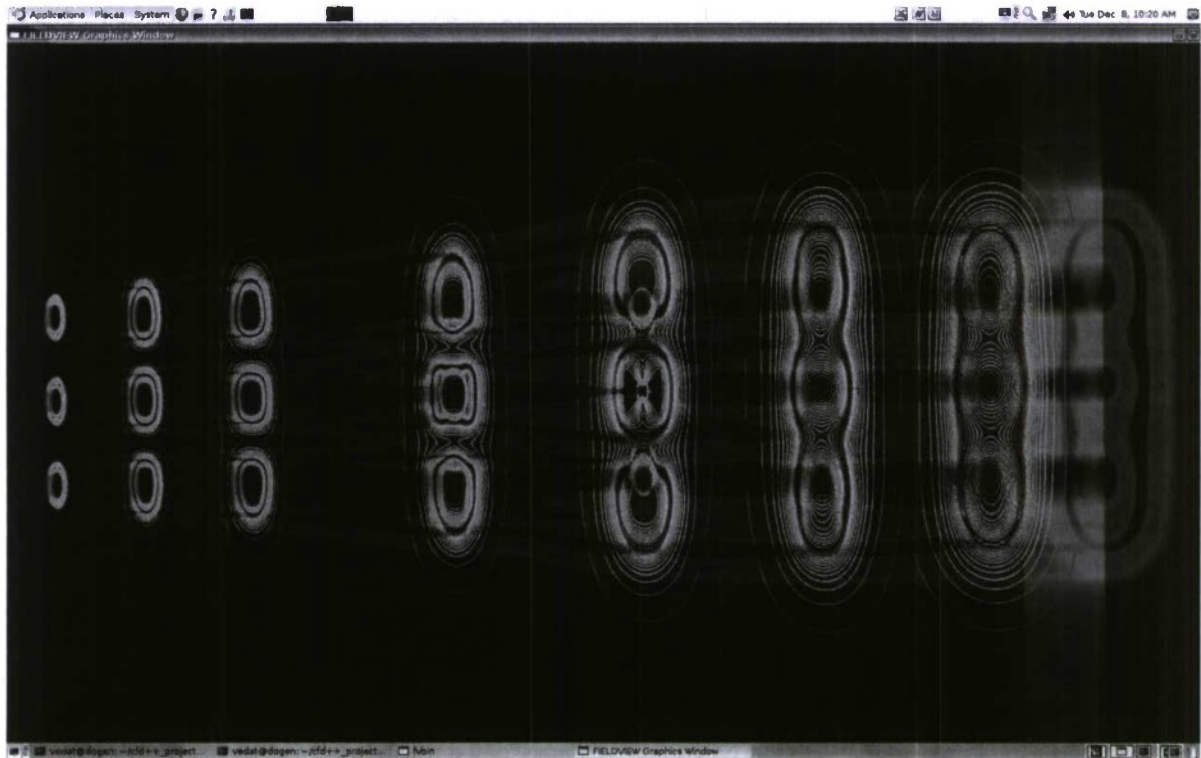


Hydrogen mass fractions (contour levels between 0 and 0.1) at the corresponding locations are shown below. About 50 % of H_2 spills in to the coolant stream and fluxes out of the domain unreacted.

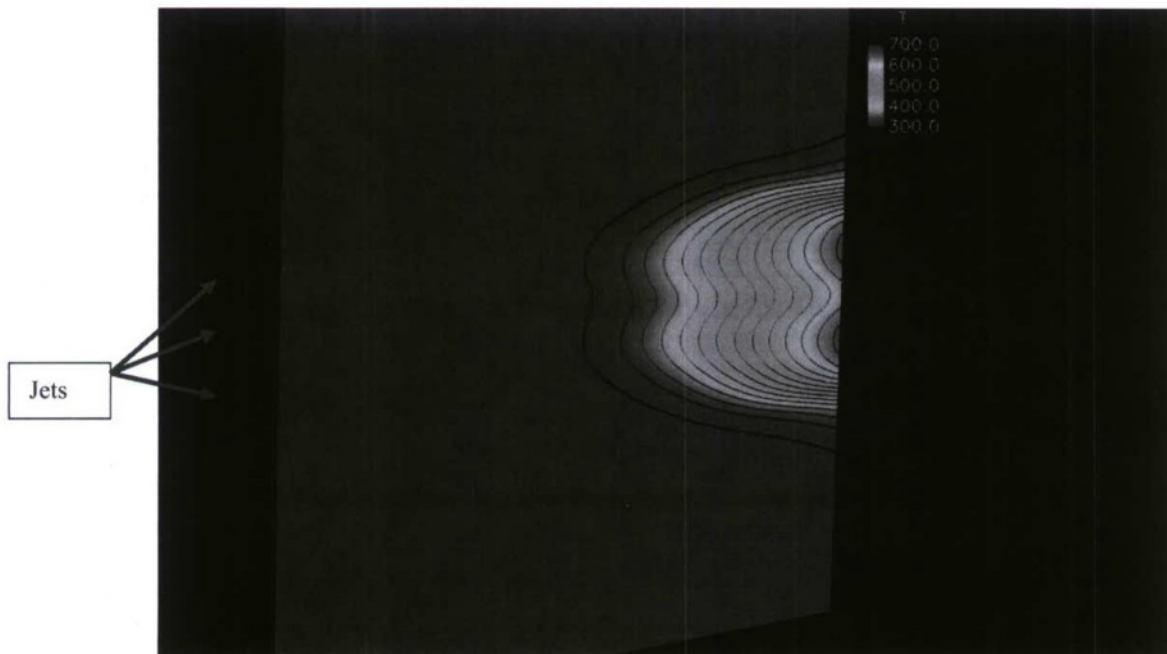


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The next figure shows temperature contours. Flame location on the symmetry plane is also visible.



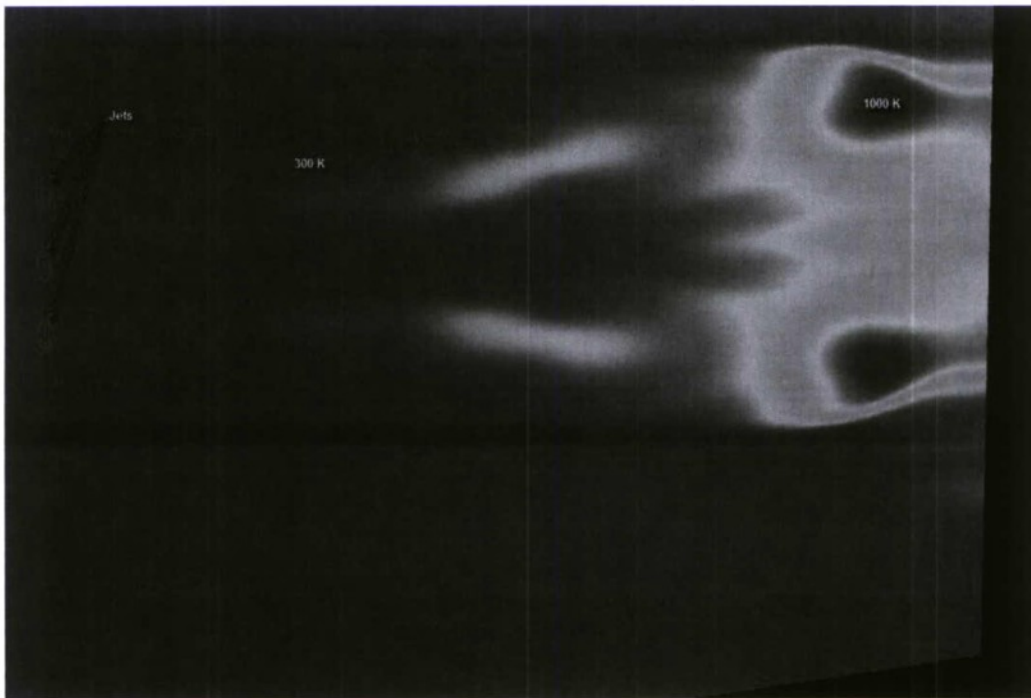
Temperature distribution on the wall is seen in the next figure. The wall temperature of almost 700 K is reached towards the exit of the domain. Adiabatic wall boundary



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condition was used at the wall for this simulation in order to estimate the maximum temperature at the wall. The coolant inflow boundary was subdivided into two sections, one closer to the walls and the other surrounding the three jets. The next set of simulations will alter the inflow velocity in the region next to the wall to estimate the effect of coolant flow rate on maximum temperature at the wall.

A second case at higher chamber pressure produced higher wall temperatures as shown below. The maximum temperature increased to 1000 K at the wall. In this case flow remained unsteady and only an



instantaneous snapshot is shown.

Conclusion

The capability in CFD++ to resolve acoustic oscillations and their coupling with reaction zones was improved. CFD++ can now resolve acoustic oscillations in combustion chambers. Acoustic modes were obtained for AFRL combustor stability test rig under quiescent conditions to study the impact of wave guide on the acoustic response of the fuel/oxidizer jets. Steady state calculations of the test facility are continuing to proceed in order to assess heat load on the wave guide for hot fire cases.

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Effort and Accomplishments at Penn State University and Georgia Tech

Cryogenic Fluid Dynamic Response of Swirl Injector to External Forcing at Supercritical Conditions

This task extends our previous study on the cryogenic fluid dynamics of swirl injectors at supercritical conditions to investigate the dynamic response of the injector to external excitations. The forcing is imposed through periodic oscillations of the mass flow rate at the injector tangential inlet over a wide range of frequencies relevant to the intrinsic flow instabilities of the injector.

The dynamic response of swirling jets to external excitations has been investigated by Panda and McLaughlin¹ using flow visualization techniques. When the jet was excited by acoustic oscillations with discrete frequencies in the upstream region, organized structures evolved from the originally weak, irregular, and large-scale structures under conditions without forcing. Cerecedo *et al.*² found that when a co-flow jet was forced at its natural or sub-harmonic frequencies, the turbulence properties were significantly changed. However, at the forcing frequency twice of the fundamental value, only modest influence was observed. In the experimental study of Gallaire *et al.*³, the vortex breakdown phenomenon was found unaffected by azimuthal forcing at the nozzle periphery since this process was governed by the dynamics in the core region. Bazarov and Yang⁴ developed a generalized linear theory on injector dynamics. Richardson *et al.*⁵ studied the dynamic response of a simple swirl injector using a boundary element method and compared the results with linear theory.

So far, very limited effort has been applied to study cryogenic fluid dynamics in a swirl injector using high-fidelity modeling and simulation techniques, especially at conditions representative of liquid rocket operation. The present task is to develop a LES (large eddy simulation) based numerical framework within which various physical processes and flow parameters dictating the dynamic response of a cryogenic-fluid swirl injector can be studied systematically. The theoretical formulation and numerical approach follow those reported in Zong and Yang.⁶ The injector geometry and boundary conditions are identical to the baseline case of our previous study.⁶ The mean mass flow rate is 0.15kg/s. External forcing is imposed by pulsating the mass flow rate at selected frequencies at the tangential inlet of the injector:

$$\dot{m} = \dot{m}_0 [1 + \alpha \sin(2\pi f_F t)] \quad (1)$$

where \dot{m}_0 and f_F denote the mean mass flow rate and forcing frequency, respectively, and α the oscillation magnitude, which is fixed to be 15%. The forcing frequency covers a range of 0.55-14 kHz, in order to capture the broadband nature of the injector flow dynamics. Turbulence with an intensity of 8% of the mean flow quantity is provided by super-imposing broadband noise onto the instantaneous mass flow rate.

Figures 1-2 show the temporal evolution of the temperature fields at forcing frequencies of 14 kHz and 3.2 kHz, respectively. The 14 kHz forcing does not show any significant

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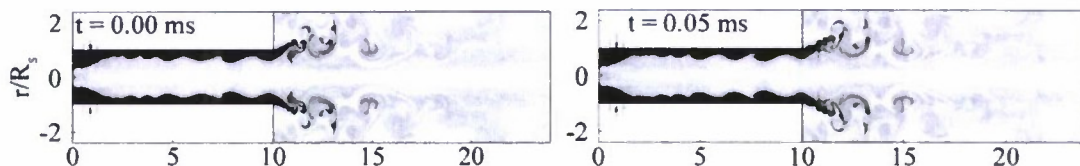
influence on the flow dynamics. The wave structure resembles that of the unforced case. Small disturbances initiated in the upstream region grow as they are conveeted downstream. As noted in our previous study⁶, the wave structure features three-dimensional hydrodynamic instability and propagates in a form similar to the shallow-water wave for an incompressible flow. The high frequency fluctuation decays rapidly and disappears as the LOX film moves downstream due to viscous dissipation. Consequently, forcing at this frequency does not affect the flow field significantly. For the 3.2 kHz forcing case, the wave structures on the LOX film lose their identities shortly after their appearance. They breakup and merge into larger billows. The frequency spectra of pressure fluctuation provide more quantitative insight into the various types of instability waves in the injector flow. Figures 3-5 indicate that the fluctuation magnitude at the forcing frequency stands up in the bulk of the LOX film. In addition, forcing makes the power of other frequency components smaller and the frequency content is reduced greatly, a situation commonly known as the frequency-locking phenomenon. Even the originally dominant fluctuation may lose most of its energy at some forcing frequencies.

Figures 6-9 show the variations of the mass flow rate at the injector inlet and exit for the cases with 3.2 kHz forcing and without oscillation. Forcing causes the mass flow rate and film thickness to vary in a more regular manner and the fluctuation magnitude of the spreading angle becomes larger. Figures 10-11 show the time-averaged film thickness and spreading angle as a function of forcing frequency. The mean film thickness and spreading angle do not change much, due to conservation of mass and momentum.

The injection dynamics can be quantified globally in terms of the mass transfer function, defined as:

$$\Gamma_m(f) = \frac{\hat{m}_e}{\hat{m}_i} \quad (2)$$

where \hat{m}^a is the Fourier component of the mass flow-rate fluctuation at the forcing frequency. The subscripts *ex* and *in* denote the injector entrance and exit, respectively. Figure 12 shows the magnitude of the injector mass transfer function as a function of the forcing frequency. This quantity reaches its maximum around 1.9 kHz, corresponding to the dominant frequency of the intrinsic injector flow instability under the condition without external forcing.



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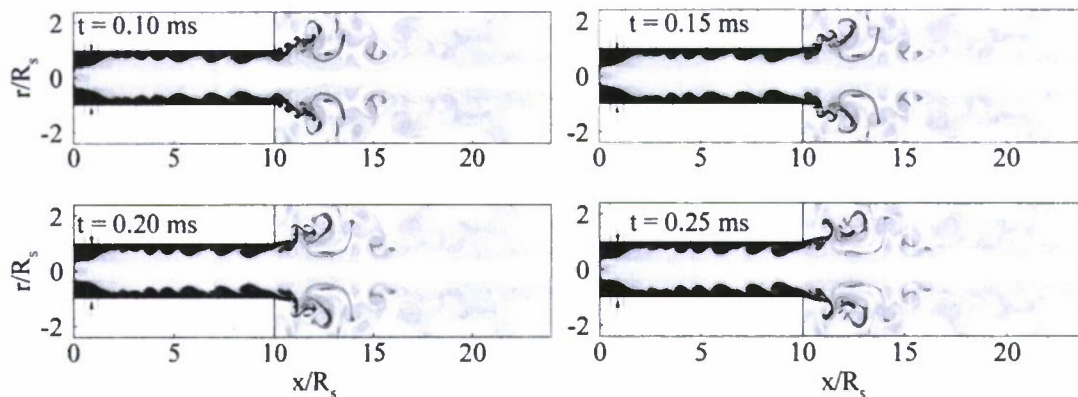
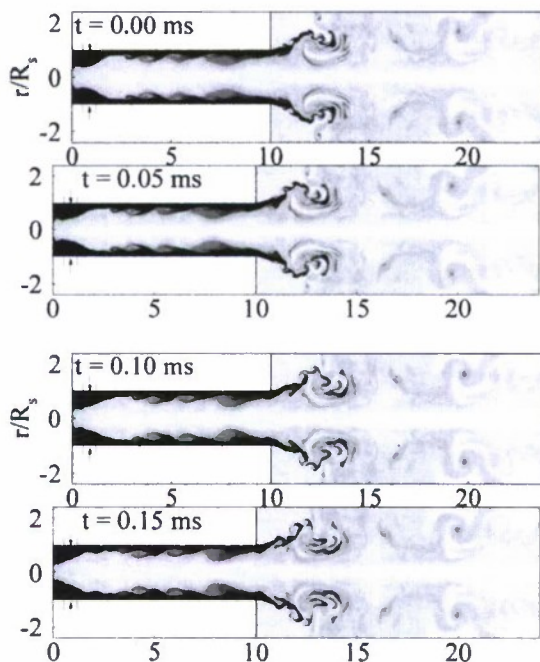


Figure 1. Temporal evolution of temperature field, external forcing at 14 kHz.



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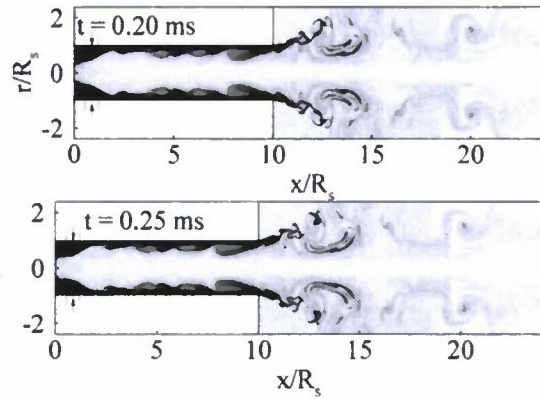


Figure 2. Temporal evolution of temperature field, external forcing at 3.2 kHz

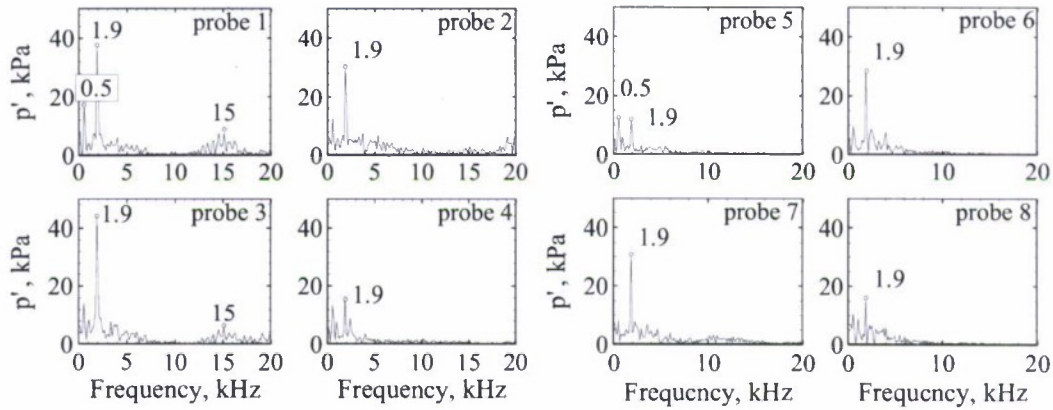


Figure 3. Power Spectral densities of pressure fluctuations at different locations inside injector, external forcing at 1.9 kHz

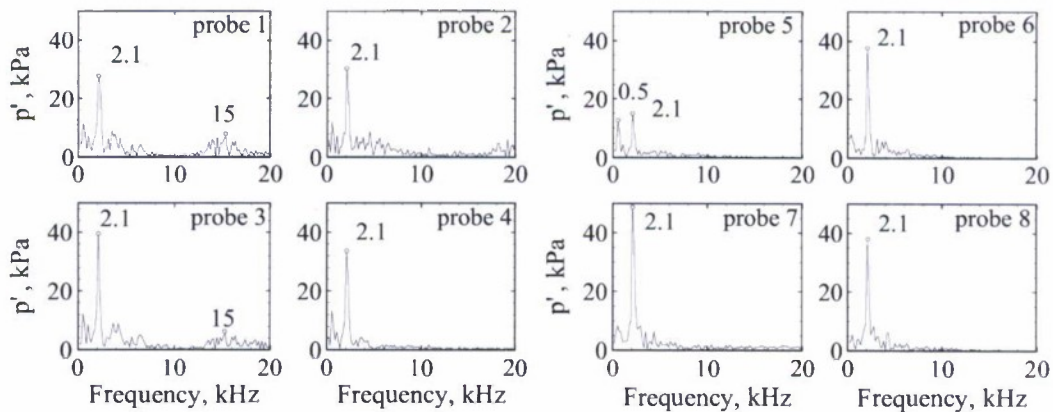


Figure 4. Power Spectral densities of pressure fluctuations at different locations inside injector, external forcing at 2.1 kHz

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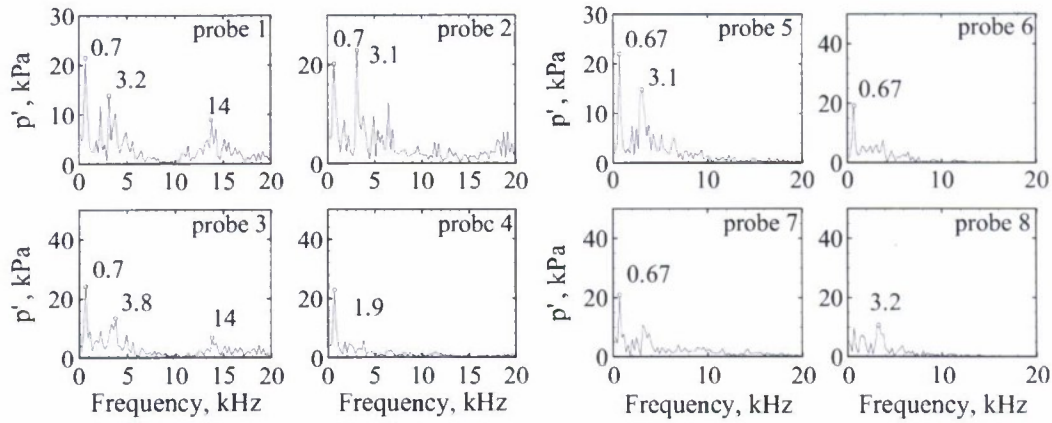


Figure 5. Power Spectral densities of pressure fluctuations at different locations inside injector, external foreing at 3.2 kHz

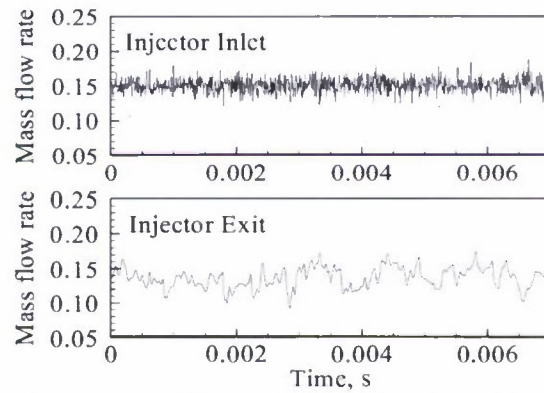


Figure 6. Mass flow rates at injector inlet and outlet without external forcing

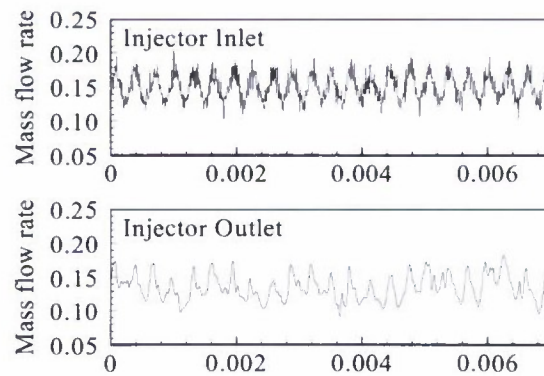


Figure 7. Mass flow rates at injector inlet and outlet with external forcing at 3.2 kHz

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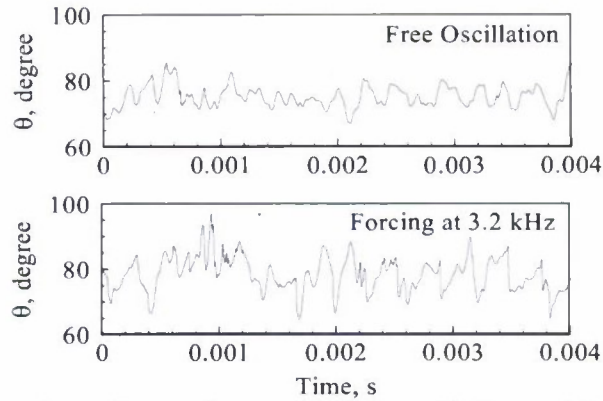


Figure 8. Comparison of spreading angle; free oscillation and 3.2 kHz forcing.

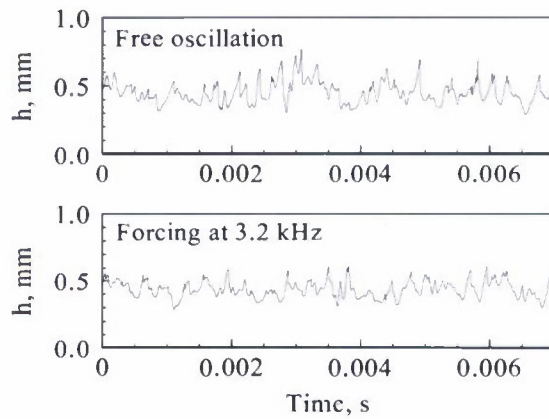


Figure 9. Comparison of injector exit film thickness; free oscillation and 3.2 kHz forcing.

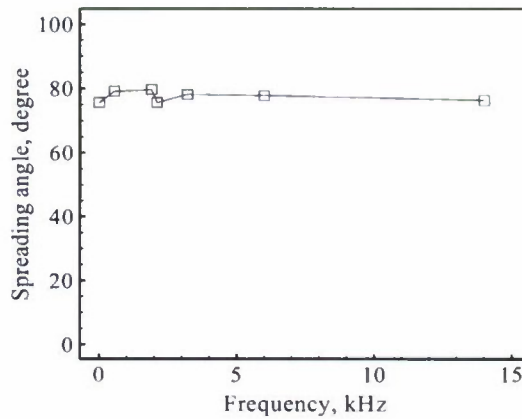


Figure 10. Variation of spreading angle with forcing frequency

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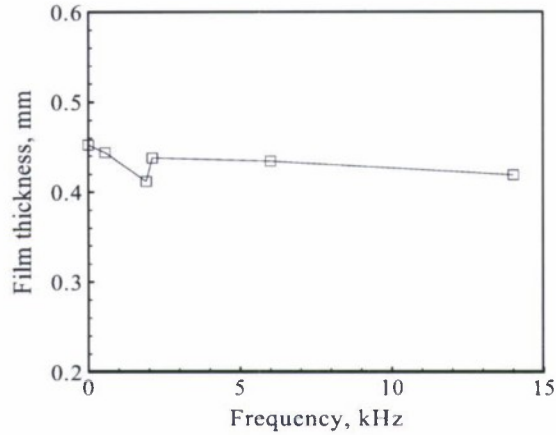


Figure 11. Variation of film thickness at injector exit with forcing frequency

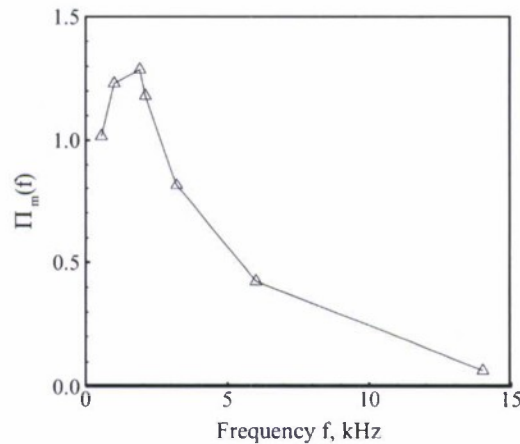


Figure 12. Frequency spectrum of magnitude of injector mass transfer function

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