



MURI Kick-off Meeting: Discovering & Modeling Turbulence and Chemistry Interactions
in High Speed Reactive Flows, December 9, 2021

CFD Modeling for Scramjet Engine Design and Evaluation: Current Practices and Future Needs

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- **Current Role of CFD in Scramjet Engine Design and Analysis**
 - Reynolds-Averaged Simulations
 - Current modeling practices
- **Physics modeling and current SoA limitations (RAS)**
 - Forebody flow physics modeling
 - Inlet flow physics modeling
 - Isolator flow physics modeling (DMRJ)
 - Combustor flow physics modeling
 - Exhaust nozzle flow physics modeling
- **Summary**
 - Where engineering application CFD stands
 - Beyond the current SoP (hybrid RAS/LES, LES, ...)

Current Role of CFD in Scramjet Development



- **Current SoA for CFD analysis of hypersonic propulsion systems are Reynolds-averaged simulations**
 - All scales of turbulence are modeled → often leading source of uncertainty
 - Boussinesq approximation → linear eddy viscosity models (LEVM)
 - Gradient diffusion assumption with constant Pr_t and Sc_t
 - Turbulence-chemistry interactions neglected (or crudely modeled)
 - Modeling strategy is relatively mature with only “evolutionary” improvements documented over the past 20+ years
- **Scale-resolved simulations have the potential to substantially reduce model-form uncertainty**
 - Only the smaller turbulence scales are modeled (larger scales resolved but with a substantial increase in computational cost)
 - Larger scales responsible for “stirring” of fuel and air streams → geometry governed mixing processes are primarily resolved
 - Smaller scales more universal in nature (presumably easier to model)
 - Model uncertainty (related to turbulence) can be reduced with grid resolution
 - SRS is less effective at reducing model uncertainty for TCI

Reynolds-averaged Equation Set



$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0$$

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j + \delta_{ij} \bar{P}) = \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} - \overline{\rho u_i'' u_j''})$$

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{E}) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{H} \tilde{u}_j) = \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} \tilde{u}_i + \overline{\tau_{ij} u_i''} - \bar{q}_j - \overline{\rho k'' u_j''} - \overline{\rho h'' u_j''} - \tilde{u}_i \overline{\rho u_i'' u_j''})$$

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{Y}_m) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{Y}_m \tilde{u}_j) = - \frac{\partial}{\partial x_j} (\overline{\rho Y_m V_j} + \overline{\rho Y_m'' u_j''}) + \bar{\dot{w}}_m$$

$$\bar{P} = \overline{\rho R T} = R_u \sum_{m=1}^{ns} \left(\frac{\bar{\rho} \tilde{Y}_m \tilde{T} + \overline{\rho Y_m'' T''}}{W_m} \right)$$

Reynolds Stress Closure Models



- **Reynolds stress typically modeled via the Boussinesq assumption:**

$$\overline{\rho u_i'' u_j''} = \frac{2}{3} \delta_{ij} \left(\bar{\rho} \tilde{k} + \mu_t \frac{\partial \tilde{u}_k}{\partial x_k} \right) - \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$

- **Typical eddy viscosity models:**
 - Zero-equation models (e.g., Baldwin-Lomax)
 - One-equation models (e.g., Spalart-Allmaras)
 - Two-equation models (e.g., k- ϵ , k- ω)
- **LEVMS are deficient in several areas:**
 - Unable to capture stress-induced secondary flow structures (Reynolds-stress anisotropies)
 - No direct avenue to incorporate pressure-strain correlation effects
 - No rigorous accounting for streamline curvature effects
- **Non-linear constitutive relationships and rotation/curvature corrections can address the above deficiencies**
 - Quadratic constitutive relationship (Spalart [2000],[2013],[2020])
 - Explicit Algebraic stress models (Rumsey et al. [2003])
 - Rotation/Curvature corrections (Shur et al. [2000])

Reynolds Flux Vector Closure Models



- Reynolds flux vectors typically modeled via gradient diffusion closures:

$$\overline{\rho g'' u_j''} = -\frac{\mu_t}{\sigma_t} \frac{\partial \tilde{g}}{\partial x_j}$$

- The rate of diffusion is controlled by the specification of σ_t
 - σ_t corresponds to the turbulent Prandtl number for the Reynolds heat flux vector
 - σ_t corresponds to the turbulent Schmidt number for the Reynolds mass flux vector

Typical Turbulent Prandtl & Schmidt Number Values

Flow Field	Pr_t	Sc_t
Planar Jets	0.2 - 3.0	0.1 - 2.2
Round Jets	0.7 - 2.0	0.1 - 2.0
Backward Facing Step	0.7 - 3.0	NA
Jet into Cross Flow	NA	0.1 - 0.5
Injection Behind a Bluff Body	NA	0.2 - 0.7

- Gradient diffusion closures intended for shear dominated scalar mixing
- Extensions to the simple gradient diffusion closures have been proposed (e.g., Bowersox [2009]) with some success

Turbulence-Chemistry Closure Models



- Common closures are mixing controlled models (Magnussen and Hjertager [1976]) or the laminar-chemistry assumption, e.g.,

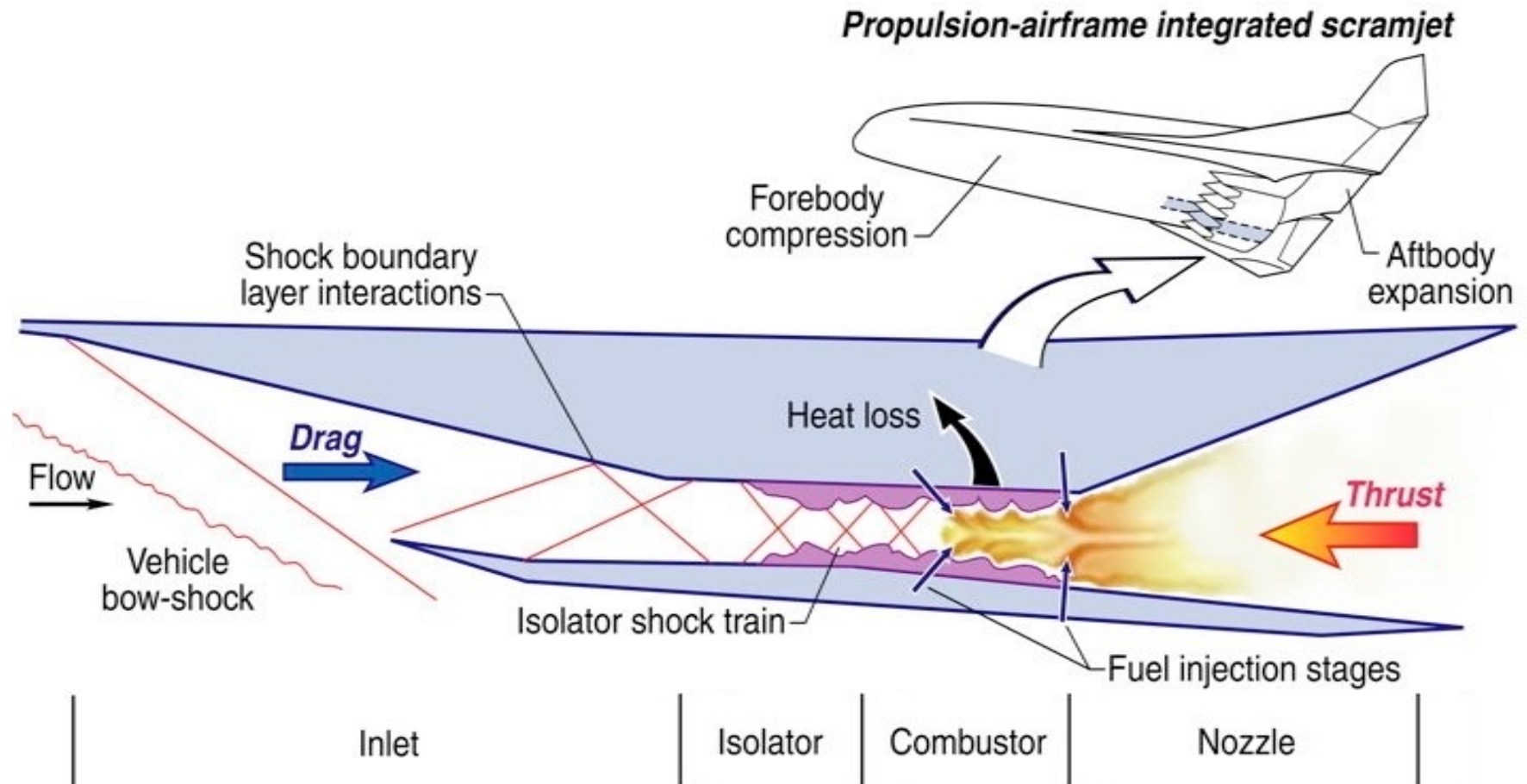
$$\overline{\dot{w}_m} \approx \dot{w}_m(\tilde{T}, \bar{\rho}_1, \dots, \bar{\rho}_{ns})$$

- Turbulent fluctuation effects on the chemistry can be more rigorously handled using PDF's:

$$\bar{\dot{w}_m} = \int \dot{w}_m(\hat{T}, \hat{\rho}_1, \dots, \hat{\rho}_{ns}) \mathcal{P}(\hat{T}, \hat{\rho}_1, \dots, \hat{\rho}_{ns}) d\hat{T} d\hat{\rho}_1 \dots d\hat{\rho}_{ns}$$

- The form of the PDF can be assumed a priori, or an evolution equation can be integrated for it
 - PDF evolution equations are theoretically sound (Pope, 1995), but computationally expensive
 - Assumed PDF approaches are relatively cheap, but lag theoretical rigor
- To reduce computational costs, the turbulent chemistry process is sometimes parameterized as a function of some number of scalars
 - Flamelet models (e.g., Terrapon et al. [2009]) typically parameterize the combustion process with mixture fraction and its variance, reaction progress variable, and pressure

Scramjet Engine Flow Features



Forebody physics & modeling limitations with RAS



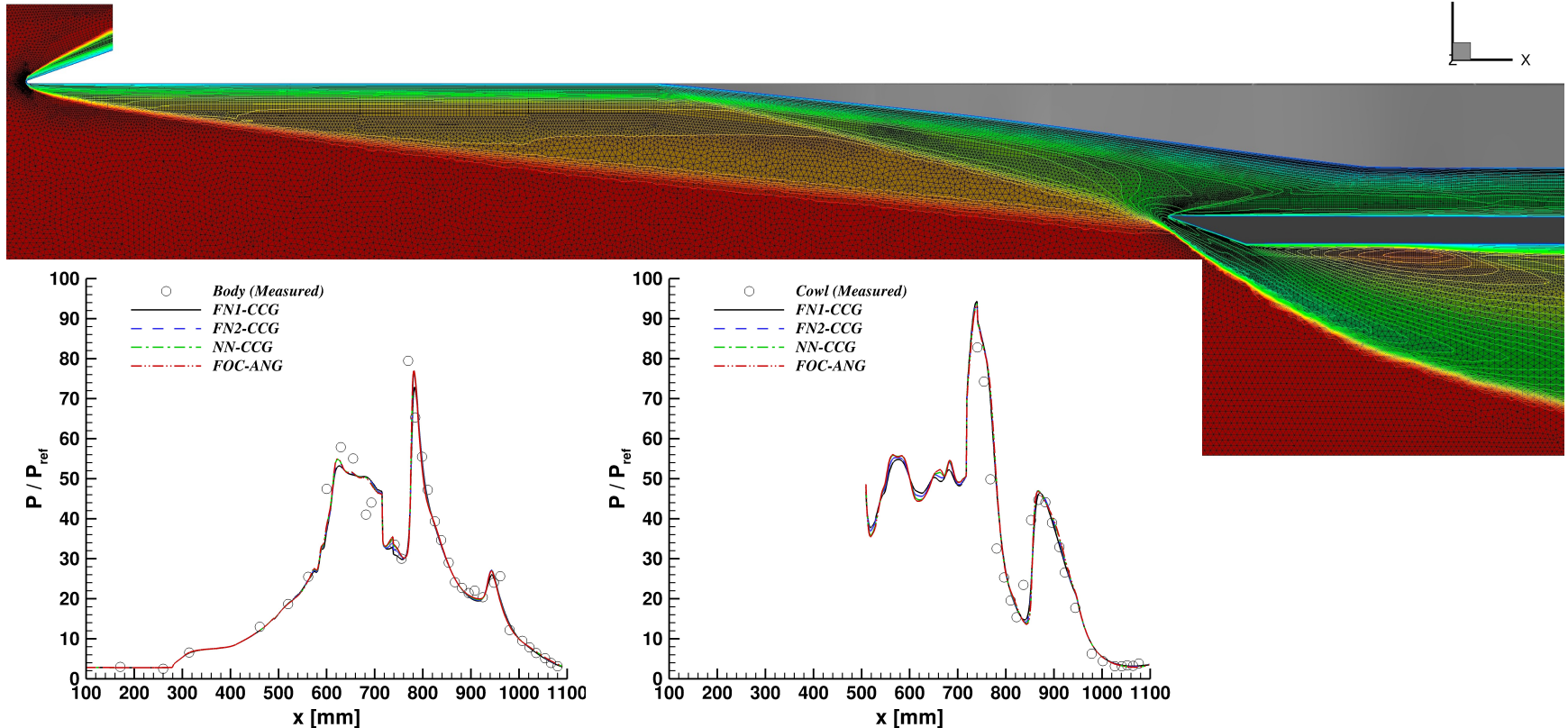
- **The forebody (if present) initiates the compression process of the propulsion system**
- **The most difficult phenomenon to predict for this scramjet engine component is the transition physics from laminar to turbulent flow**
 - Boundary layer instabilities (e.g., Gortler vortices) are typically not captured with RAS approaches and these effects can persist over long distances and affect engine performance.
 - Commonly used RAS based transition models (e.g., Langtry-Menter 4-equation model [2009]) have been formulated on the basis of low-speed measurements/database correlations, and cannot be relied upon for transition prediction in hypersonic flows.
 - Transition predictions based on off-line linear stability analyses have been more successful in the context of natural transition on smooth surfaces (likely transition scenario on forebodies in the absence of tripping).
 - **Can data-driven models based on LST be formulated to improve the SoA in a RAS context or maybe ROM's in a coarse-grid scale-resolving context?**

Inlet physics & modeling limitations with RAS



- **The role of the inlet in a hypersonic air-breathing propulsion system is to capture and compress a portion of the exterior airflow to provide the oxidizer (at sufficiently high pressure without excessive dissociation) to furnish favorable conditions for combustion within the engine**
- **CFD simulations of the inlet system are used to provide information about the following metrics across the entire flight envelope:**
 - 1) Mass capture (1st-order impact on engine thrust)
 - 2) Inlet compression efficiency (speaks to the losses of the inlet compression process)
 - 3) Inlet starting (at what Mach number will the inlet self-start?)
 - 4) Inlet unstart (how resilient is the inlet to remaining started during maneuvers?)
- **To answer these questions, the following physical phenomenon must be predicted adequately:**
 - Shock / Boundary Layer Interactions ... the prediction of whether the SBLI leads to flow separation, and if so how much, impacts both the 2-4 above.
 - Vortical structures caused by surface curvature effects and/or corners
 - pressure gradient induced vortical structures typically dominate, but stress-induced vortices may be important as well → this latter phenomenon cannot be predicted by standard linear eddy viscosity models.

Inlet physics & modeling limitations with RAS



- Existing RAS closures are typically adequate for on-design inlet performance analysis
 - Off-design more problematic due to stronger SBLI → separation more likely
- Inlet unstart (or starting) dynamics is an inherently unsteady process with massive flow separation
 - Uncertainty with URAS unacceptable → SRS typically required

Isolator physics & modeling limitations with RAS

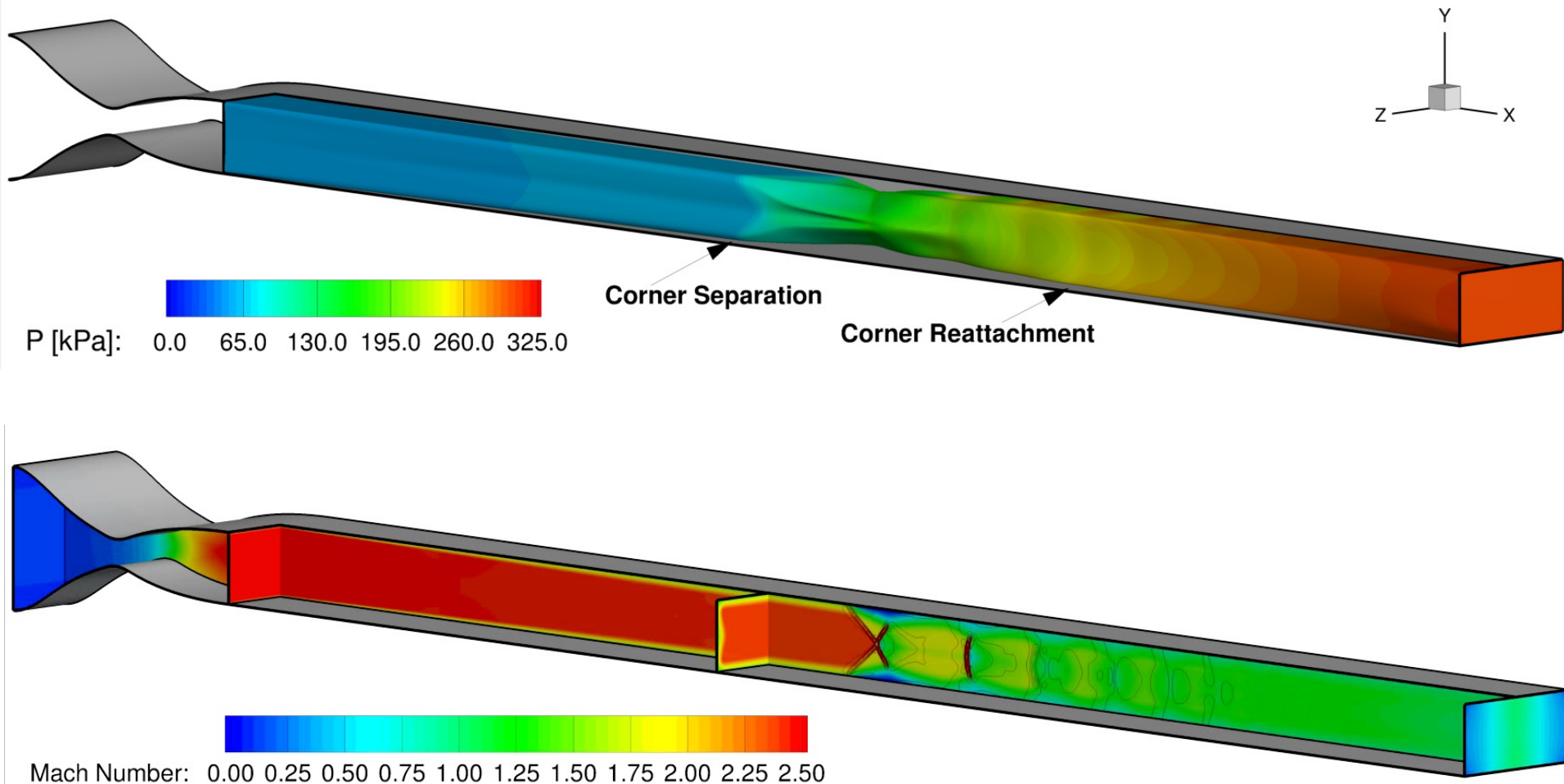


- **The role of the isolator is to contain the combustion induced pressure rise during DMRJ operation ($M_\infty < 7$) to prevent the resulting shock train from propagating into the inlet and causing the engine to unstart**
- **The primary metric of importance for the engine isolator is the maximum allowable pressure rise that the isolator can withstand**
- **In order to predict this quantity, the turbulence model must accurately capture:**
 - Skin friction distribution after the inlet compression process
 - Resistive force that controls the position of the shock train
 - Massively separated flow that results from multiple Shock / Boundary Layer Interactions through the shock train
 - Determines the strength of the incident shock and each shock reflection
 - Boundary layer recovery during the diffusion process downstream of the shock train
 - Governs the rate of post-shock system pressure rise
- **RAS turbulence closures struggle with proper prediction of massively separated flow ... typical uncertainty in predicting the incident shock train position at high pressure ratios is on the order of 5-8 δ , which can translate to several isolator duct heights for smaller scramjet engines**

Isolator physics & modeling limitations with RAS



- Isolator flow structure present during DMRJ operation

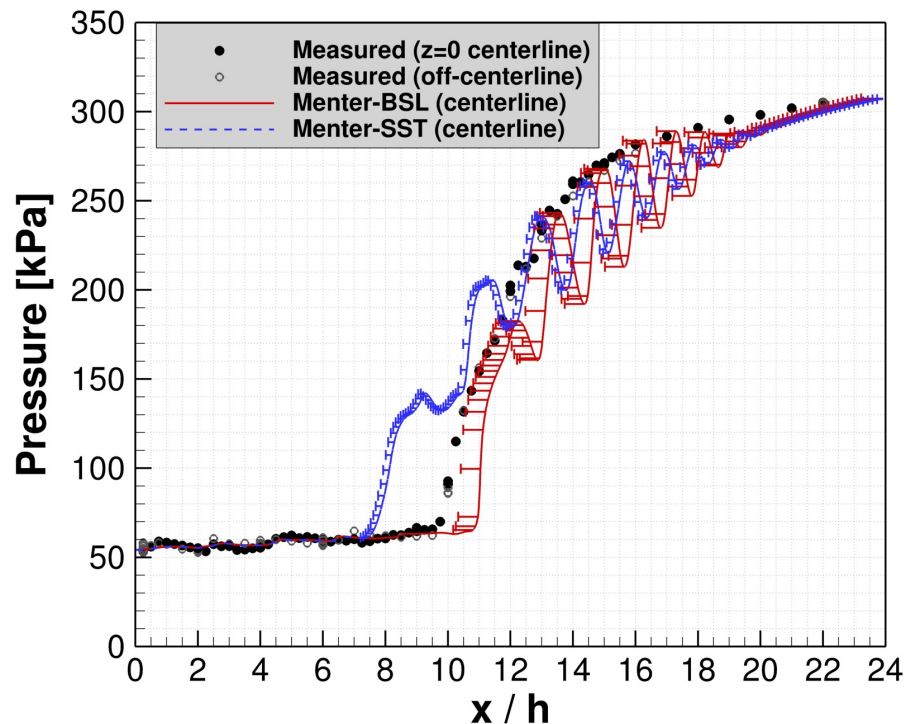


Isolator physics & modeling limitations with RAS

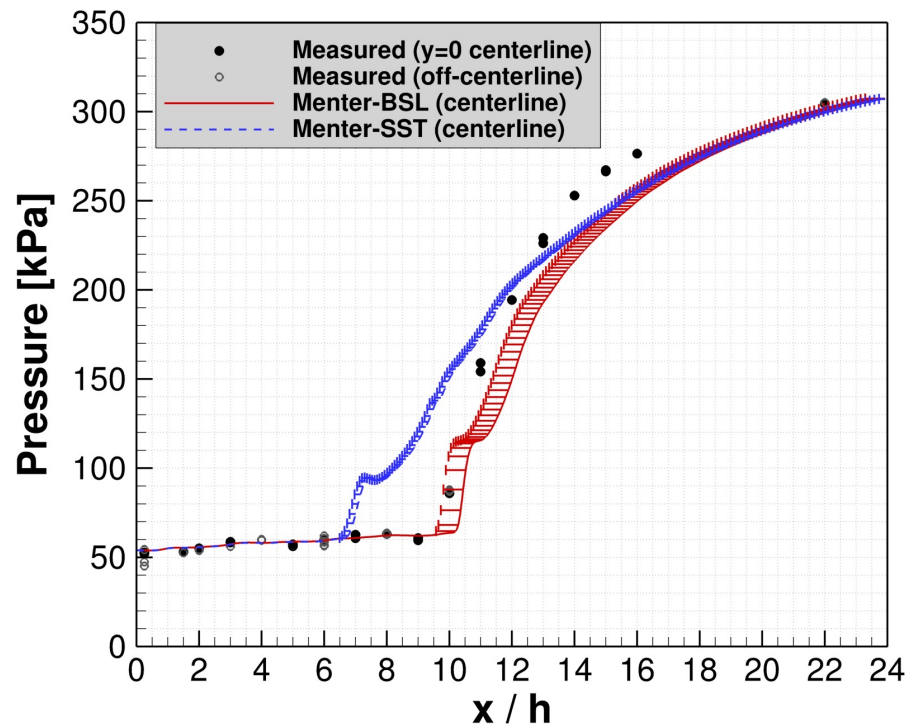


- Isolator shock train predictions from 2 common RAS closures
 - Shock train position differs by nearly 4 duct heights
 - Detailed shock/boundary layer separated flow structure by both models show discrepancies

Contoured Wall



Side Wall

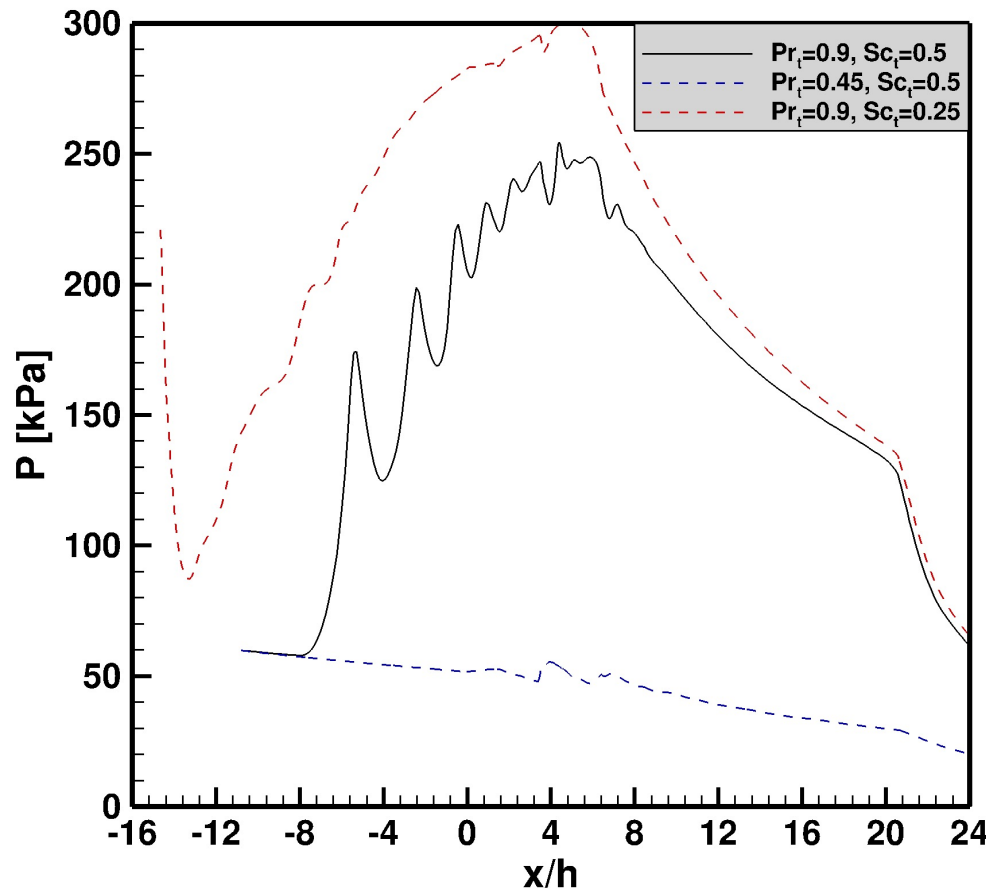
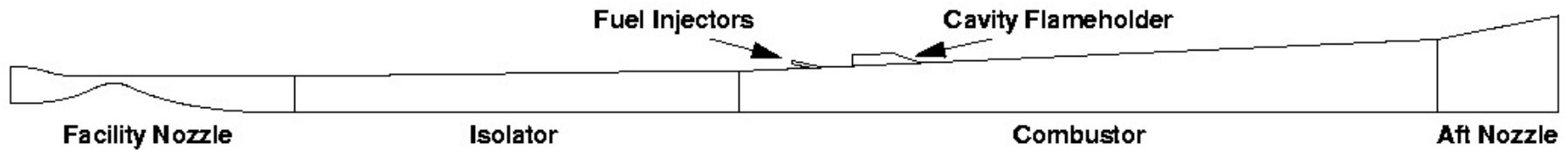


Combustor physics & modeling limitations with RAS



- **The scramjet engine combustor is tasked with adding chemical energy to the flow to enable thrust generation when the engine flow is expanded through the exhaust nozzle**
- **CFD simulations of the combustor need to provide information on some (or all) of the following metrics:**
 - How efficient the fuel and air are mixed and the losses associated with mixing
 - Robustness of flameholders used to sustain combustion
 - How much chemical energy is released
 - Distribution of the heat release
 - Information on ignition (where to place ignitors and what ignition system to employ)
 - Heat loads and distribution to inform the cooling system design
- **The following physical phenomenon must be predicted adequately:**
 - Turbulent fuel/air mixing rates (limited residence times imply low margin of error)
 - Chemical kinetics (residence time similar to ignition delay time)
 - TCI → under what circumstances is this a leading modeling concern?
 - Heat transfer to walls will be severe and using fuel as a coolant must be balanced with required fuel rates for combustor operation

Combustor physics & modeling limitations with RAS

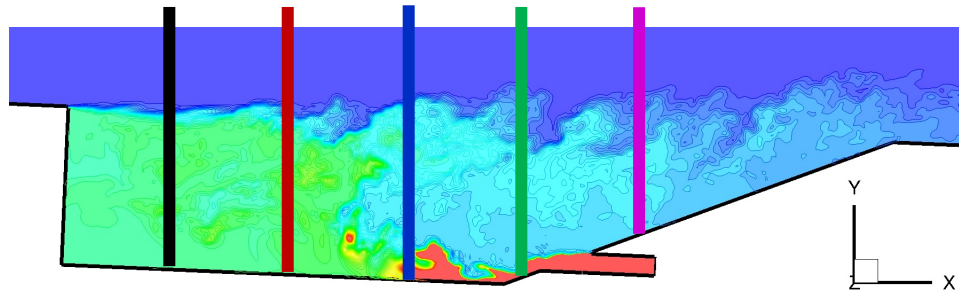


Physical process time scales can be very similar making scramjet combustor predictions extremely sensitive to modeling choices!

RAS models applied to scramjet combustors are unreliable and rely on calibrations (typically) to offer any predictive value.

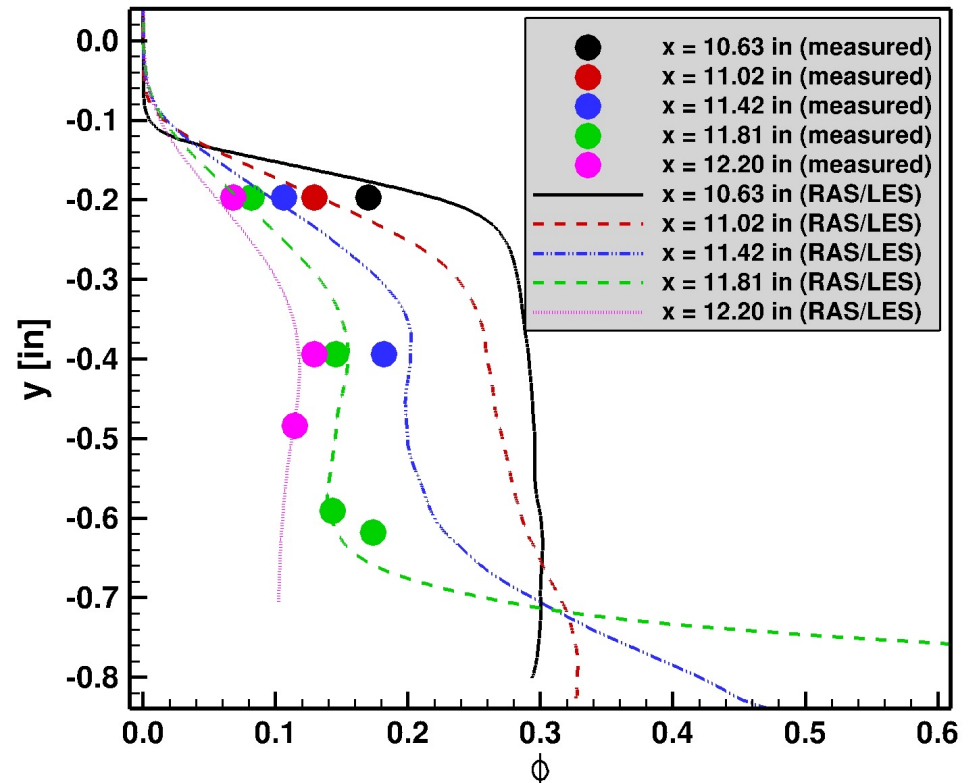
Scale-resolving simulations likely required to significantly improve combustor predictions.

Use of SRS to Calibrate RAS Closure Constants

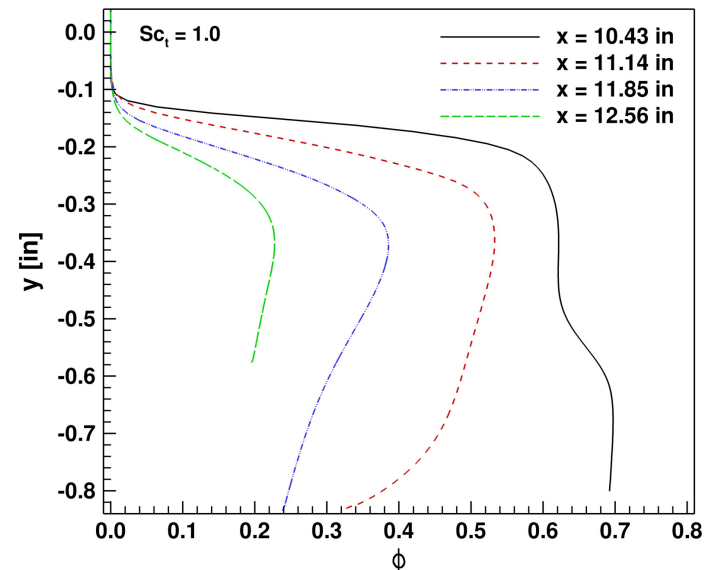
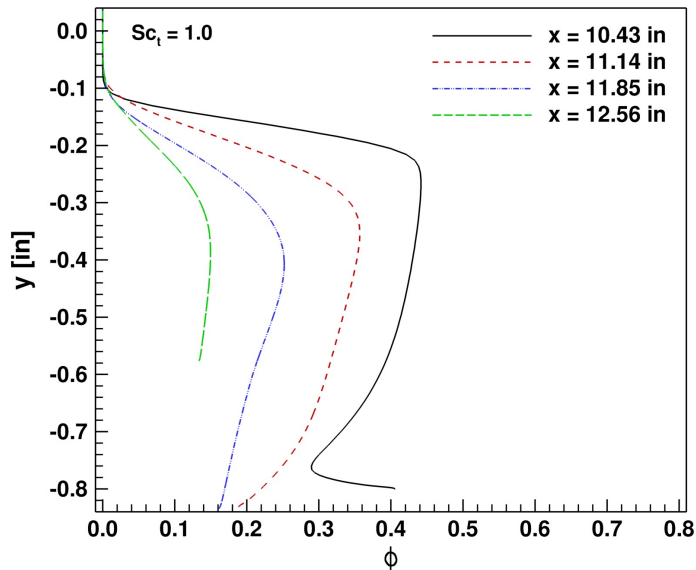
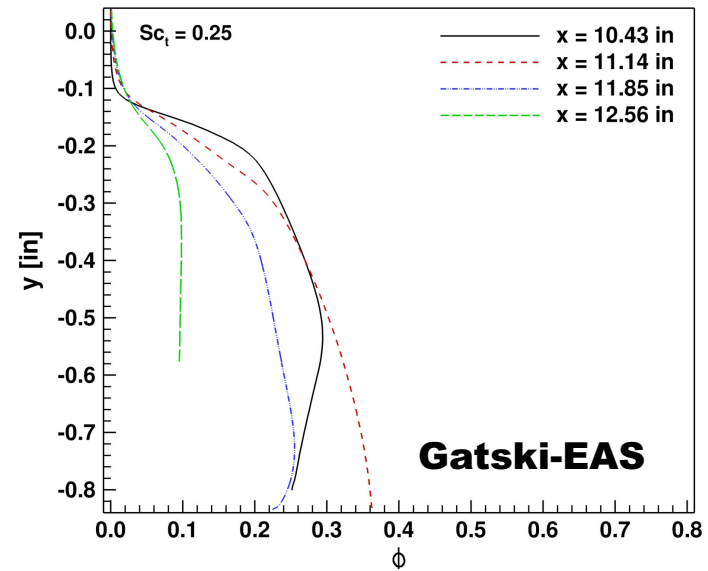
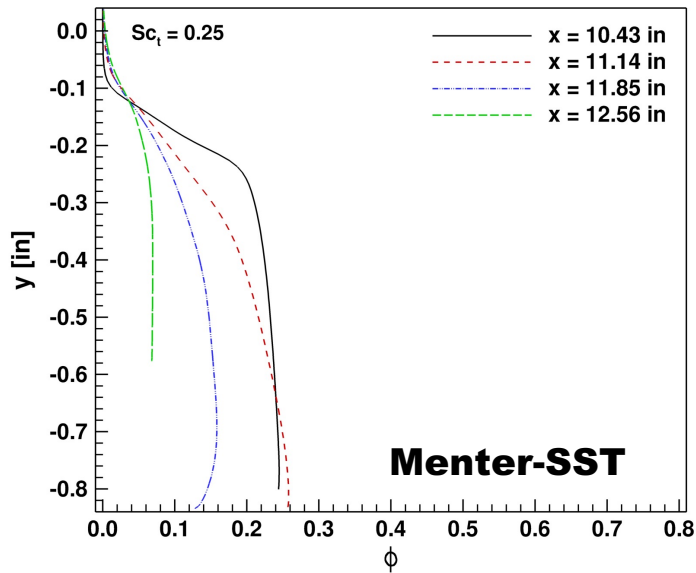


ϕ : 0.00 0.25 0.50 0.75 1.00 1.25

- Hybrid RAS/LES for Mach 2 flow past a fueled recessed cavity
- Ethylene fuel conditions:
 $\dot{m} = 56$ SLPM, $T_o = 310$ K
- Fuel/Air Equivalence Ratio measured via LIBS



Use of SRS to Calibrate RAS Closure Constants

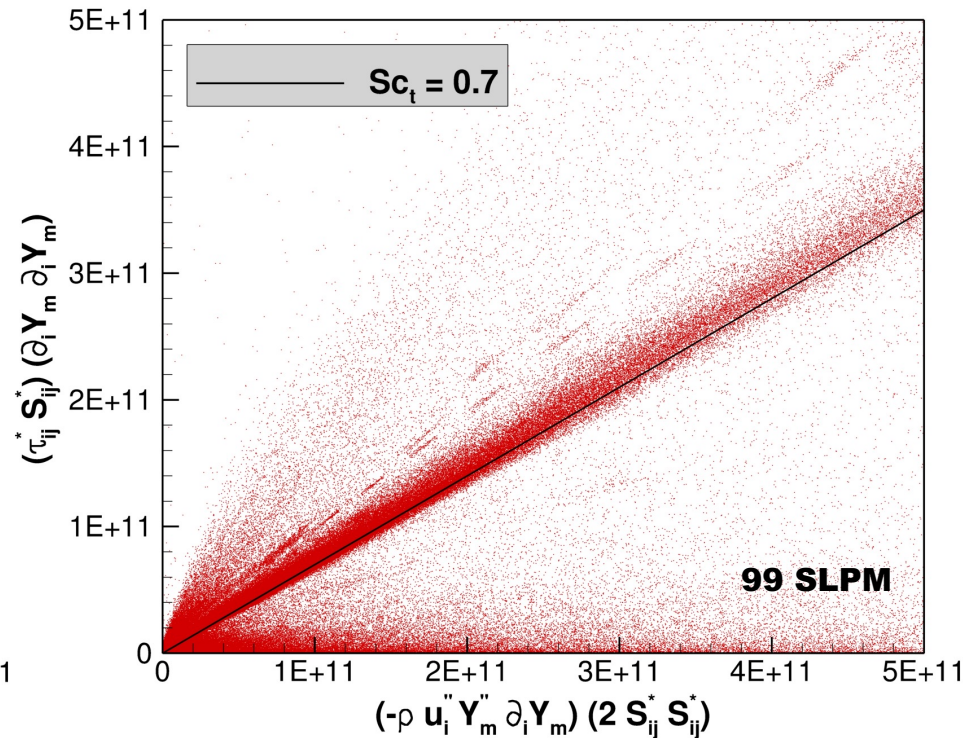
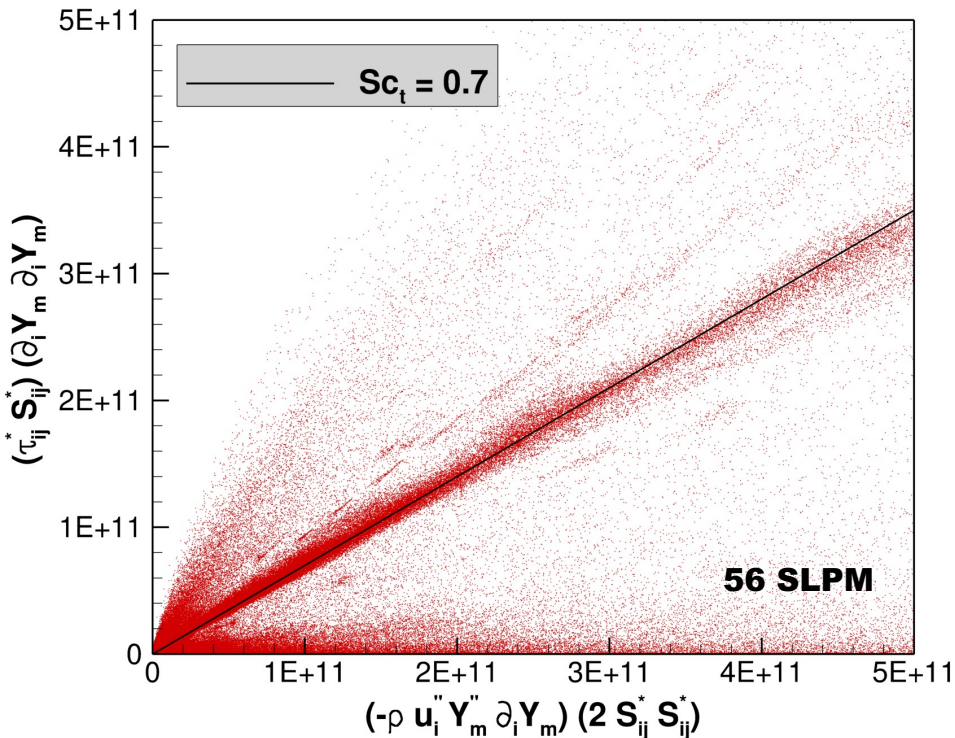


Use of SRS to Calibrate RAS Closure Constants

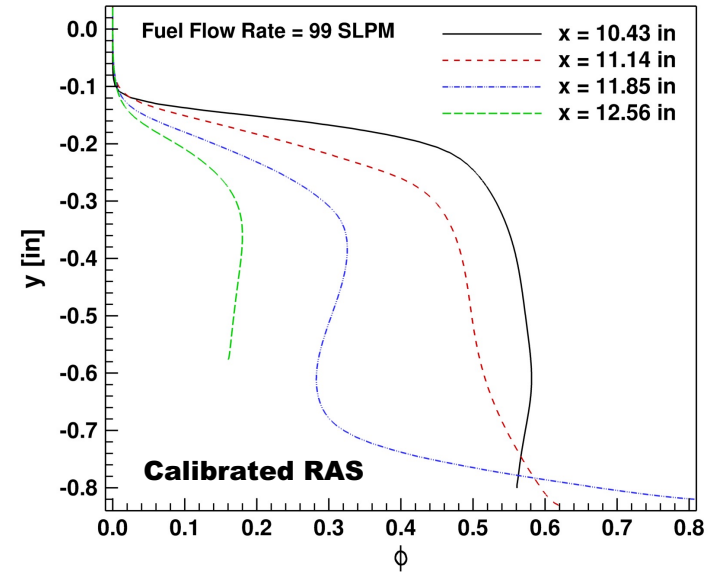
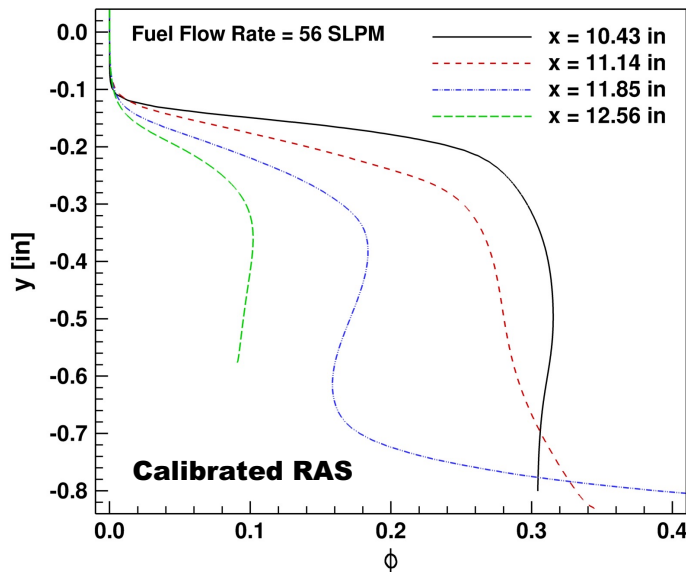
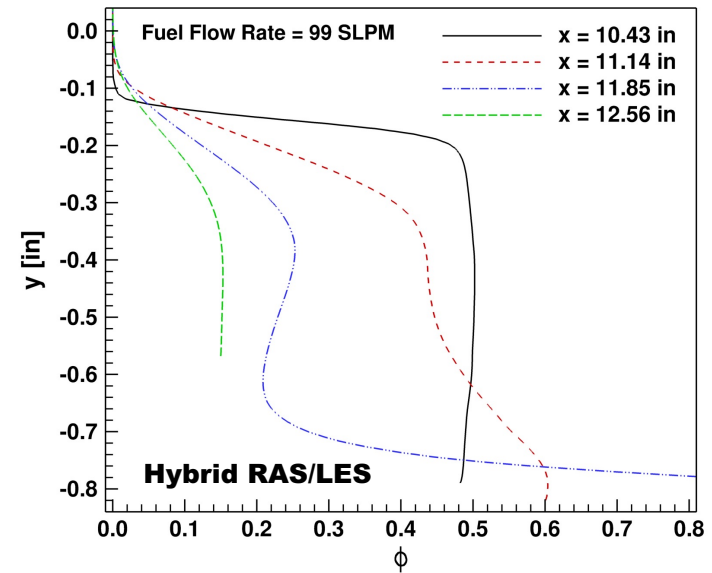
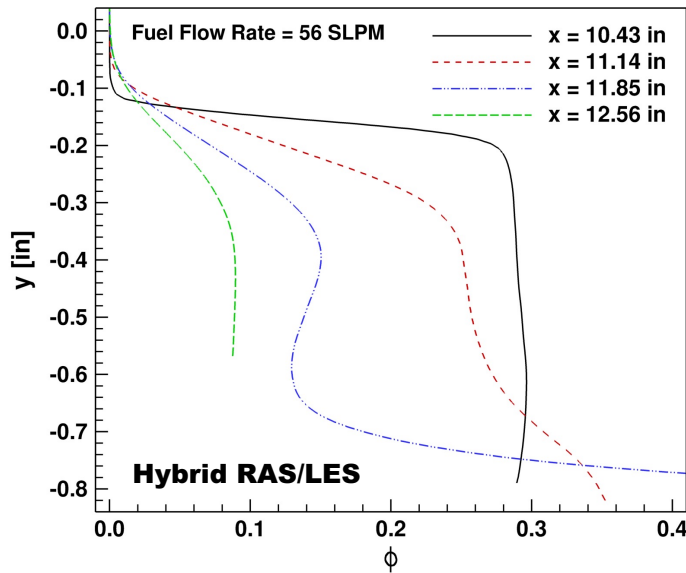


$$\tau_{ij} = 2\mu_t \left(S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right) - \frac{2}{3} \delta_{ij} \bar{\rho} \tilde{k}, \quad \bar{\rho} \widetilde{u_i'' Y_m''} = -\frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}_m}{\partial x_i}$$

$$\mu_t = \frac{\left(\tau_{ij} + \frac{2}{3} \delta_{ij} \bar{\rho} \tilde{k} \right) \left(S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right)}{2 \left(S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right) \left(S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right)} \equiv \frac{\tau_{ij}^* S_{ij}^*}{2 S_{ij}^* S_{ij}^*}, \quad \frac{\mu_t}{Sc_t} = \frac{-\bar{\rho} \widetilde{u_i'' Y_m''} \frac{\partial \tilde{Y}_m}{\partial x_i}}{\frac{\partial \tilde{Y}_m}{\partial x_i} \frac{\partial \tilde{Y}_m}{\partial x_i}}$$



Use of SRS to Calibrate RAS Closure Constants



Engine nozzle physics & modeling limitations with RAS



- **The role of the engine exhaust nozzle is to convert the potential energy of the propulsion system airflow exiting the combustor into kinetic energy to generate thrust for the scramjet engine**
- **The primary difficulty in predicting the flow physics of this portion of this engine component is the potential of flow relaminarization due to rapid expansion**
 - Relaminarization can significantly reduce heat loads in the nozzle and standard turbulence closure models are incapable of capturing this phenomenon accurately.
 - Incomplete combustion within the combustor may allow some level of chemistry to continue during the nozzle expansion (i.e., chemistry may not be frozen and radical recombination may affect nozzle performance).
- **CFD based on RAS can usually be relied upon to predict the performance of this component with considerably less uncertainty than the upstream portions of the engine flowpath**

- **Scramjet propulsive flowpaths are extremely challenging to model accurately.**
- **Current SoA for CFD analysis of high-speed propulsion flow paths are Reynolds-averaged simulations:**
 - All scales of turbulence are modeled → often leading source of uncertainty
 - Boussinesq approximation (LEVM)
 - Gradient diffusion assumption with constant Pr_t and Sc_t
 - Turbulence-Chemistry interactions neglected (or crudely modeled)
 - Modeling strategy is relatively mature with only “evolutionary” improvements documented over the past 15-20 years → Current focus is primarily on UQ
- **Full vehicle simulations (or even matrices of simulations) are computationally tractable for problems of programmatic interest on current supercomputers (typically several weeks to solution) when using Reynolds-averaged simulations.**

- **Scale-resolved simulations (LES or hybrid RAS/LES) have the potential to substantially reduce turbulence model uncertainty:**
 - Only the smaller turbulence scales are modeled (larger scales resolved)
 - Smaller scales more universal in nature (presumably easier to model)
 - Model form uncertainty (related to turbulence) can be reduced with grid resolution
 - Computational cost is excessive (at least 100 times that of RAS)
- **Expected trend is to continue leveraging RAS capabilities (can ML offer measureable improvements?) for the design and analysis of high-speed reacting flows.**
- **SRS likely to remain limited to specific situations:**
 - improve fundamental physics understanding (universities routinely do this)
 - investigate impact of unsteady effects
 - RAS scenarios with unacceptably high uncertainty (e.g., operability bounds)
 - calibration of RAS closure models

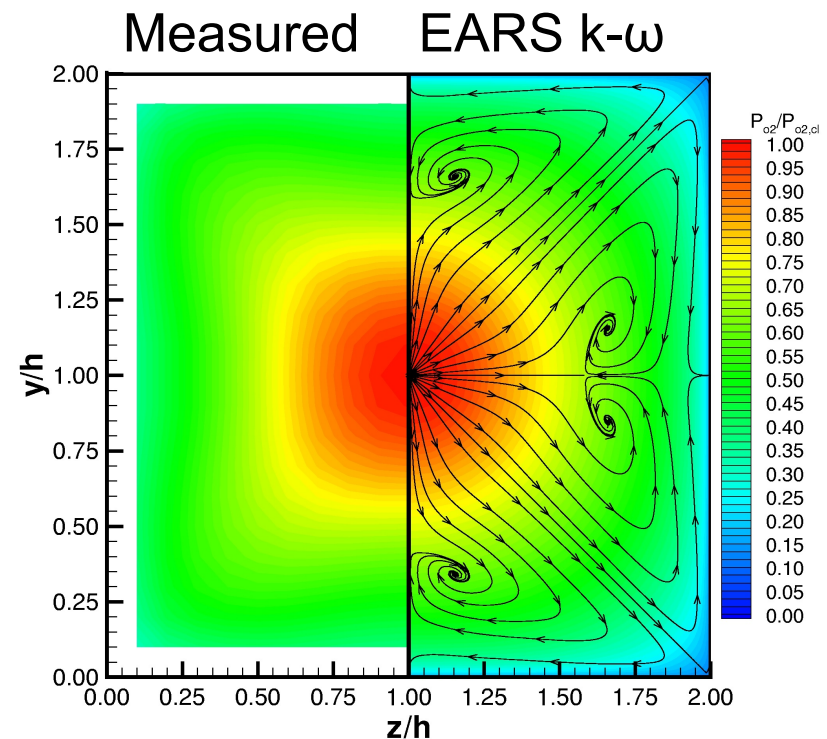
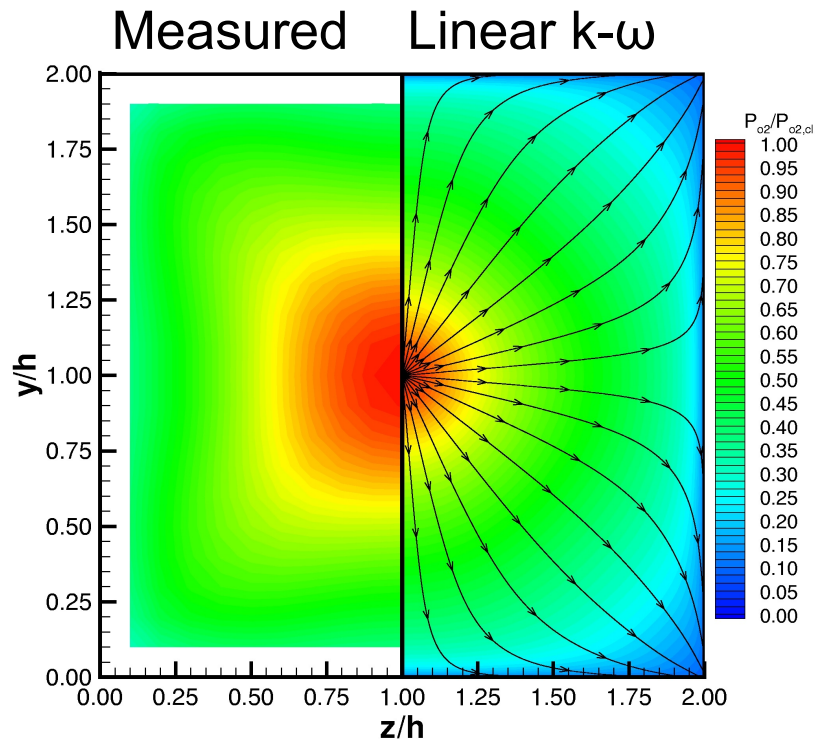
Back-up Slides ...



Inlet physics & modeling limitations with RAS



- **Example of the potential impact of stress-induced corner vortices is illustrated below for Mach 3 flow through a square duct:**
 - Linear eddy viscosity models (i.e., the Boussinesq approximation) are incapable of capturing this phenomenon
 - Nonlinear models (e.g., EARS, QCR) or Full Reynolds stress closures are required



- Present formulation can be regarded as a wall-modeled LES
 - SBLI require resolved turbulent content in the attached boundary layer
 - Flush wall injection likely will require resolved content as well
- Hybrid RAS/LES modeled viscosity
 - (F) [RAS eddy viscosity] + $(1-F)$ [SGS viscosity]
- Blending function (F) designed to transition near the outer edge of the log layer (AIAA 2010-0111) :

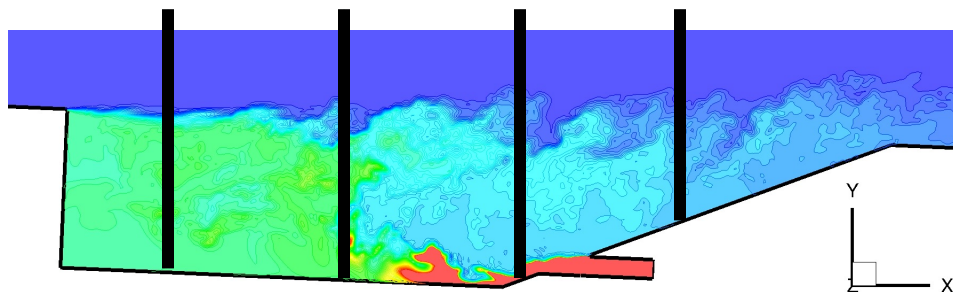
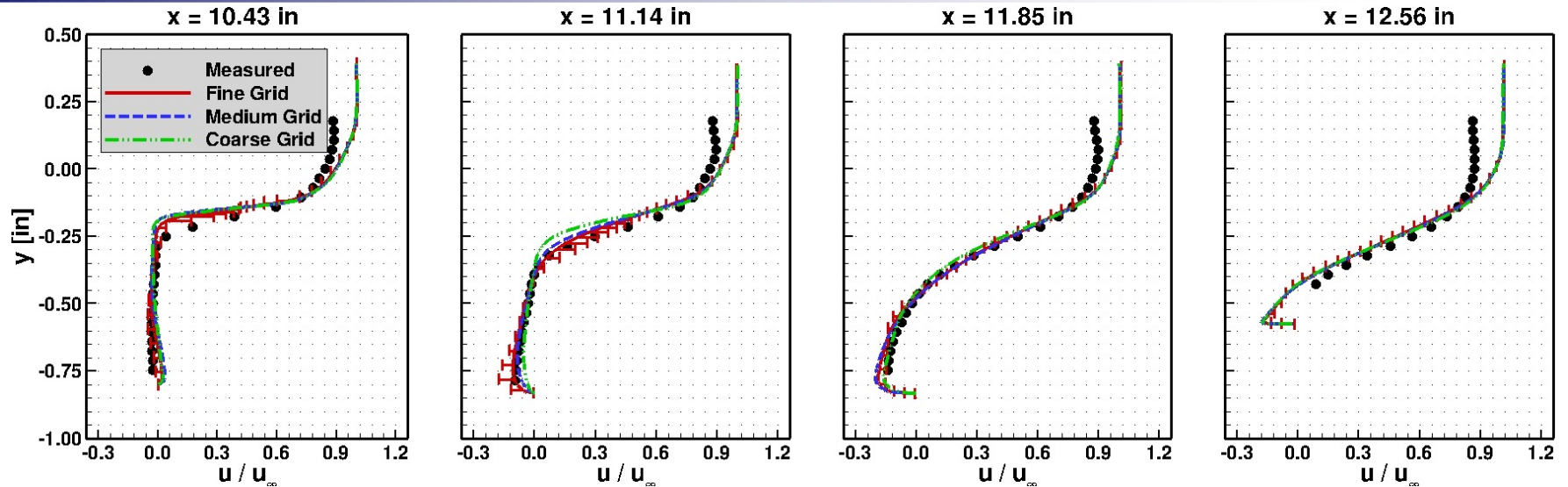
$$F = \frac{1}{2} \left\{ 1 - \tanh \left[5 \left(\frac{\kappa}{\sqrt{C_\mu}} \eta^2 - 1 \right) - \phi \right] \right\}$$
$$\ell = \sqrt{\frac{\nu}{C_\mu \omega}}$$
$$\eta = \frac{d}{\alpha \ell}$$

- Plan to implement a more recent blending strategy that is not BL specific and free of user-specified input (AIAA Journal, Vol. 49, 2011)

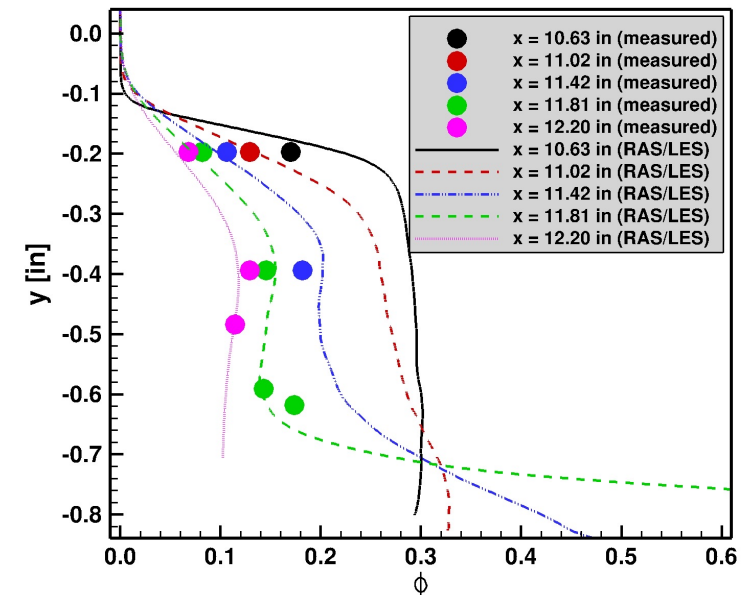


- Recycling/Rescaling to allow development and sustainment of resolved turbulent structures (AIAA 2010-1099)
 - The idea is to extract the solution at some downstream station, properly rescale the data, and recycle the turbulent content back to the inflow plane.
 - Only the fluctuations are recycled to avoid any drift in the inflow mean flow properties.
 - Velocity fluctuations are recycled and scaled based on known boundary layer scaling properties.
 - Temperature fluctuations are obtained from the velocity fluctuations using Morkovin's hypothesis that total temperature fluctuations are negligible.
 - Pressure fluctuations are recycled without any rescaling.
 - An intermittency function is applied near the edge of the inflow boundary layer to prevent recycled fluctuations from corrupting the freestream.
 - A random spanwise shift procedure is used to mitigate the formation of large-scale structures (rollers) during the recycling process.

Scramjet Combustor Flameholder SRS



ϕ : 0.00 0.25 0.50 0.75 1.00 1.25

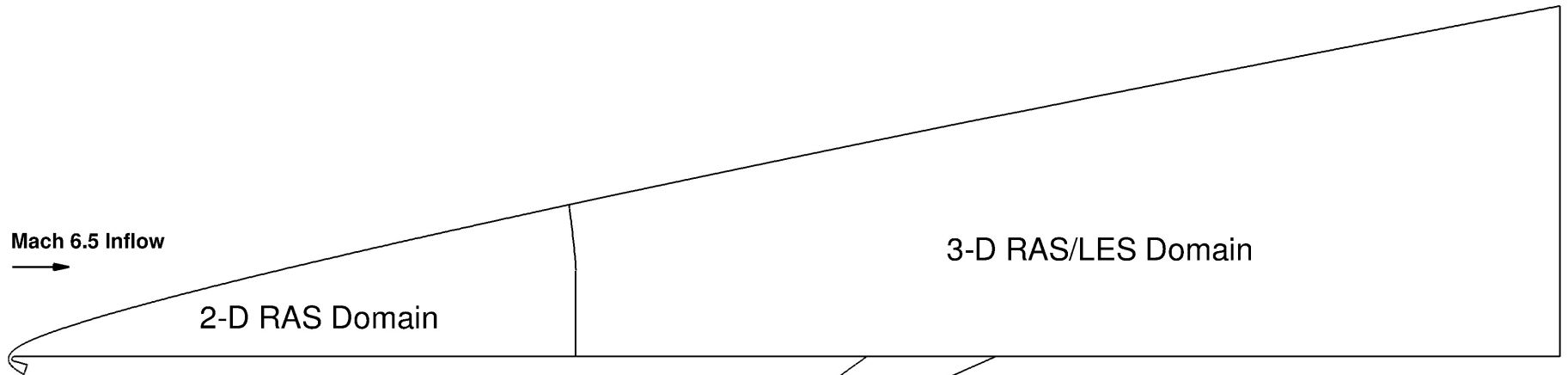


Hybrid RAS/LES Numerical Framework

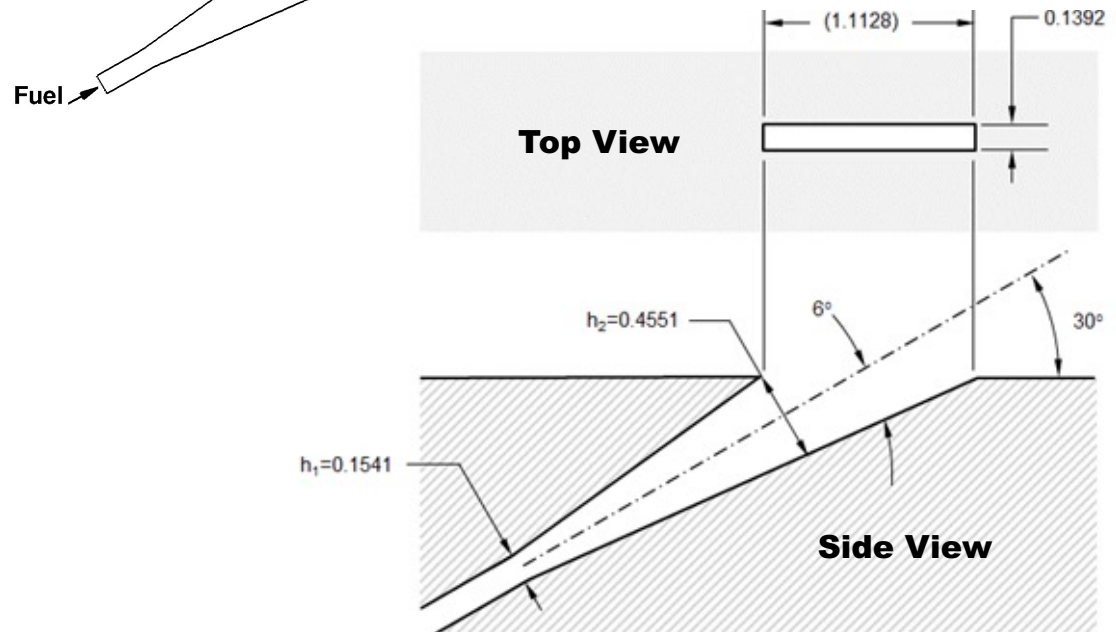


- Hybrid RAS/LES formulation blends the RAS and SGS viscosity values
 - (F) [RAS eddy viscosity] + $(1-F)$ [SGS viscosity]
- Dissipative and non-dissipative schemes are blended such that the standard dissipative formula is applied in inviscid regions and a non-dissipative formula is applied in viscous regions
 - Dissipative flux scheme: MUSCL ($\kappa=1/3$) reconstruction with 2nd order ENO limiter
 - Nondissipative flux scheme: Symmetric 4th-order reconstruction (i.e., a centered stencil)
- The hybrid flux at the cell faces is based on a weighted average of each reconstruction:
 - $q_h^{L,R} = (\psi) q^{L,R} + (1-\psi) q_{SR}$
- The Ducros (JCP-1999) switch, ψ , is used to detect inviscid (divergence dominated) regions and viscous (vorticity-dominated) regions

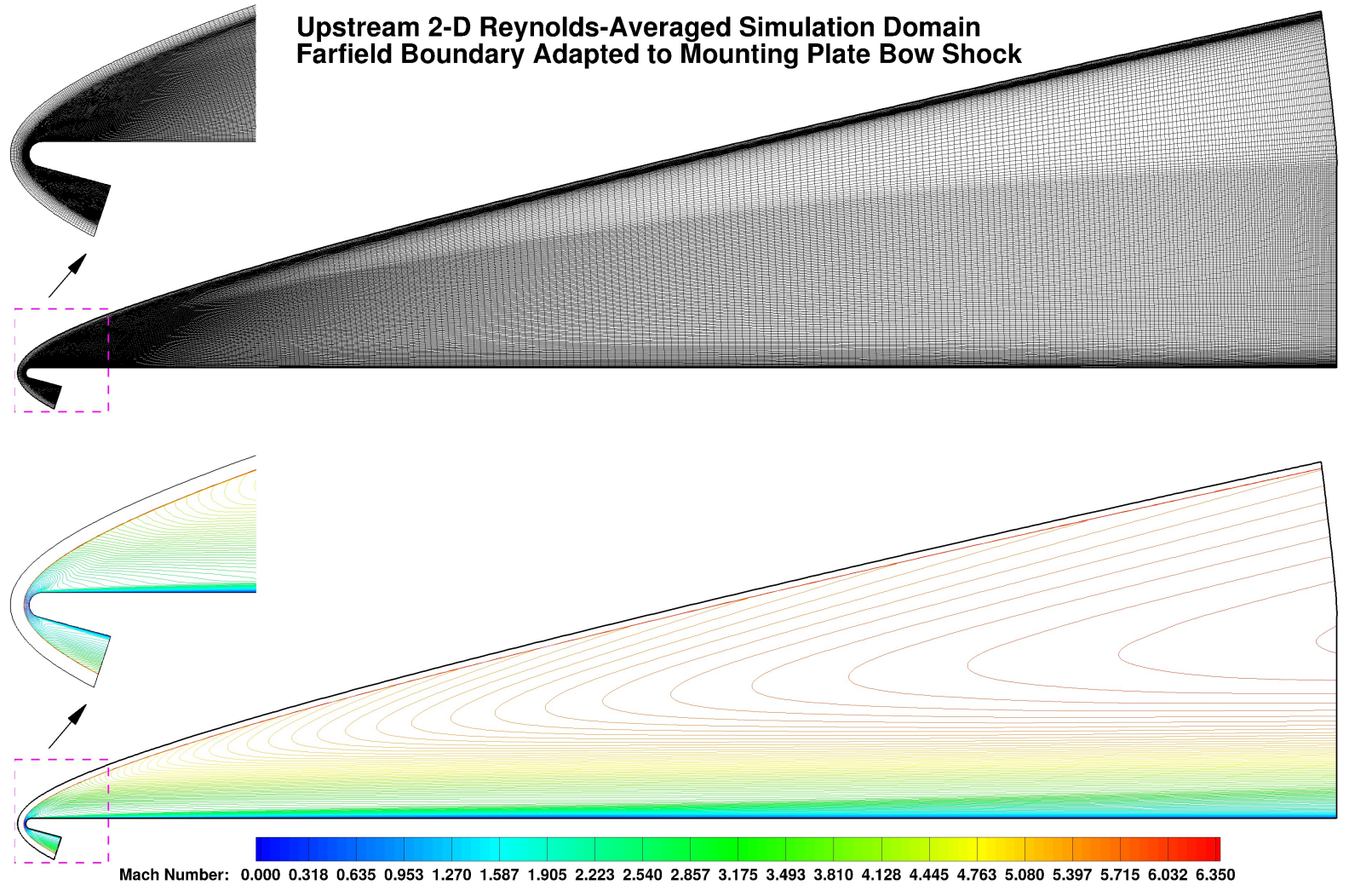
EIMP Flush-wall Injector Geometry



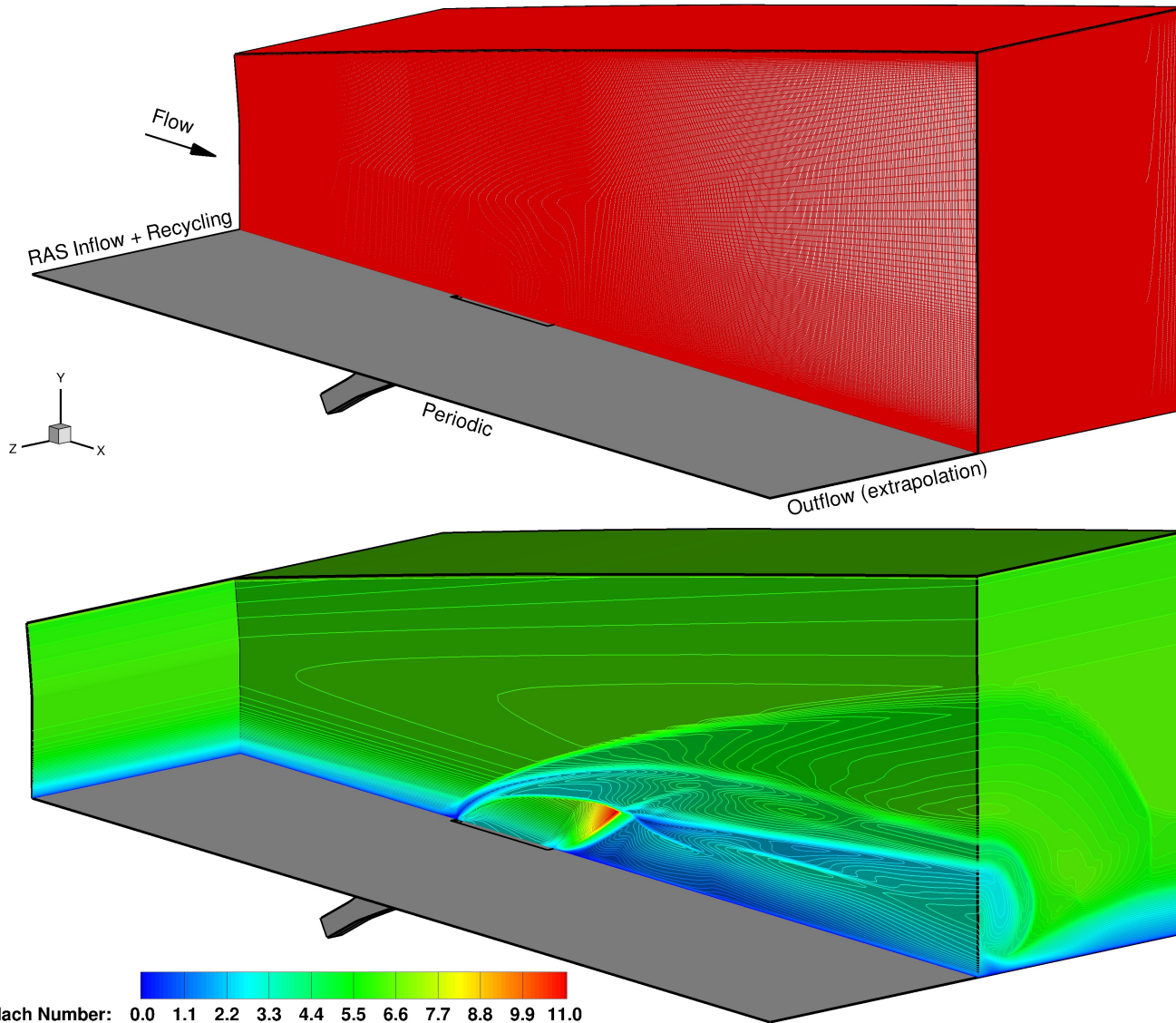
- Inflow corresponds to a Mach 15 flight condition (Mach 6.5, $T_o = 977.8$ K, $Re = 9 \times 10^6/m$)
- Helium used as an H_2 fuel simulant ($\dot{m} = 5.17 \times 10^{-3}$ kg/s, $T_o = 293.15$ K)



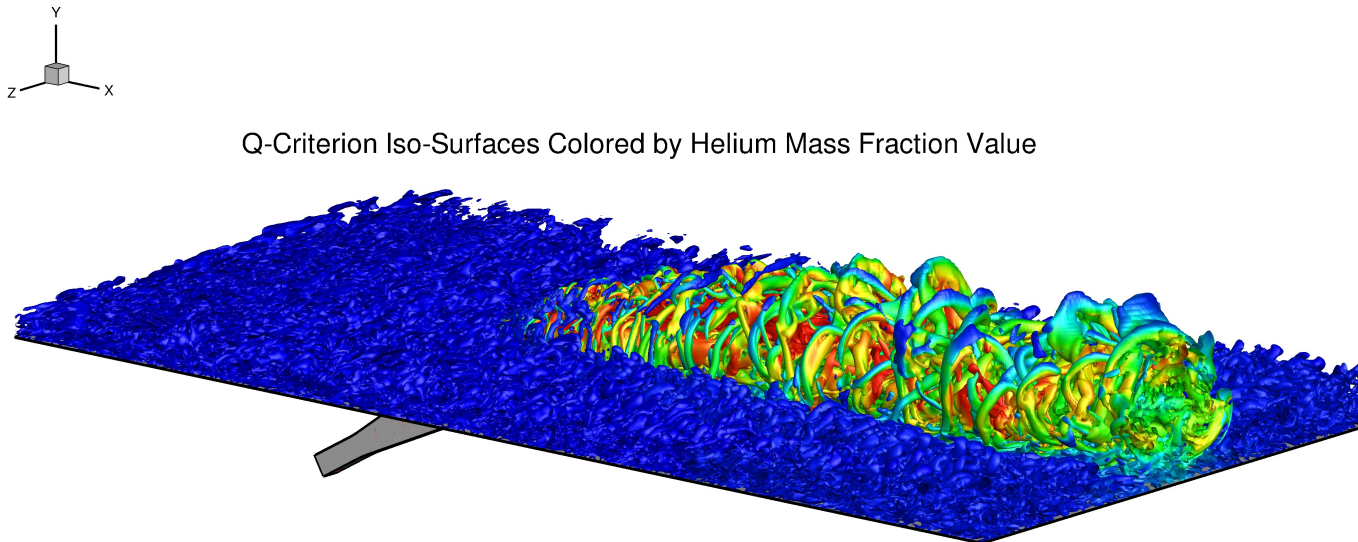
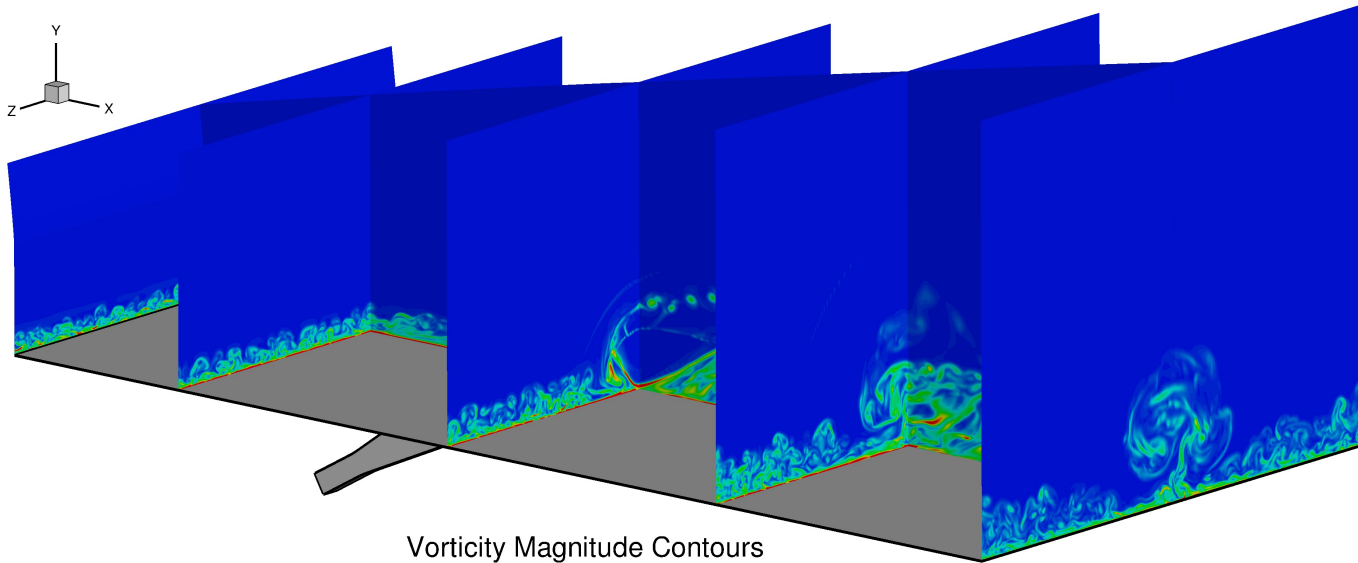
Injector Grid (2D upstream section)



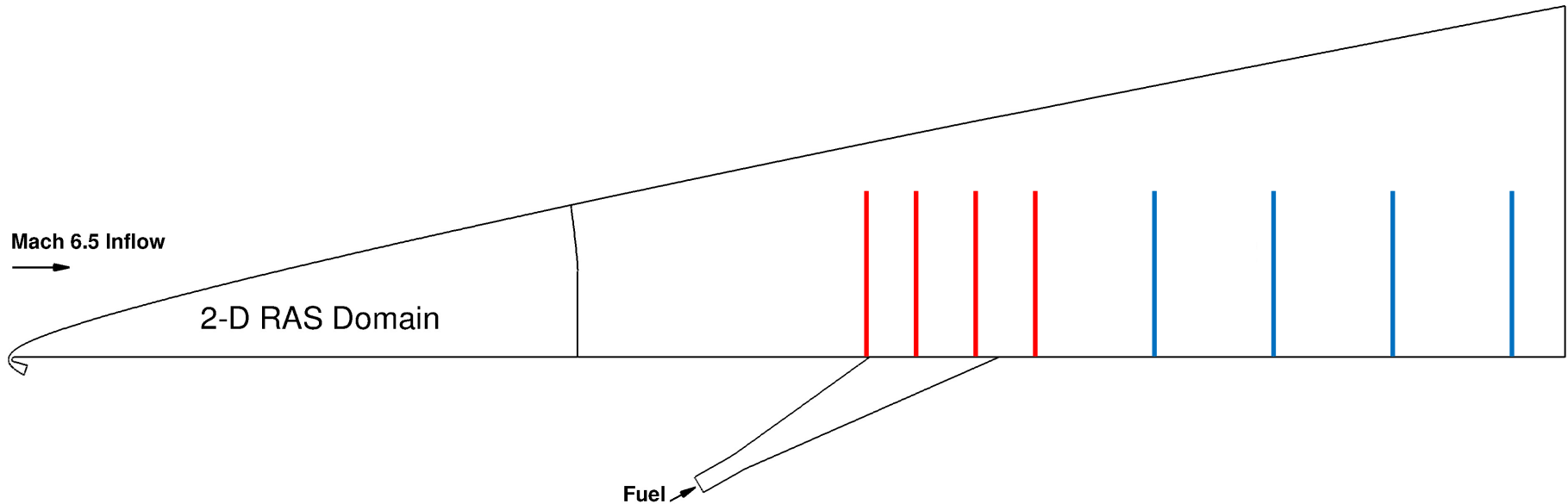
Injector Grid (3D downstream section)



Visualization of Turbulence Structures



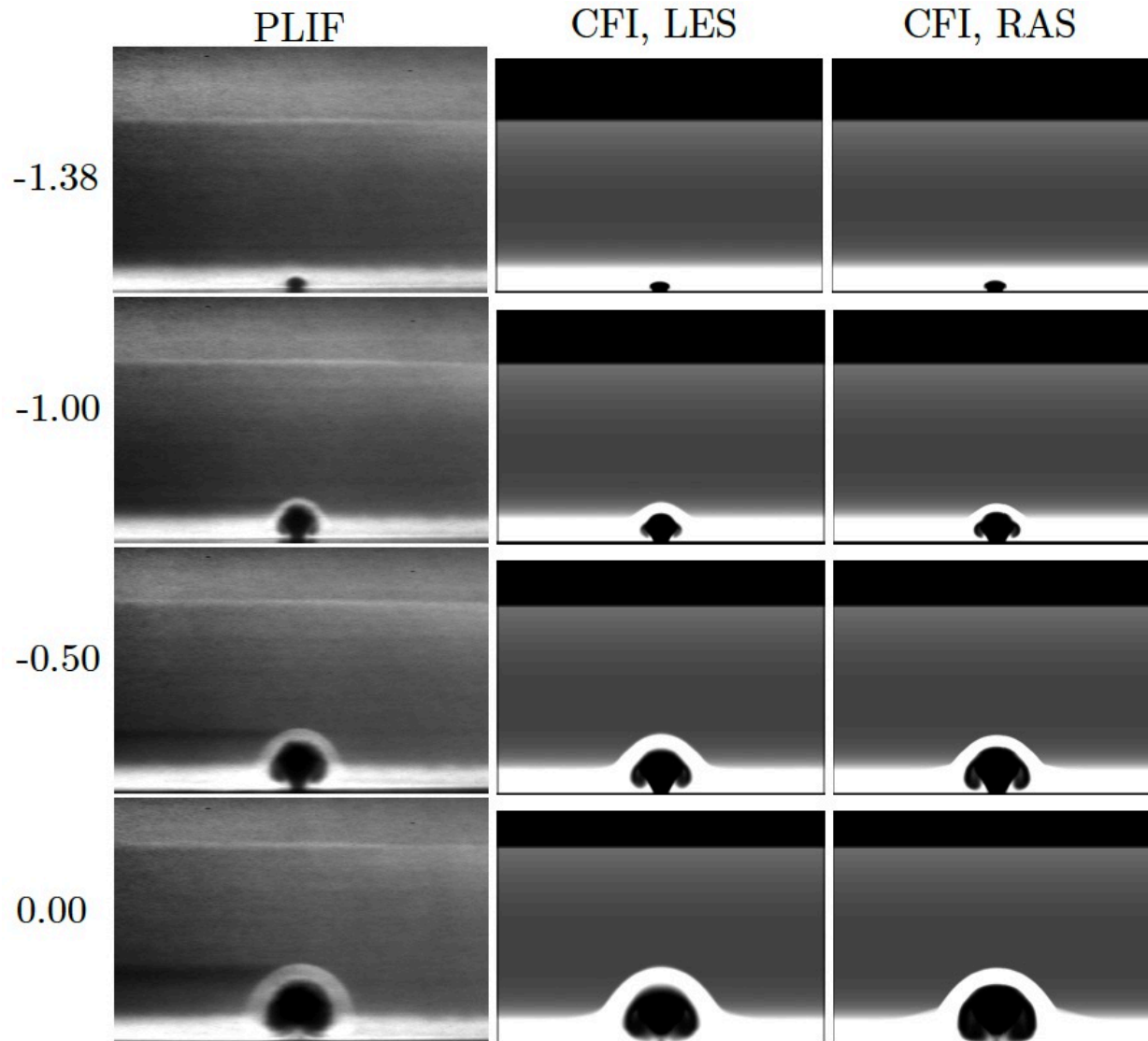
Plume Characterization via (NO PLIF)



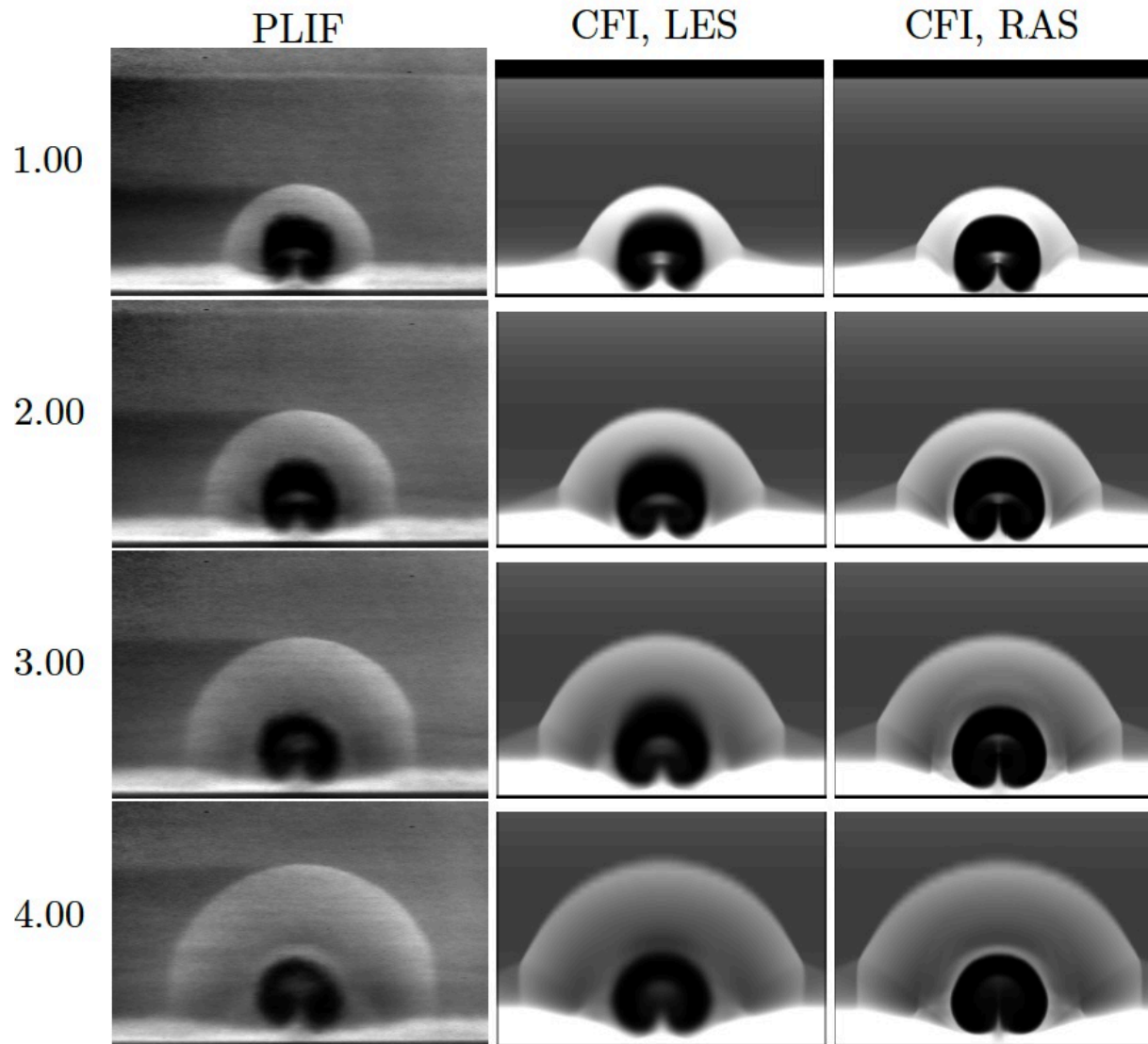
- Nitric Oxide Planar Laser-Induced Fluorescence (NO PLIF) chosen to visualize the injected fuel plume structure
 - NO is naturally present in the NASA Langley Arc-Heated Scramjet Test Facility
- CFD data processed using a theoretical fluorescence model to compare with the NO PLIF visualizations (Computational Flow Imaging)
 - Fluorescence model sensitive to NO composition, pressure, temperature and velocity

Plume Visualization via NO PLIF

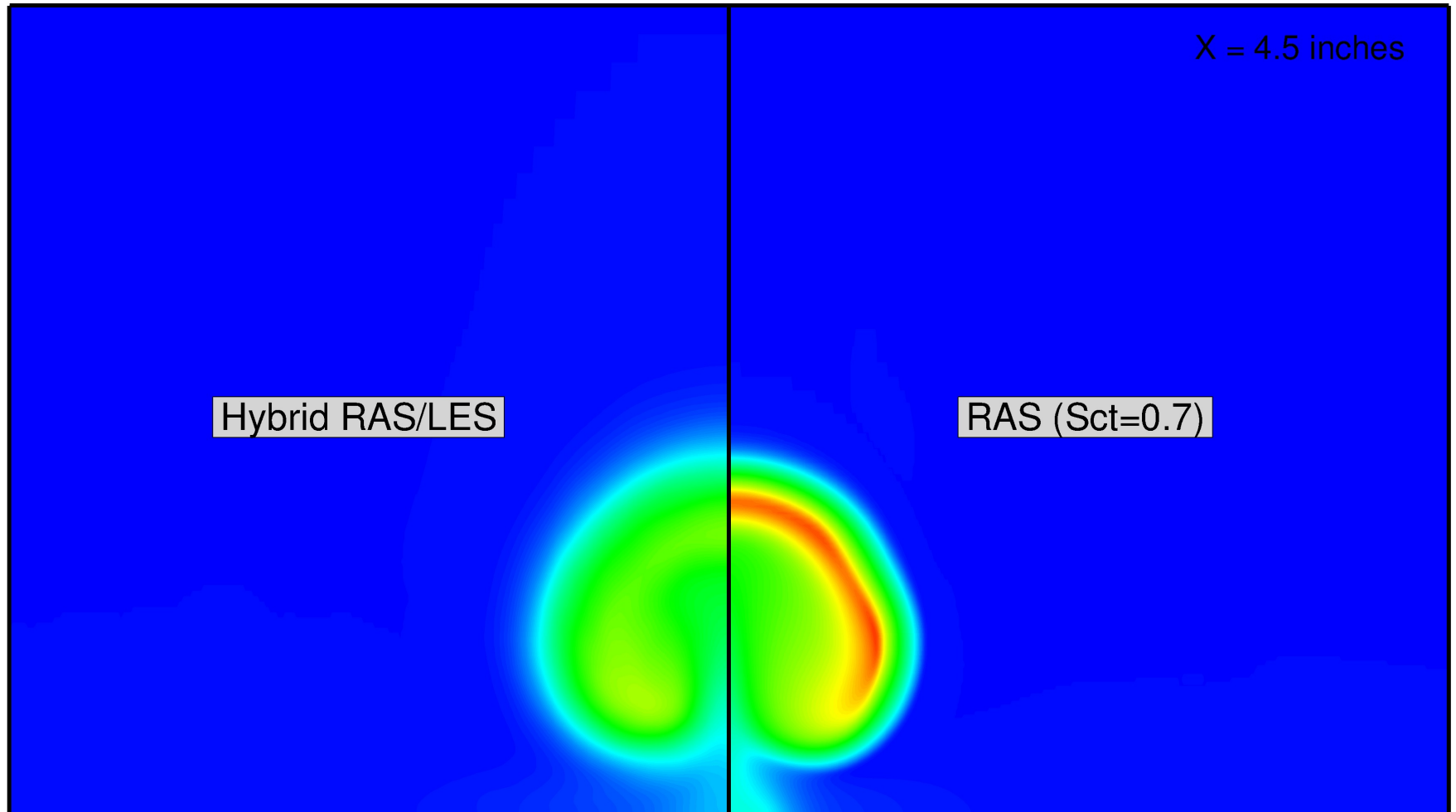
(Drozda et al., AIAA 2018-5379)



Plume Visualization via NO PLIF



RAS and Hybrid RAS/LES Helium Plumes



He Mass Fraction: 0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50 0.55 0.60 0.65 0.70 0.75 0.80 0.85 0.90 0.95 1.00

