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Understanding the Role of CFD, Including RANS, DES, LES and DNS, in Hypersonic Propulsion Design and Analysis

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Outline

- **Role of CFD in Scramjet Engine Design and Analysis**
  - Historical perspective
  - Current role
- **Physics modeling and current SoA limitations (RANS/RAS)**
  - Forebody flow physics modeling
  - Inlet flow physics modeling
  - Isolator flow physics modeling (DMRJ)
  - Combustor flow physics modeling
  - Exhaust nozzle flow physics modeling
- **Beyond steady-state RAS (hybrid RAS/LES, LES, …)**
  - Where (and under what circumstances) is it best utilized
    - DNS
    - LES
    - Hybrid RAS/LES or WMLES
- **Summary**

Historical Perspective of Scramjet CFD Tools

- **Potential benefits of scramjets were first identified in 1960**
  - Performance gains were based on simple analytical arguments
  - Ground test capability was limited → need for computational tools
- **Modular or quasi-one-dimensional cycle analysis codes**
  - Initial development began in the early 1960s
  - Allowed rapid evaluation of potential scramjet concepts
  - Allow for effects of area change, wall friction, heat transfer, fuel injection, and chemistry
  - Examples: RJPA, GASL1D, SRGULL
- **Multi-dimensional analysis codes**
  - Initial development began in the middle 1960s with viscous MoC
  - Some PNS formulations appeared at GASL (1969) and ATL (1970)
  - 2D and 3D Euler solvers appeared in the early 1980s
  - 2D and axi VSL and PNS, Scramp, Scrint, Scorch and Snoz during the NASP
  - 2D RANS with (3D RANS w/out) chemistry appeared in the mid 1980’s
  - 3D RANS with equilibrium and finite rate chemistry appeared in the late 1980s

Current Role of CFD in Scramjet Development

- **Current SoA for CFD analysis of hypersonic propulsion systems are Reynolds-Averaged Simulations (RAS)**
  - All scales of turbulence are modeled → often leading source of uncertainty
    - Boussinesq approximation with 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)
    - 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

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

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

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

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

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

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 linear 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)
- **Linear eddy viscosity models 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
- **Nonlinear constitutive relationships and rotation/curvature corrections can address the above deficiencies**
  - Quadratic constitutive relationship (Spalart [2000])
  - 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 are 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.,**

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

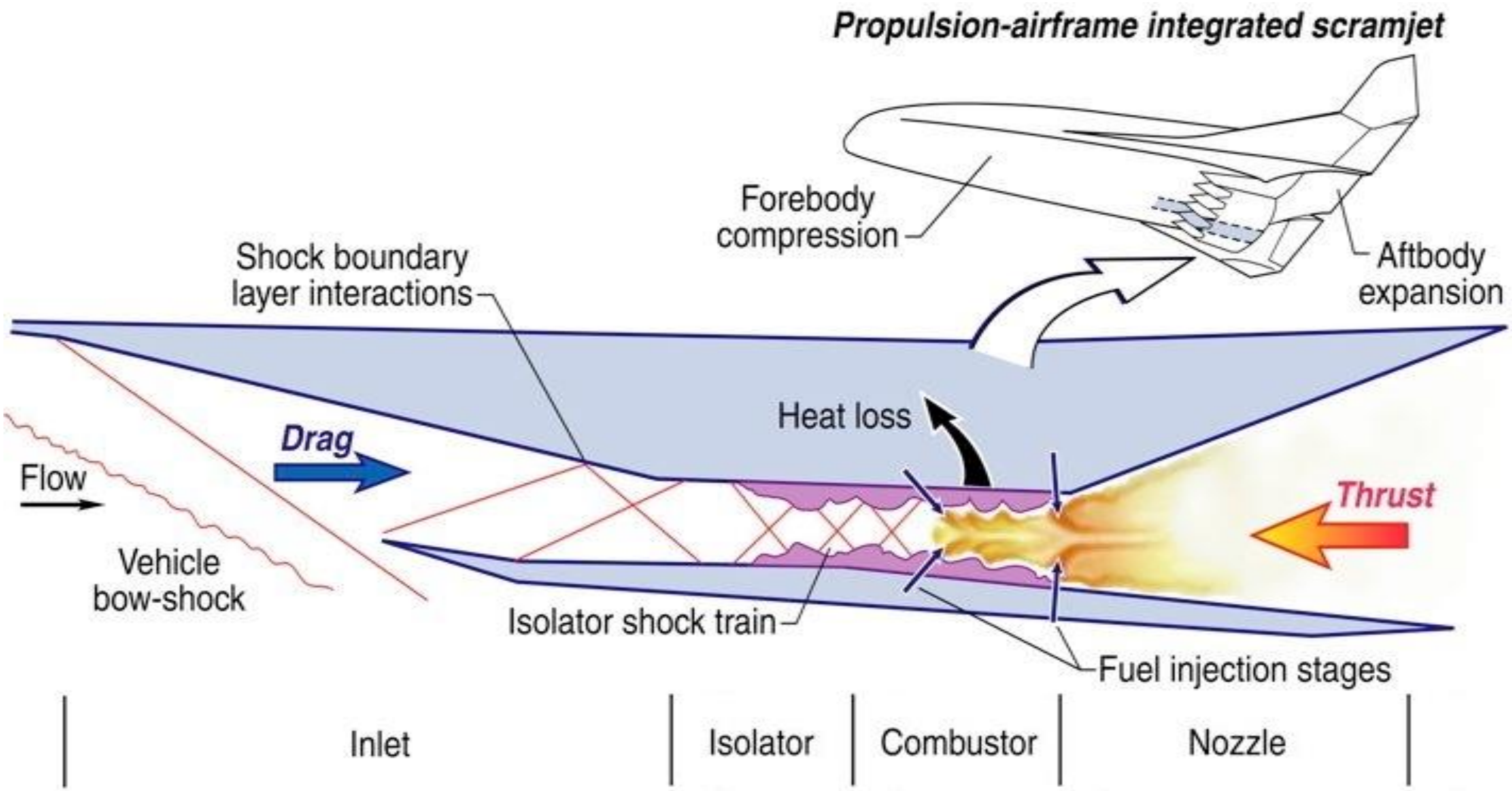
- **Turbulent fluctuation effects on the chemistry can be more rigorously handled using PDF's:**

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

- **The form of the PDF can be assumed a priori, or an evolution equation can be integrated for it**
  - PDF evolution equations are theortically sound (Pope, 1995), but computationally expensive <u>What about the treatment of pressure, also coupling problems with the Eulerian Eqs.</u>?
  - 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 combution process with mixture fraction and its variance, reaction progress variable, and pressure

Scramjet Engine Flow Features



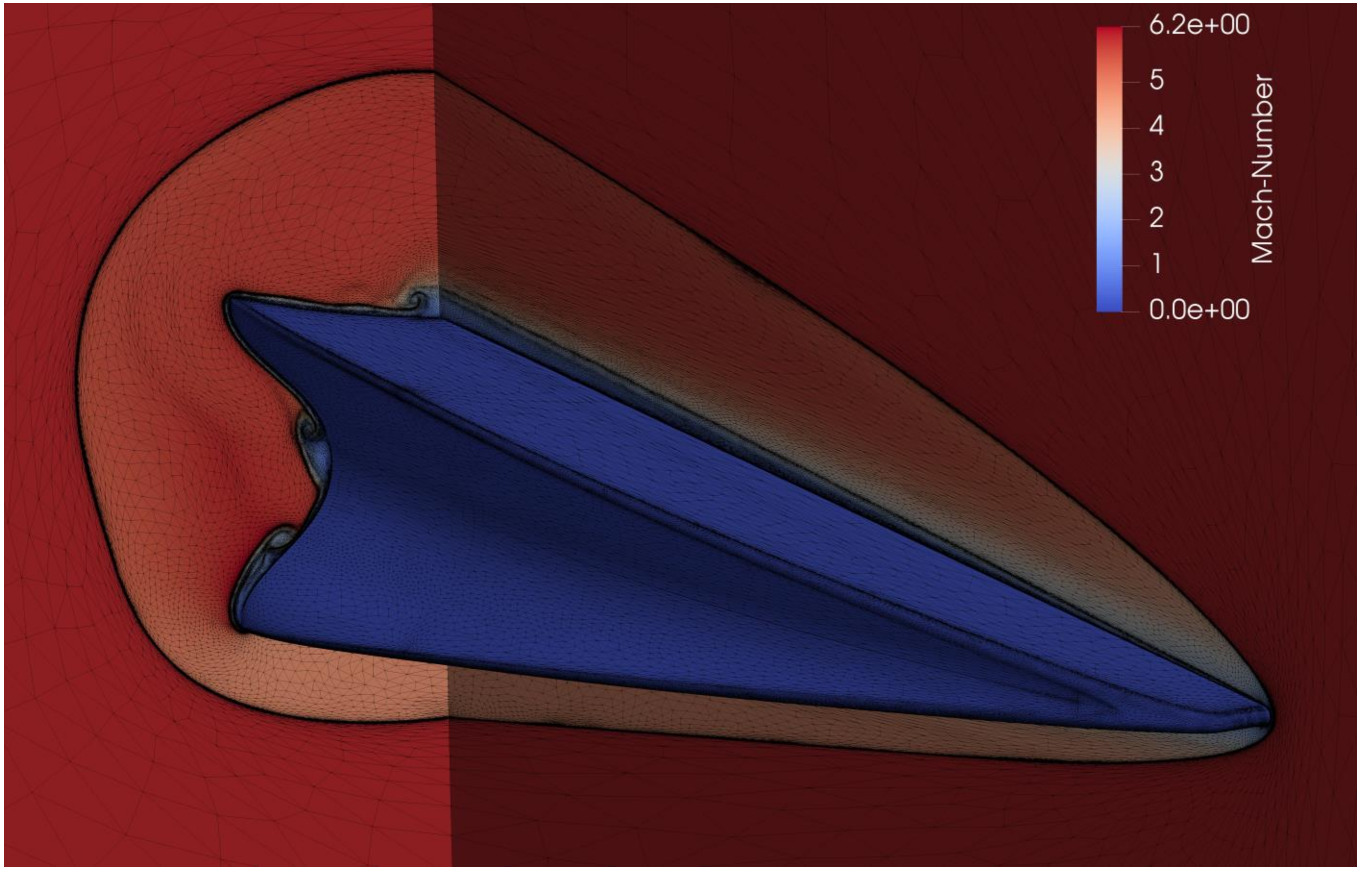
Heiser, W. H. and Pratt, D. T. "**Hypersonic Airbreathing Propulsion,**" AIAA Education Series,1994

Forebody physics and modeling limitations with RAS

- **Laminar flow instabilities and laminar to turbulent flow transition**
  - 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, therefore, cannot be relied upon for transition prediction in hypersonic flows.
    - Attempts to extend transport-equation based transition models to hypersonic flows (e.g., Papp and Dash [2008], Wang et al., [2016], Guo et al. [2019], Zhou et al. [2019], Qiao et al. [2021], Kang et al. (2021)], have been made, but these models have primarily been used for demonstration purposes by the model developers over a narrow range of geometry/flight conditions and have not been incorporated into mainstream codes.
    - Algebraic correlations based on integral boundary layer parameters are also not reliable except when the target application falls within the range of the underlying database.

Forebody physics and modeling limitations with RAS

- **Transition from laminar to turbulent flow continued …**
  - 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).



Forebody physics and modeling limitations with RAS

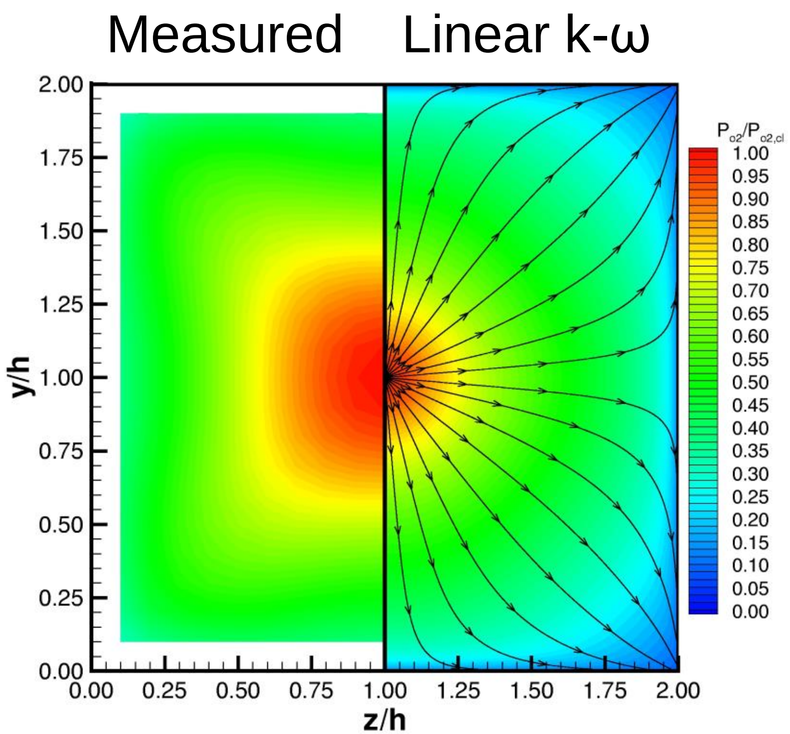
- **Transition from laminar to turbulent flow continued …**
  - High fidelity laminar flow CFD solutions (often termed basic state solutions) are required to perform the linear stability analysis.
    - Accuracy requirements are much more stringent for this purpose than what would normally be required engineering performance assessment.
  - Transition models derived from linear stability analysis can be incorporated into RAS based CFD predictions in different ways:
    - Zero-equation transition models (based on analytical curve fits/database lookup procedures/machine learning/automated linear stability computations) that couple with RAS via intermittency factor (e.g., Tufts et al. [2018]).
    - Transport-equation-based transition models based on linear stability correlations (e.g., Qiao et al. [2021], Xu et al. [2017]).

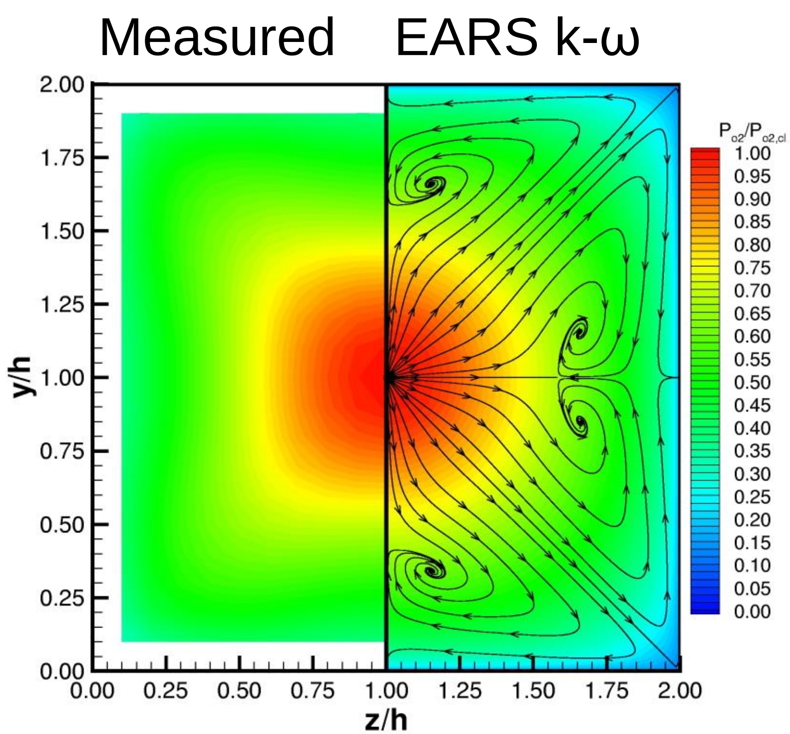
Inlet physics and modeling limitations with RAS

- **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 provide favorable conditions for combustion within the engine.**
- **CFD simulations of the inlet system are used to provide information about the following metrics:**
  1) Mass capture (1^{st}-order effect on engine thrust)
  2) Inlet compression efficiency (speaks to the efficiency 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 sudden maneuvers?)
- **To answer these questions, the following physical phenomenon must be predicted adequately:**
  – Shock / Boundary Layer Interactions … the predicition 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 affects and/or corners
    - pressure gradient induced vortical structures typically dominate, but stress-induced vortices may be important as well → this latter effect can not be predicted by standard linear eddy viscosity models.

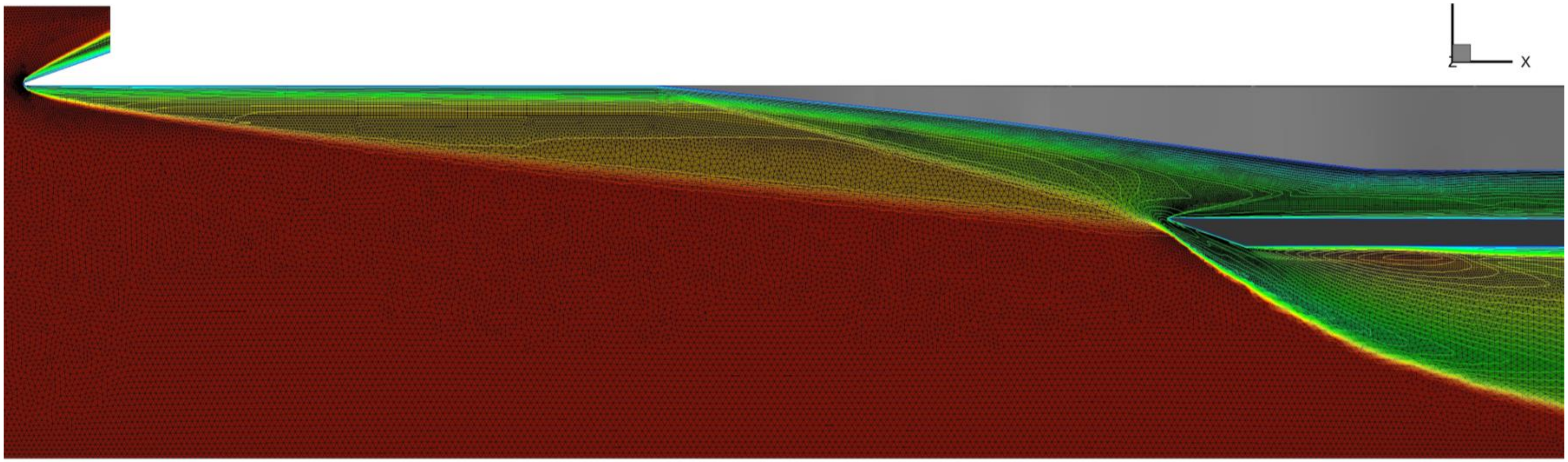
Inlet physics and modeling limitations with RAS

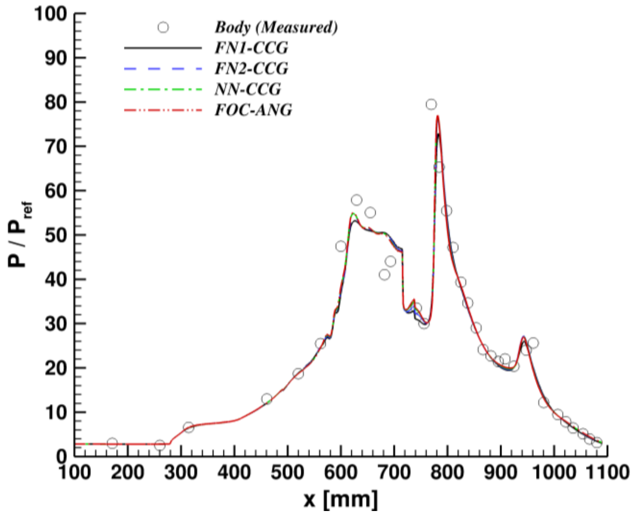
- **Example of the potential impact of stress-induced corner vortices is illustrated below for Mach 3 flow through a square duct:**
  - Linear eddy viscosity models (i.e., the Bousinesq approximation that invokes a linear relationship between the turbulent stress tensor and the strain rate tensor) are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

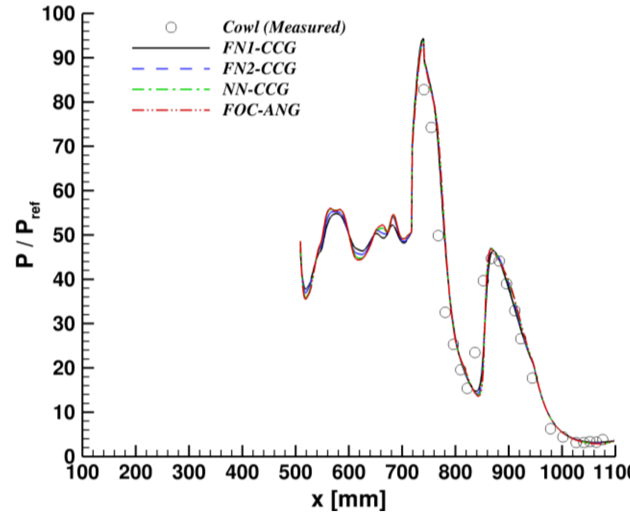




Inlet physics and modeling limitations with RAS





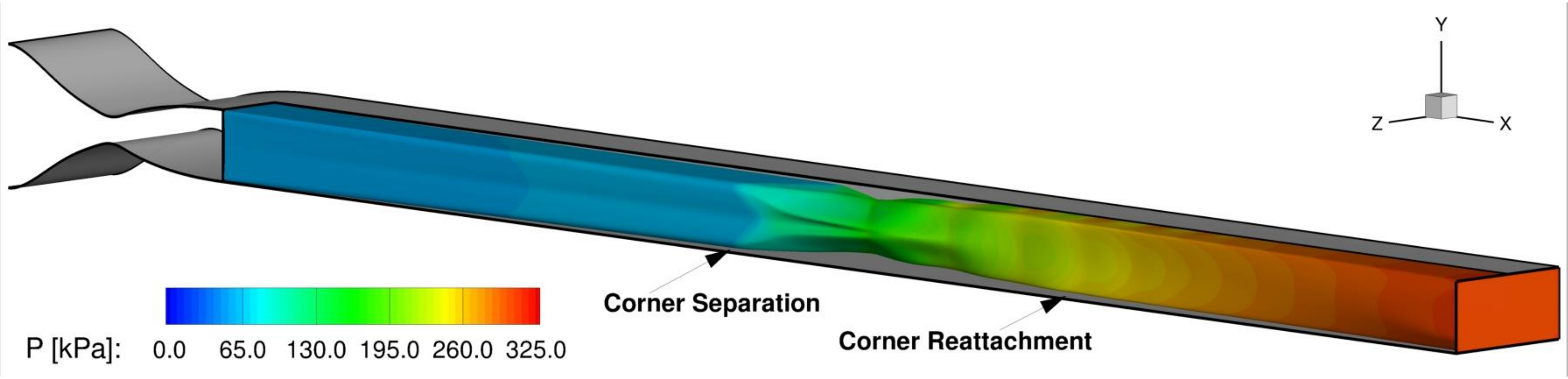


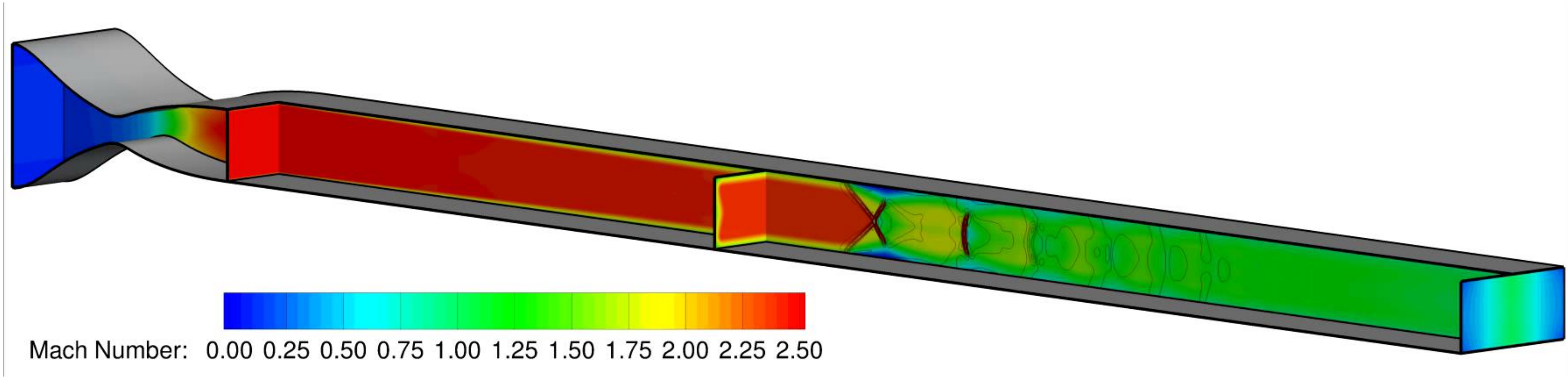
Isolator physics and modeling limitations with RAS

- **The role of the isolator is to contain the combustion induced pressure rise during DMRJ operation (M_∞ < 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 operational pressure rise (OPR) 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 separted 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 near the maximum OPR is on the order of 5-8 δ, which translates to several isolator duct heights for smaller scramjet engine applications.**

Isolator physics and modeling limitations with RAS

- **Isolator flow structure present during DMRJ operation**

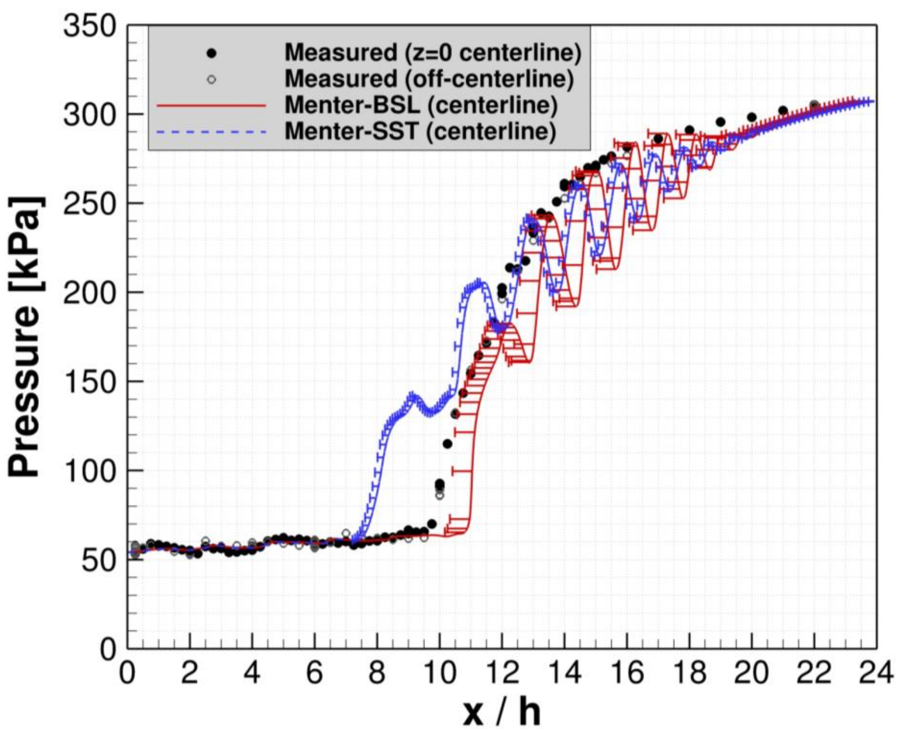




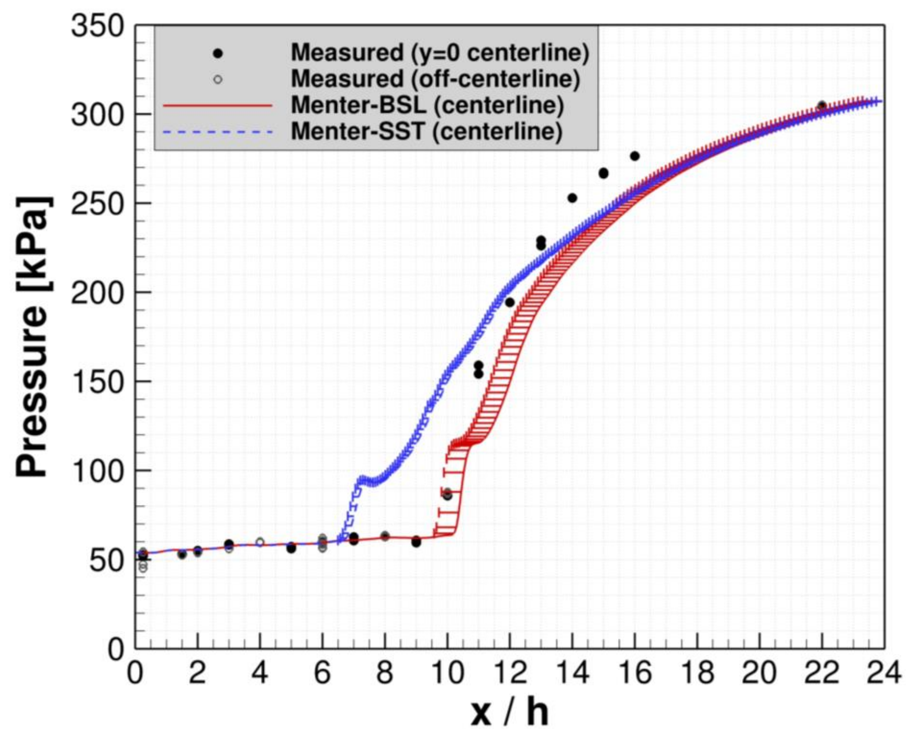
Isolator physics and modeling limitations with RAS

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

Contoured Wall



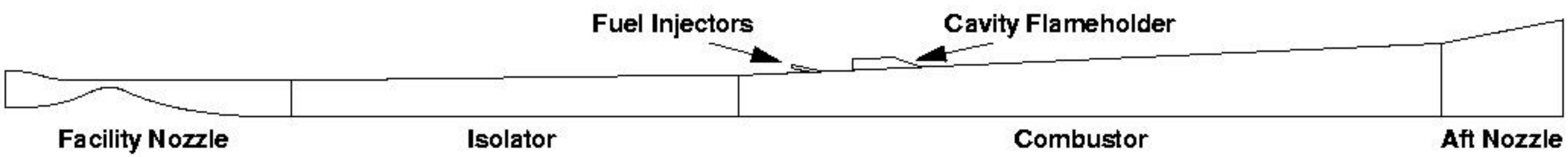
Side Wall

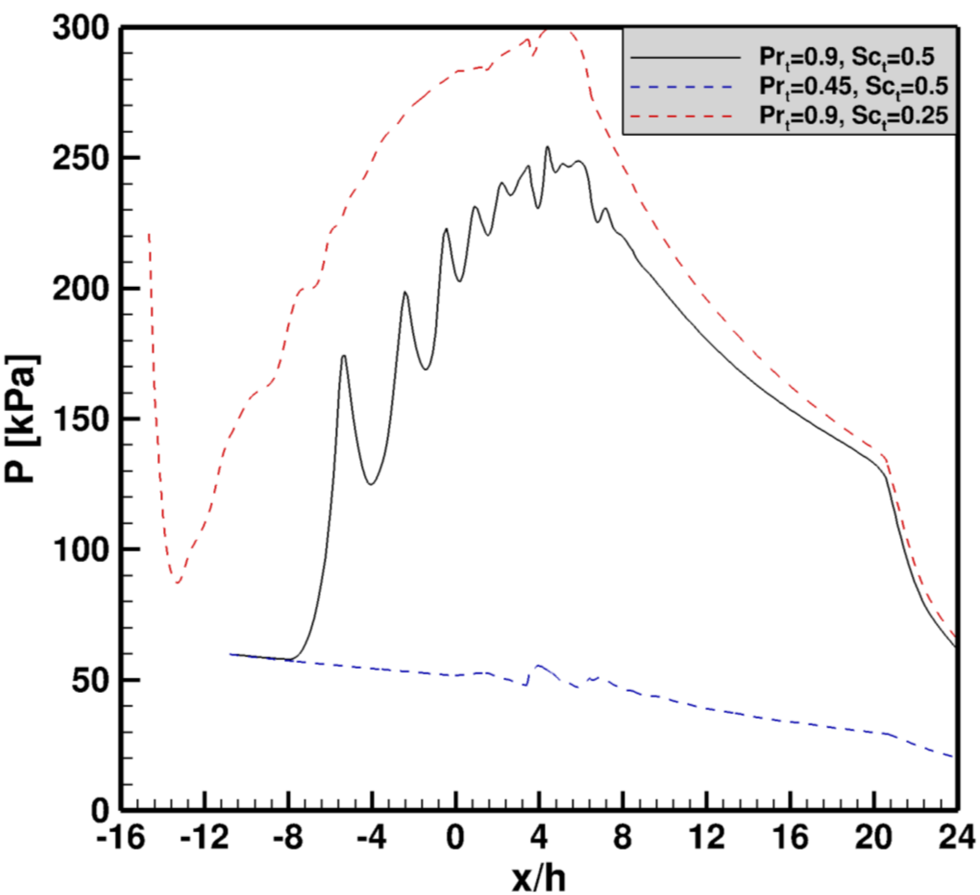


Combustor physics and modeling limitations with RAS

- **The scramjet engine combustor is tasked with adding chemical energy to the flow to enhance 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 the flameholders use 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 and effects of TCI (residence time similar to ignition delay time)
  - 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 and modeling limitations with RAS



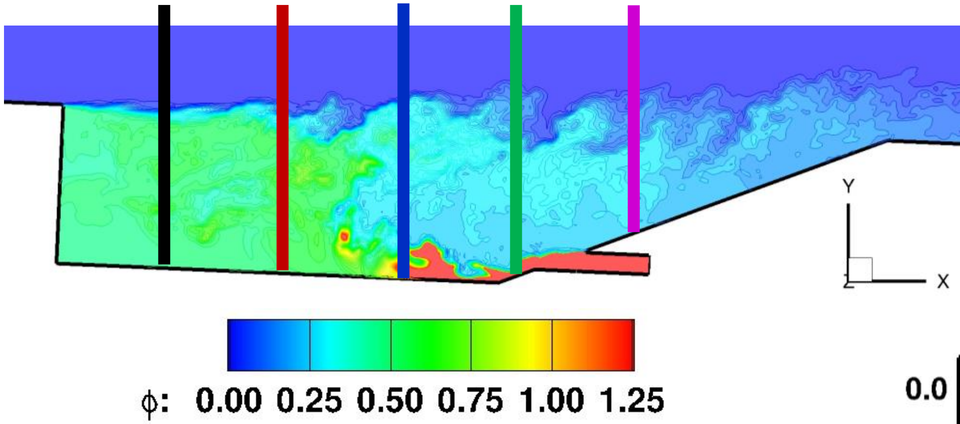


Physical process time scales can be very similar making scramjet combustor predictions extremely sensitive to modeling choices!

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

Scale-resolving simulations have shown some promise in this regard.

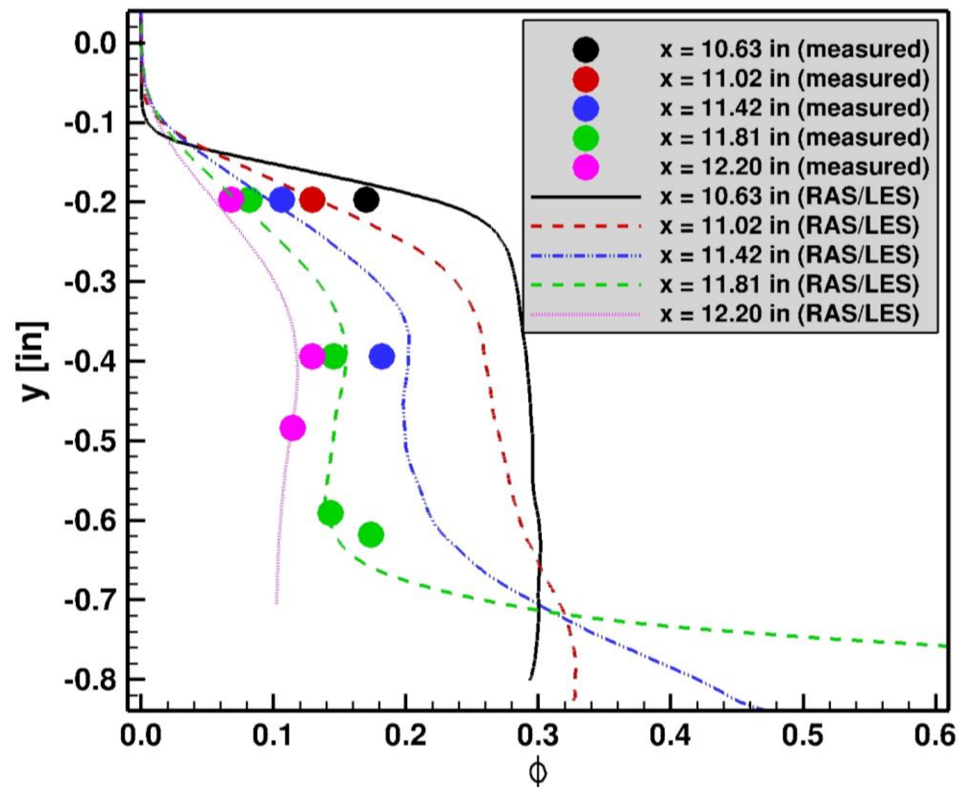
SRS of a Scramjet Combustor Flameholder



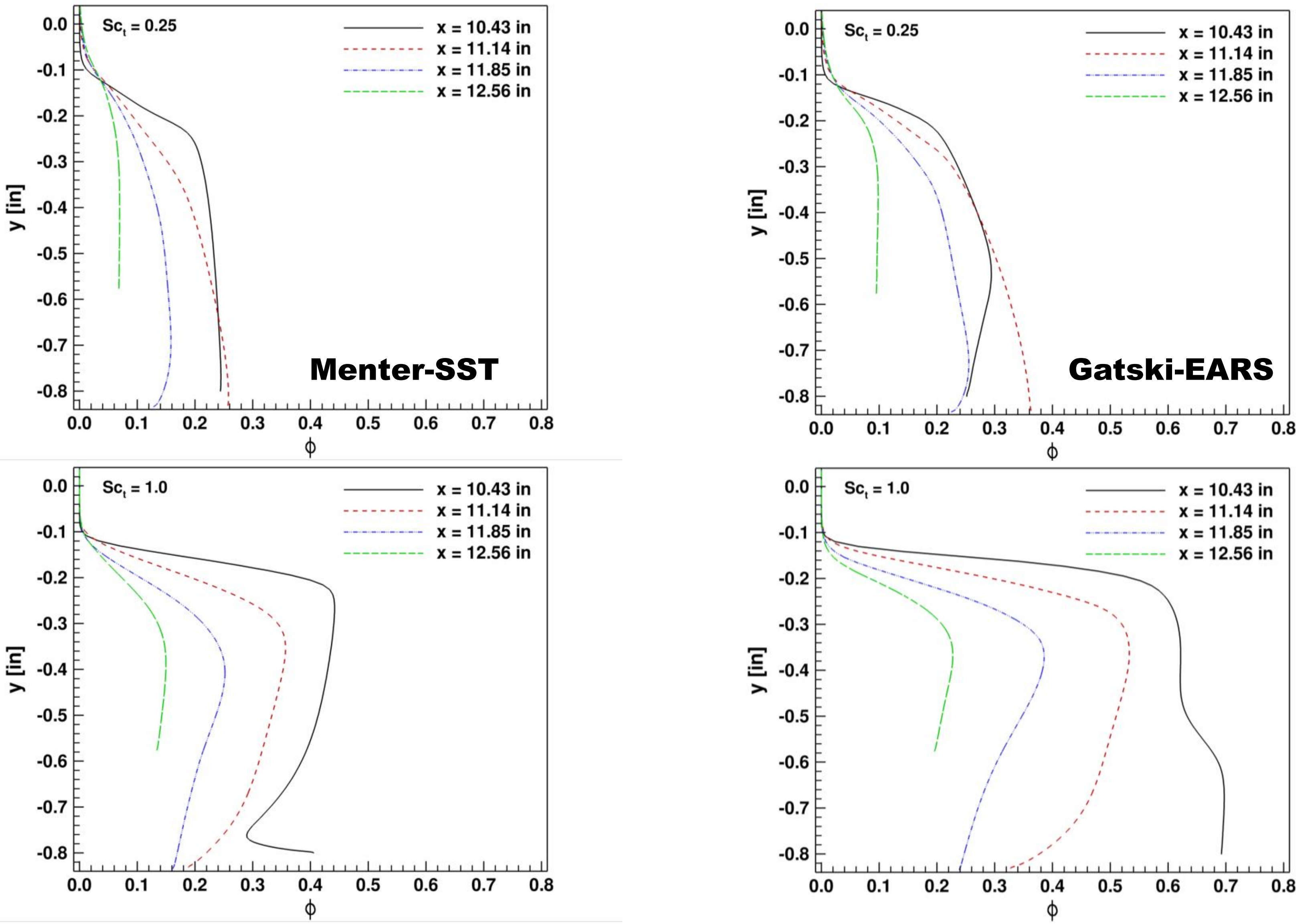
- Hybrid RAS/LES for Mach 2 flow past a fueled recessed cavity

- Ethylene fuel conditions: $\dot{m}$ = 56 SLPM, T_o = 310 K

- Fuel/Air Equivalence Ratio measured via LIBS



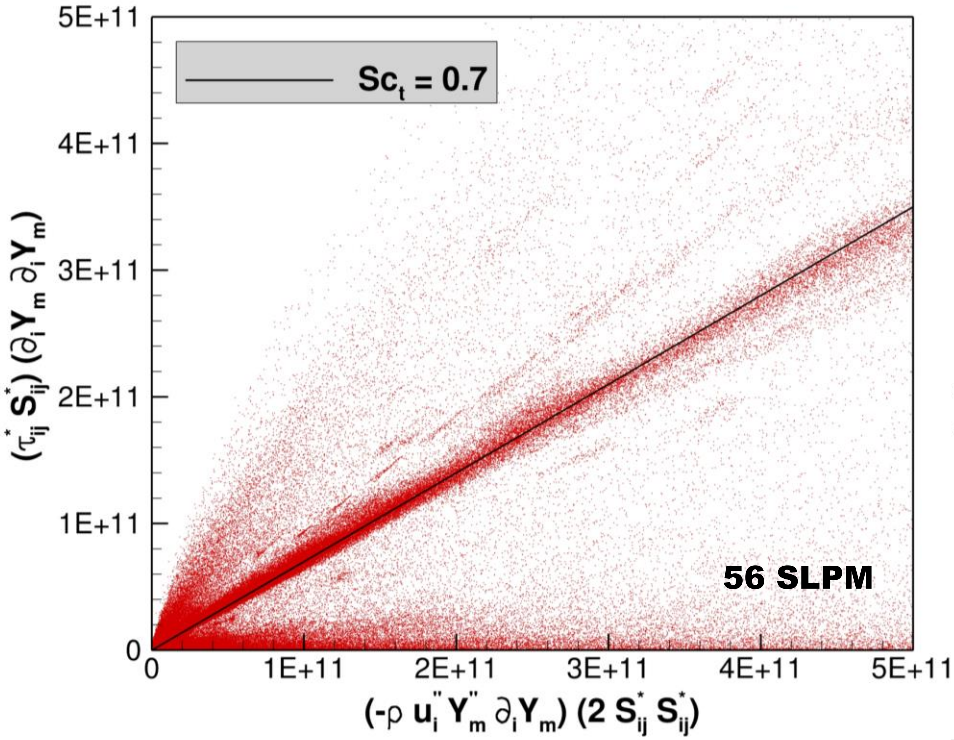
Sensitivity to RAS Turbulence/Mixing Model

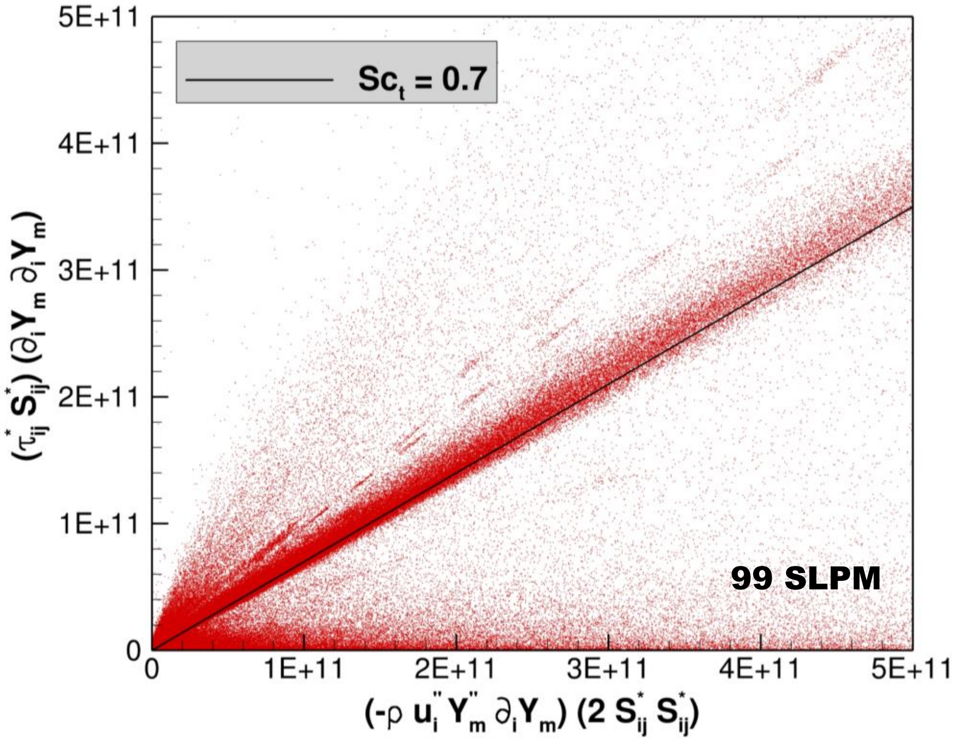


Turbulent Transport Correlation Calibration

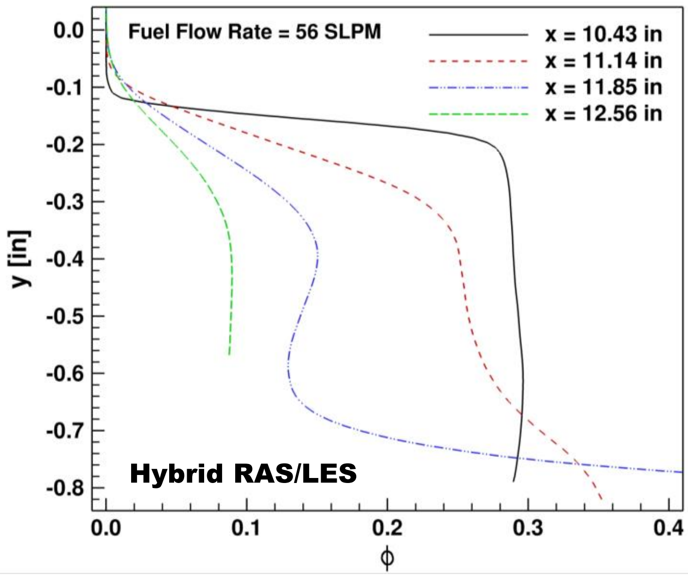
$$\tau_{ij} = 2\mu_t\left(S_{ij} - \frac{1}{3}\delta_{ij}\frac{\partial\tilde{u}_k}{\partial x_k}\right) - \frac{2}{3}\delta_{ij}\bar{\rho}\tilde{k}\,, \qquad \bar{\rho}\widetilde{u_i'' Y_m''} = -\frac{\mu_t}{\mathrm{Sc}_t}\frac{\partial\tilde{Y}_m}{\partial x_i}$$

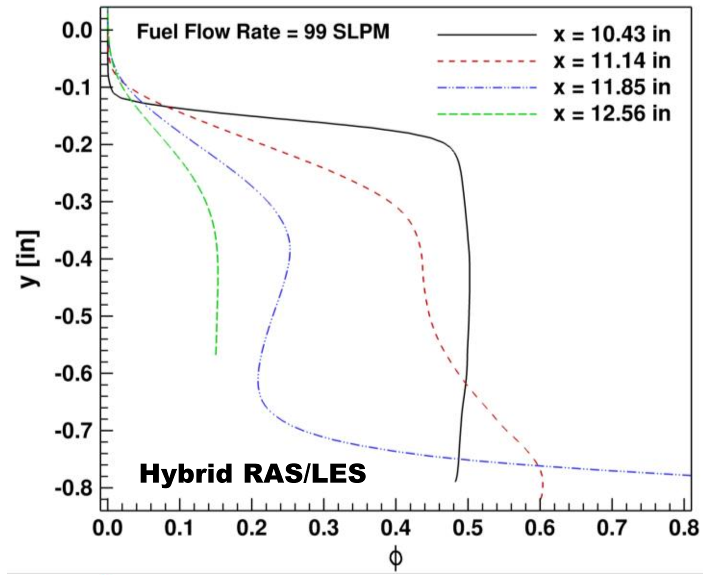
$$\mu_t = \frac{\left(\tau_{ij} + \frac{2}{3}\delta_{ij}\bar{\rho}\tilde{k}\right)\left(S_{ij} - \frac{1}{3}\delta_{ij}\frac{\partial\tilde{u}_k}{\partial x_k}\right)}{2\left(S_{ij} - \frac{1}{3}\delta_{ij}\frac{\partial\tilde{u}_k}{\partial x_k}\right)\left(S_{ij} - \frac{1}{3}\delta_{ij}\frac{\partial\tilde{u}_k}{\partial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

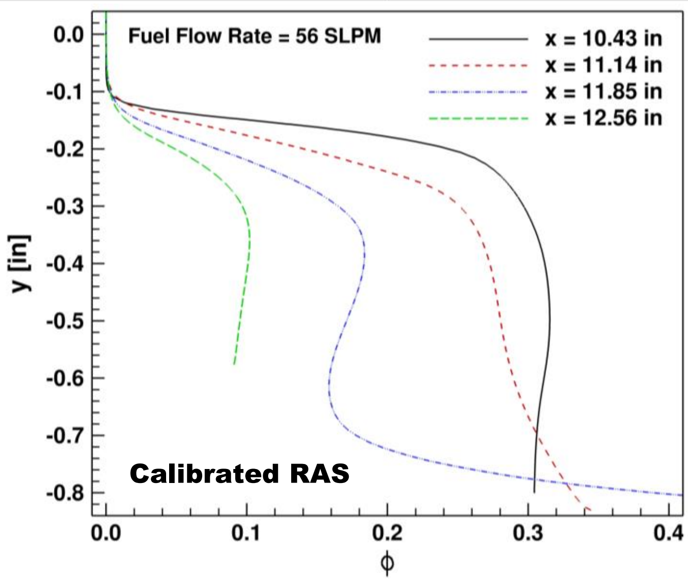


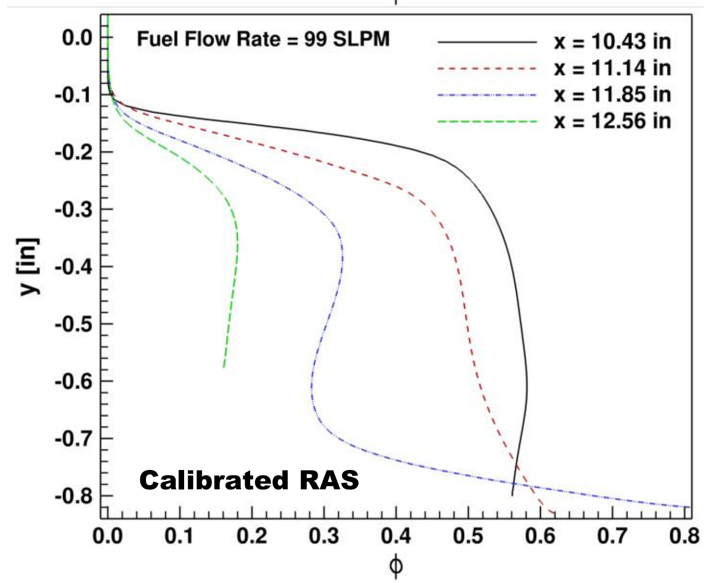


ϕ Comparison of RAS with Hybrid RAS/LES









Engine nozzle physics and modeling limitations with RAS

- **The role of the engine exhaust nozzle is to convert the potential energy of the propulsion system flow 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.
  - Standard turbulence closure models are incapable of capturing this phenomenon accurately.

- **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.**

Available Sources of CFD Software

- **A plethora of options are now available for Scramjet CFD Analysis**
  - Commercial software (many to choose from)
    - Pros: Extensive user support
    - Cons: Cost
  - Open source / public domain software (e.g., OpenFoam)
    - Pros: Free (or almost free)
    - Cons: Often require modular builds to combine libraries to construct the desired CFD capability
  - Government developed software (DOD: Kestrel, DOE: SPARC, NASA: VULCAN-CFD, FUN3D, LAURA, DPLR)
    - Pros: Free
    - Cons: Distribution and support often limited
  - University developed software (e.g., US3D)
    - Pros: Free
    - Cons: Distribution, Documentation, and support are limited

Summary

- **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 with 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.**

Summary

- **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 in design and analysis of high-speed reacting flows while systematically investigating modeling sensitivities.**

- **SRS likely to remain limited to specific situations:**
  - improve fundamental physics understanding (universities routinely do this)
  - investigate impact of unsteady effects
  - RAS scenerios with unacceptably high uncertainty (e.g., operability bounds)
  - calibration of RAS closure models