Advanced Modeling & Simulation (AMS) Seminar Series

NASA Ames Research Center, June 23rd, 2022

https://www.nas.nasa.gov/pubs/ams.html

High-Speed Combustion/Reacting Flows Current Solutions and Development

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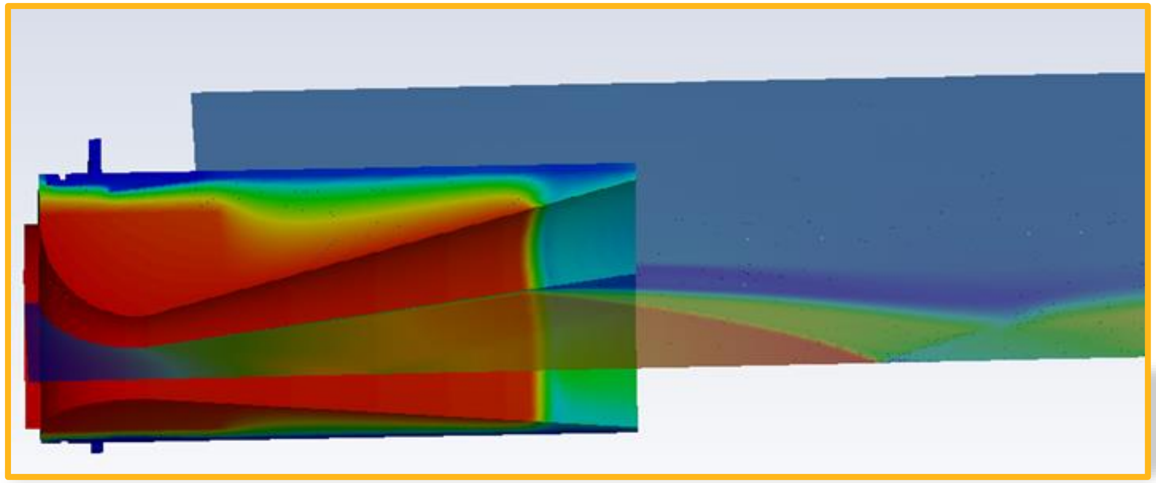
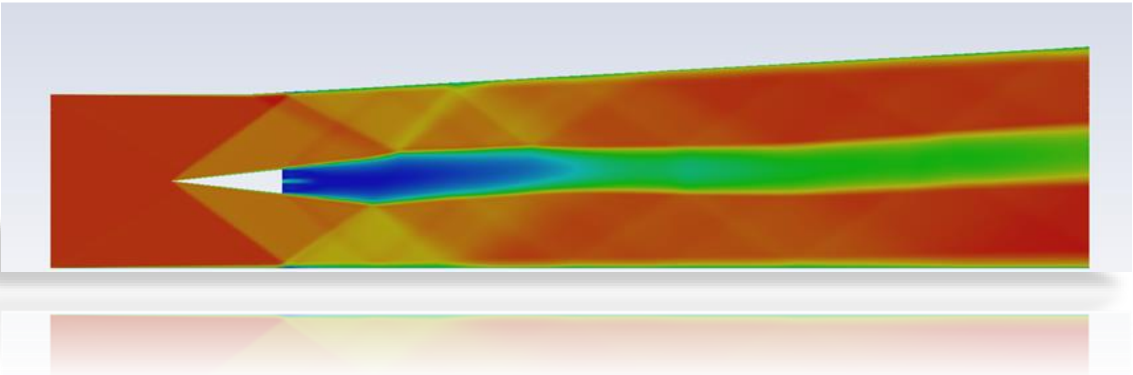
June 23, 2022

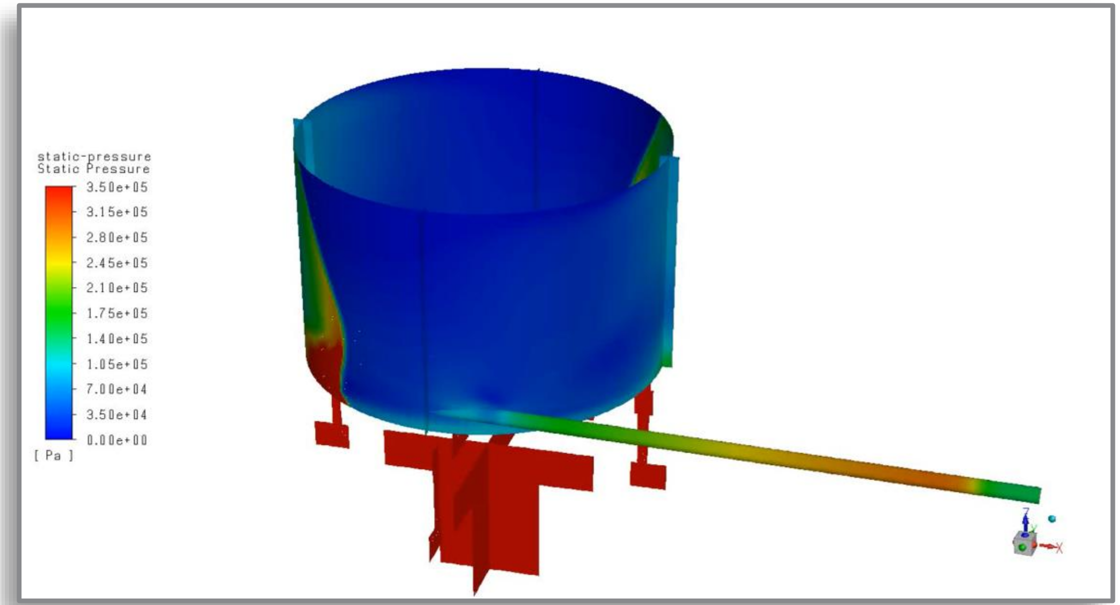
Ansys

Agenda

- Motivation
- Current Status of Technology
- Types of propulsion/reacting flows
- Core Ansys Technology and Roadmap
- Collaborations
- Validations and Case Studies
  - DLR SCRAMJET
  - Burrows&…
  - Babu Scramjet
  - AFRL RDE
  - Rockets/ NAVY
  - Ablation modeling







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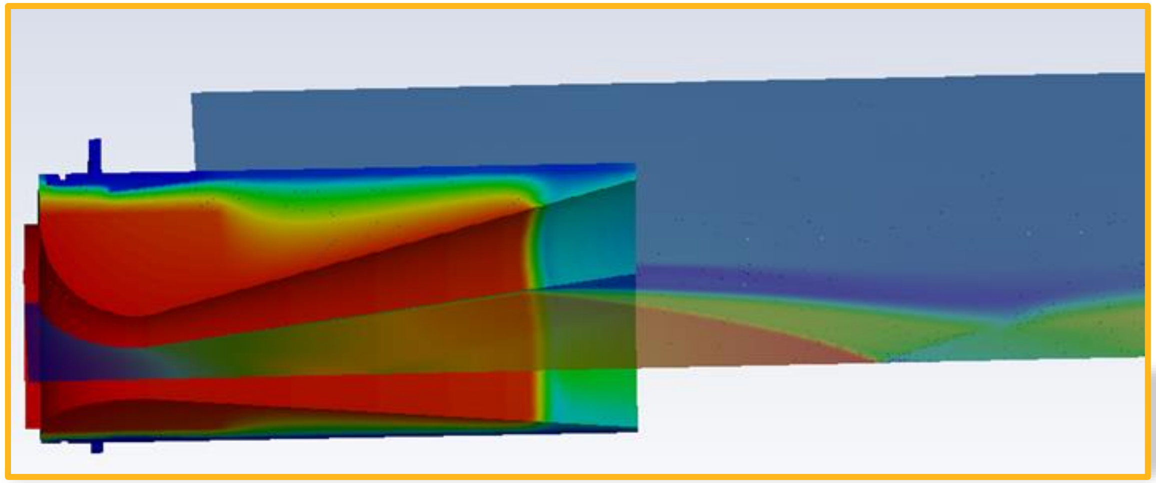
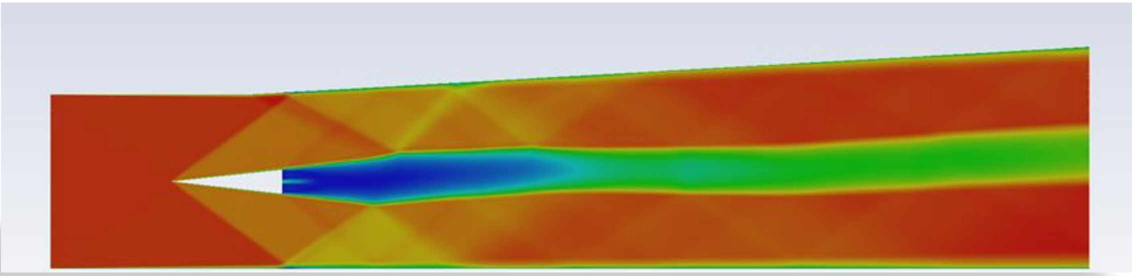
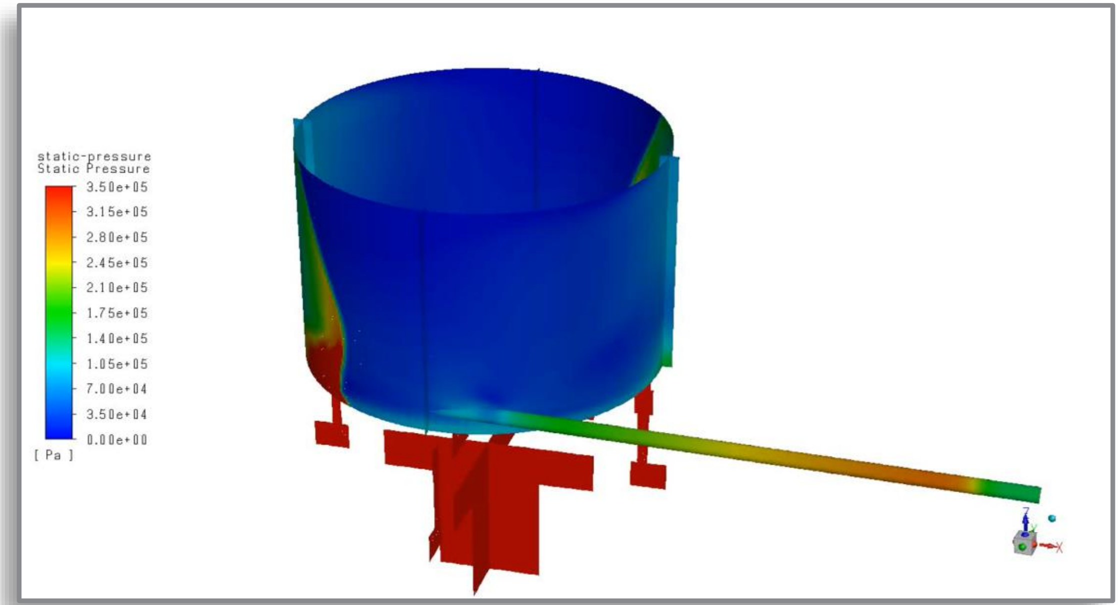
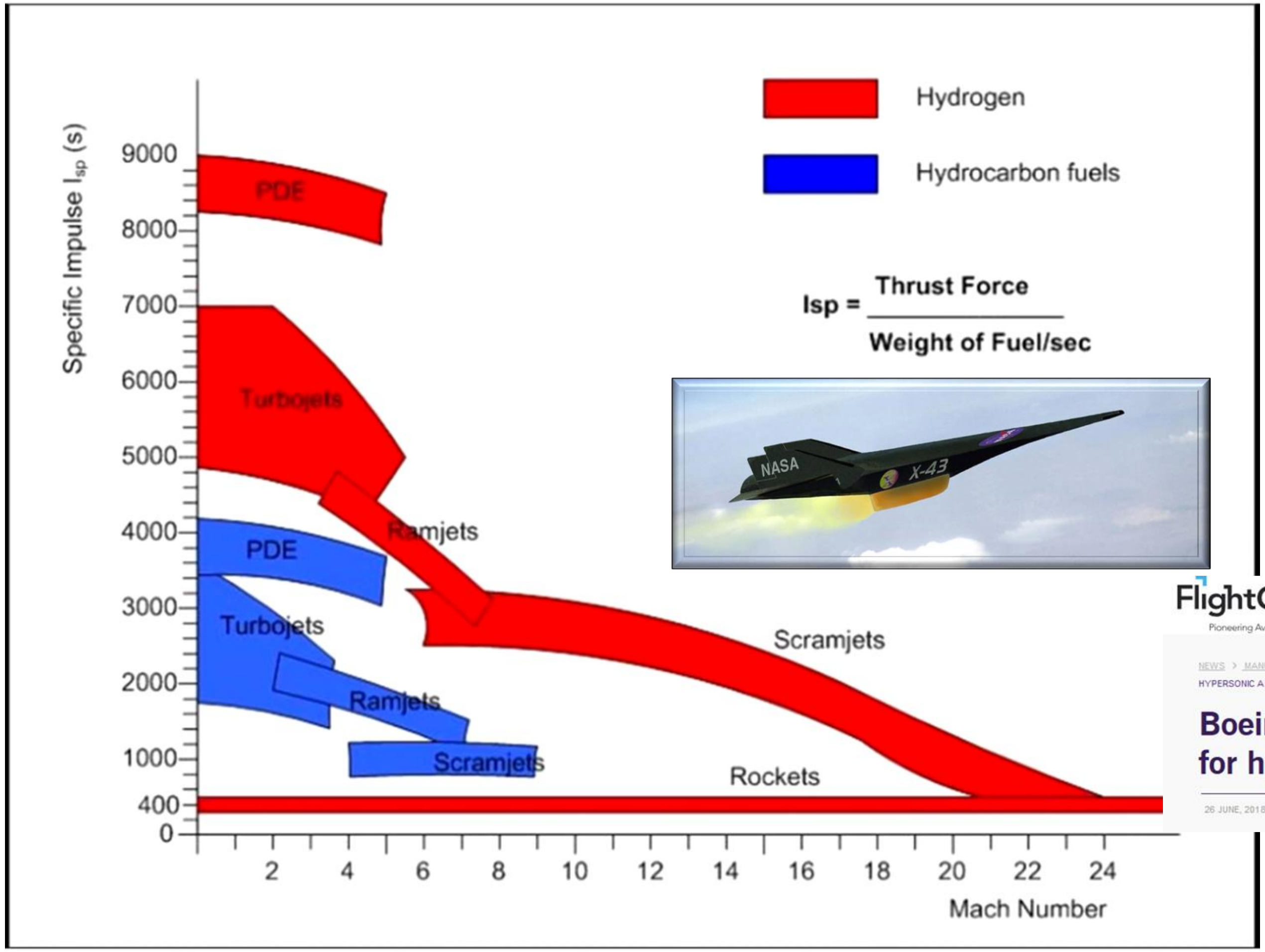






Motivation

- **With the resurgence in interest supersonic and hypersonic vehicles, there is a need on develop the propulsion to reach those speeds.**



- Improved efficiency
- Higher impulse propulsion
- Re-entry materials
- New technologies

Flight Global/Boeing

European States Plan For Hypersonic Defense

Tony Osborne January 10, 2020

AVIATION WEEK NETWORK

Ansys

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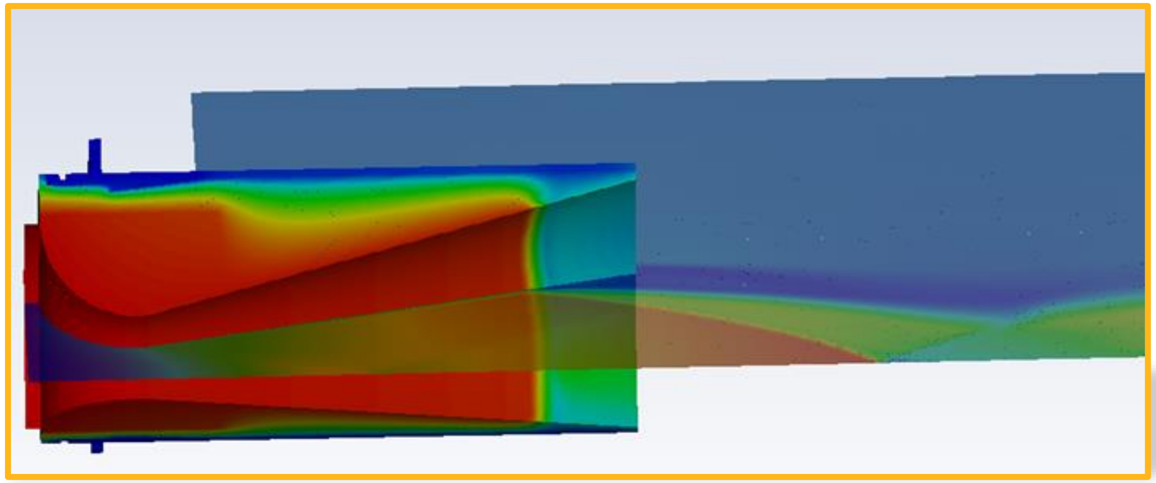
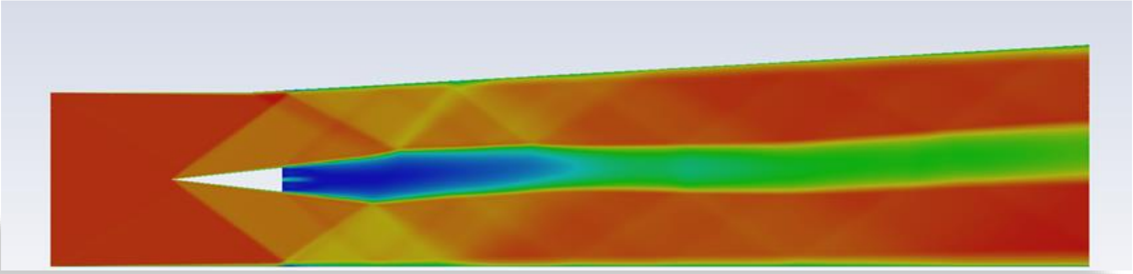
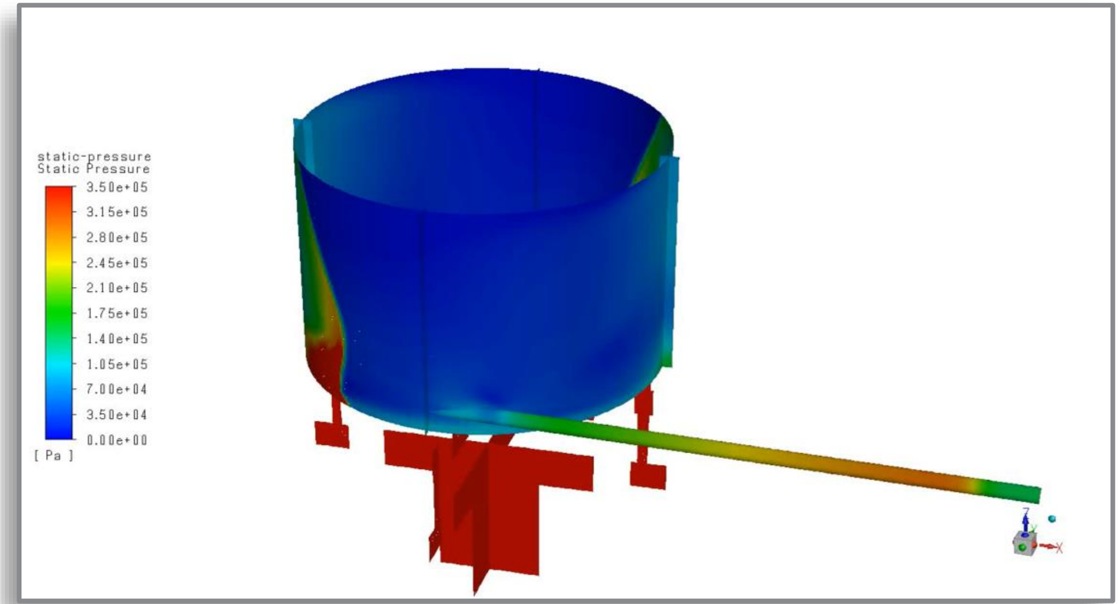




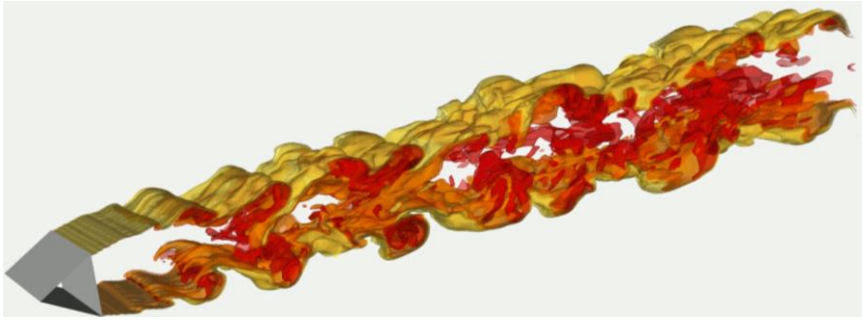


High-Speed Combustion/Reactions

- Ansys CFD has been the leader for over 20 years Combustion and Reacting flows
- Applying these experiences to the high-speed propulsion and re-entry flow simulations
- Current focus areas are the foundation for all High-Speed Combustion/Reacting flow simulations
  - Improve flame capturing and solver numerics for robust, efficient, and accurate solutions
  - Extended modeling to improve physical phenomena predictions
- Multi-faceted and multi-team effort
  - Fluids Development, Applications, Documentation, Testing, and Technical Support (ACE)

Real Gas EOS

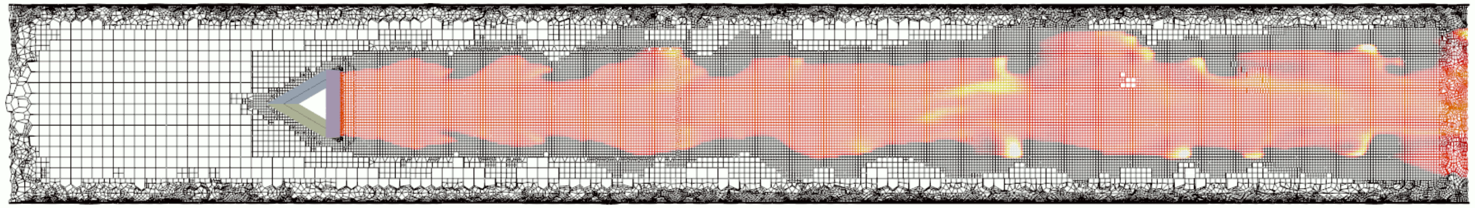
Finite rate kinetic reactions



Ablation

Pyrolysis/ Surface Reactions

Turbulence



Non-equilibrium thermodynamics

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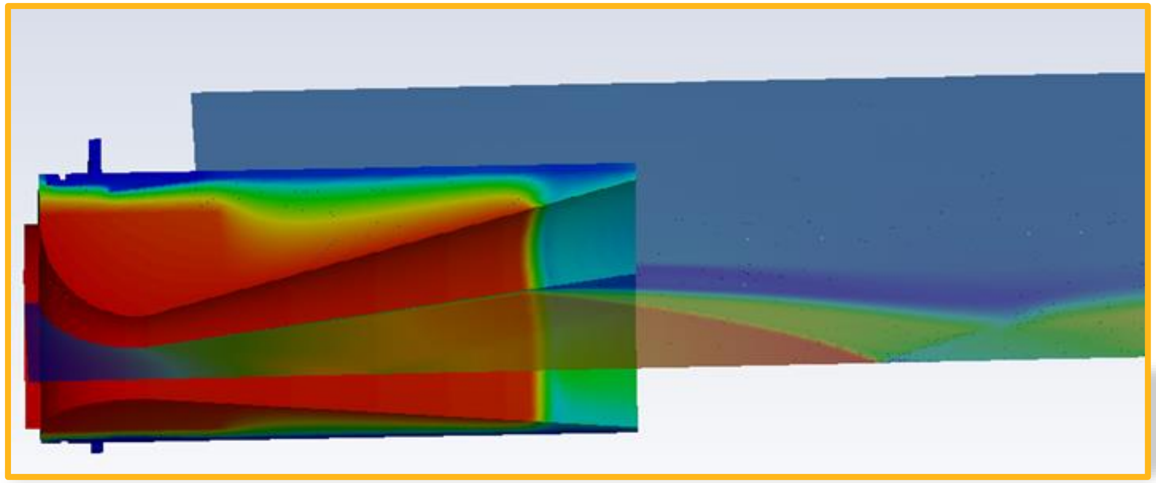
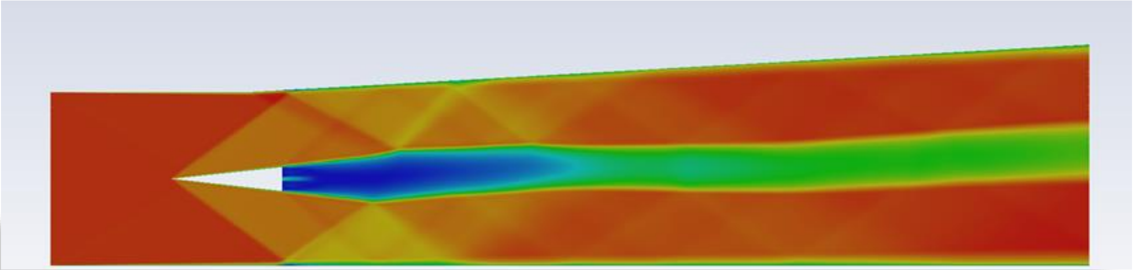
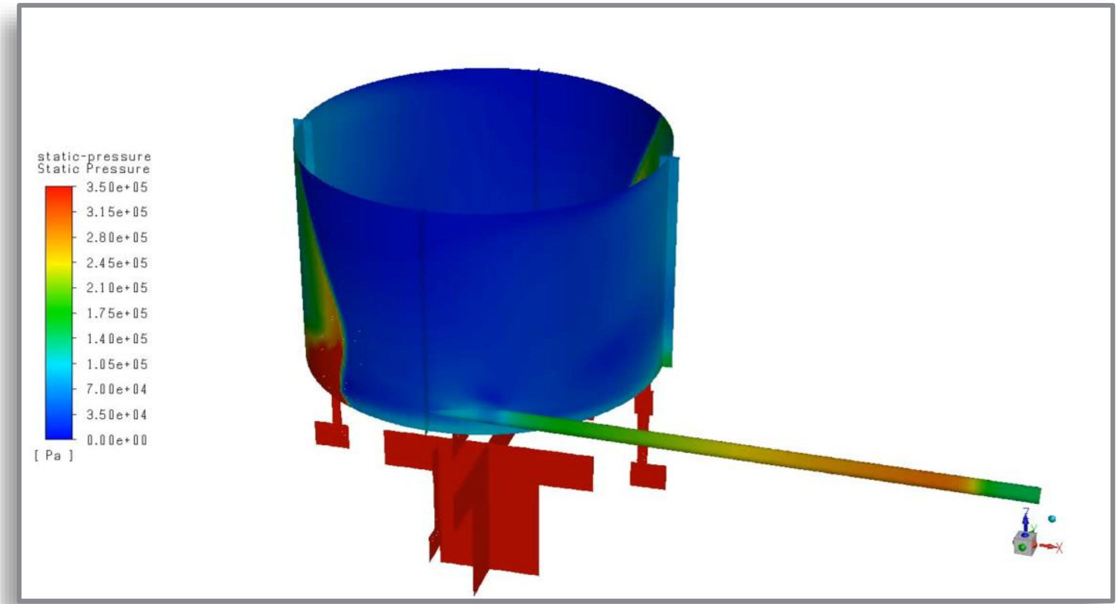






What type of highspeed reacting flows are we talking about?

Propulsion

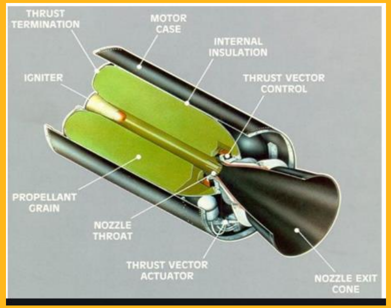
Air Breathing | Internal Oxidizer

RAM/SCRAM jets

- Mach < ≈12.0
- DBNS/PBNS solvers
- Finite Rate Chemistry (Fluent/CHEMKIN)
- Turbulent Combustion Interaction (TCI)
- Equilibrium Chemistry (RTE, Gibbs)
- Fuel Droplet/ Solid Particle Injection
- Transpiration cooling/combustion

Liquid/Solid Rocket Motors

- ≈1 < Mach < ≈18.0
- DBNS/PBNS solvers
- Vielle's Law Modeling
- Surface Reactions
- Pyrolysis Reaction in Porous Media
- Particle Erosion (flow injection)
- Solid recession modeling (MDM)
- PDF Combustion
- Real Gas EOS



Re-entry

- Mach > ≈18.0
- DBNS Solver
- Modeling Air Chemistry NASA 9C thermo data format
- Finite Rate Chemistry(Fluent/CHEMKIN)
- Equilibrium Chemistry
- Two Temperature model
- Ionization Predictions
- Surface Ablation
- Pyrolysis reaction

Photo: Courtesy of ESA

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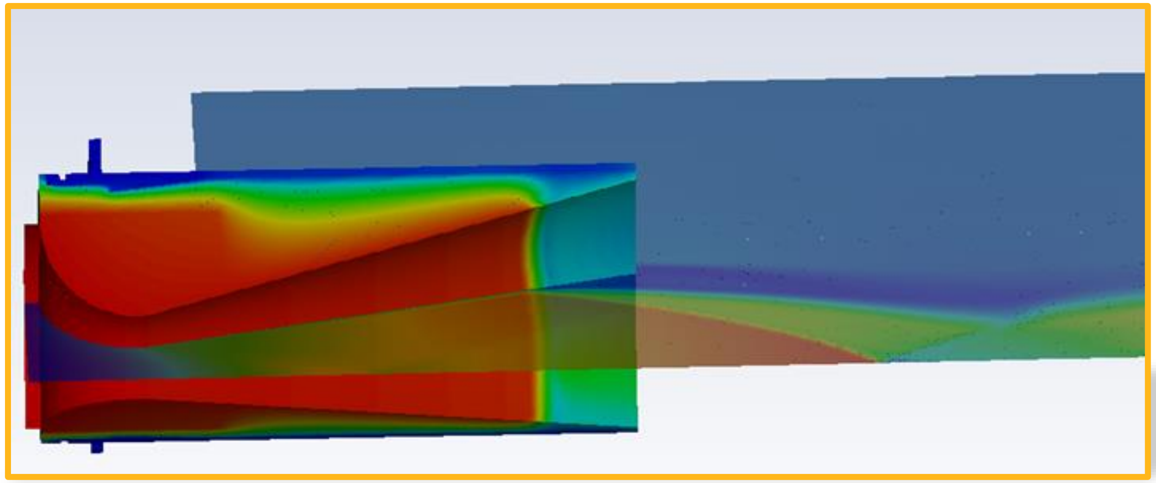
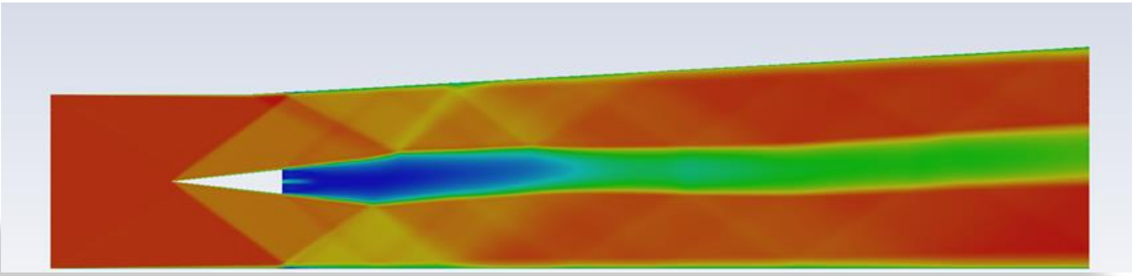
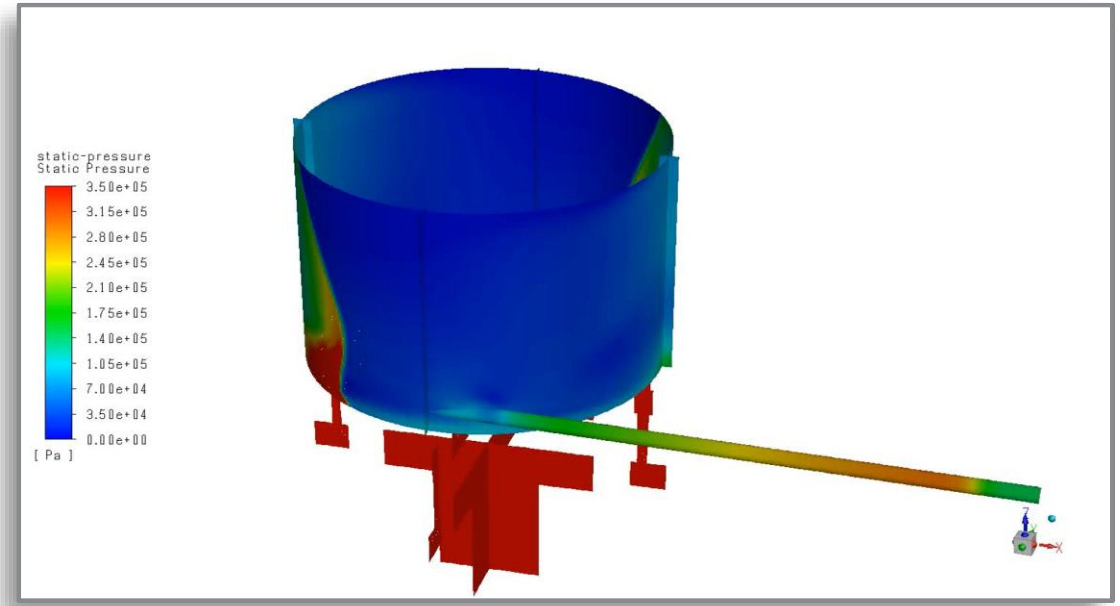
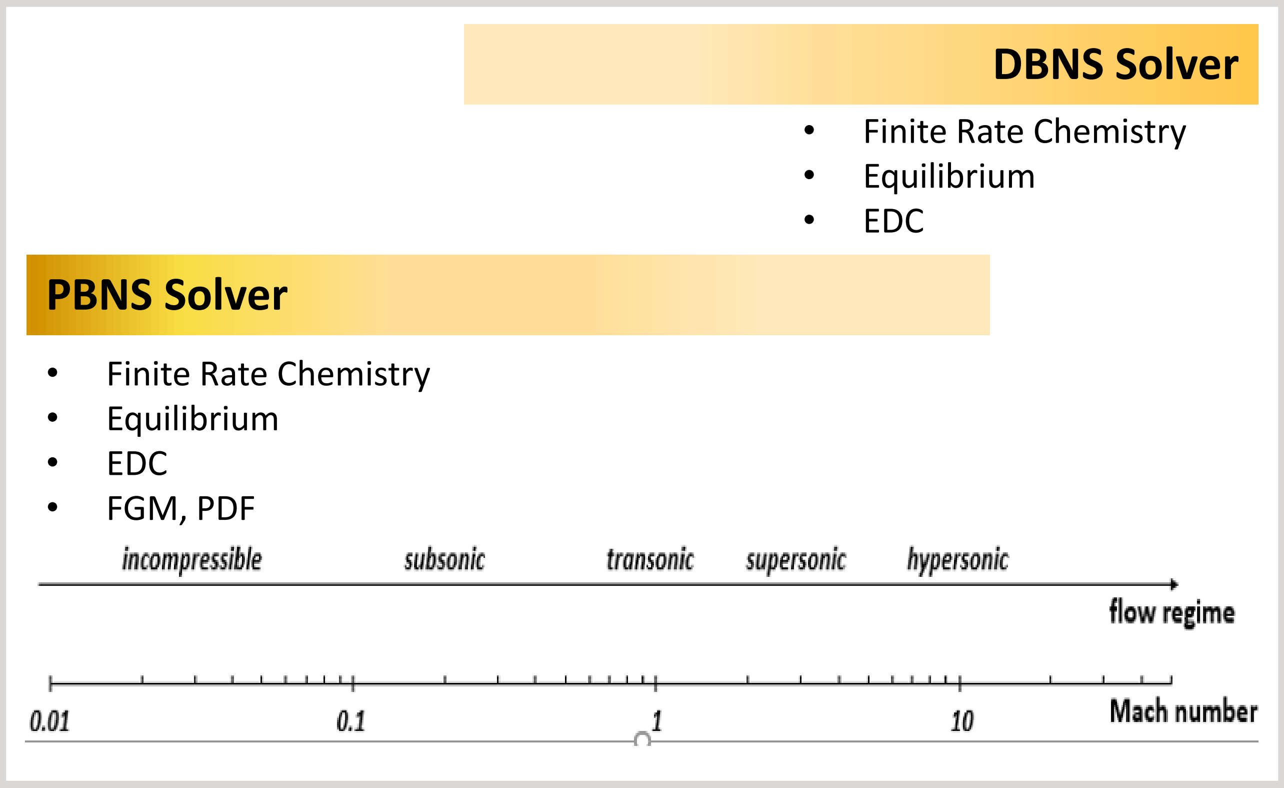






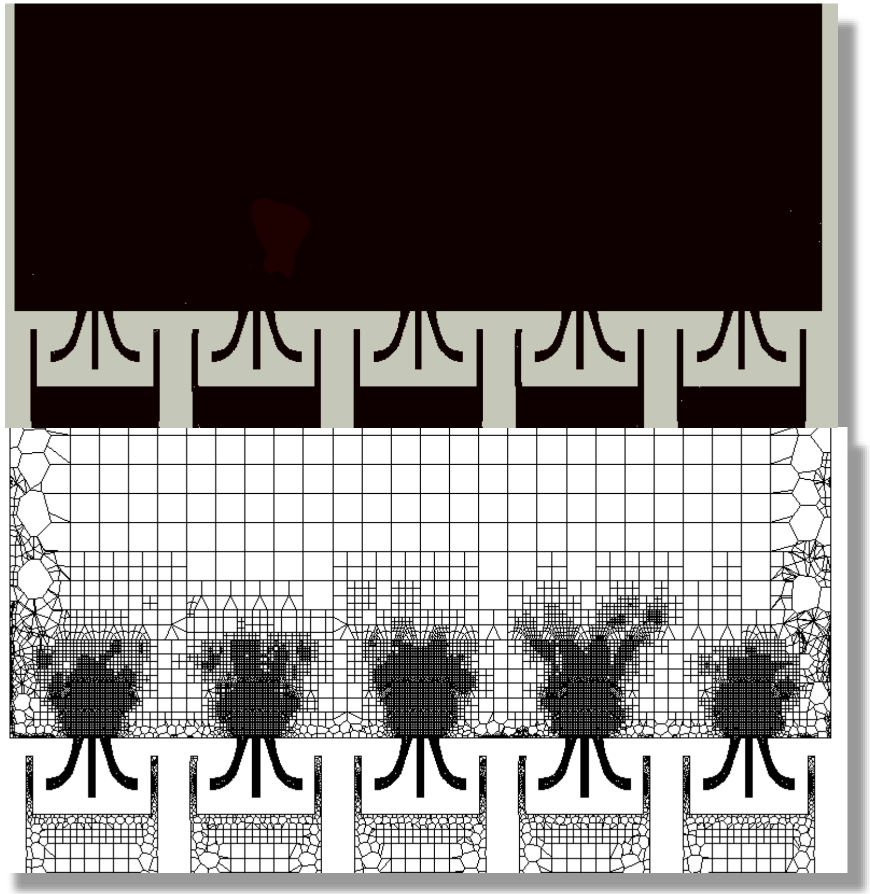
Ansys Fluent for High-Speed Combustion/Reactions

- Coupled Finite Volume Method with higher order discretization
- Using both pressure-based and density-based solution method
  - Depending on flow Regime and Combustion process, Different Combustion/Reaction models are currently available
- Leverage and build on existing broad capabilities and infrastructure of Fluent
  - turbulence and transition, Radiation, solid conduction, mesh motion and deformation, ...



Fluids Developments and Roadmap for High-Speed Combustion/Reaction

- **Physics Modeling** Combustion/Reaction Applications
- **Numerics** Enhancements for Highly Compressible Flow with Species and Reactions
- **Mesh Adaptation** for Efficient Capturing of Reactions zones/Shocks
- **Collaborations** on High-Speed Combustion/Reaction Flow Simulation
- **Validation** and Testing of High-Speed Combustion/Reaction Developments



Physics Modeling: High-Speed Combustion/Reaction Applications

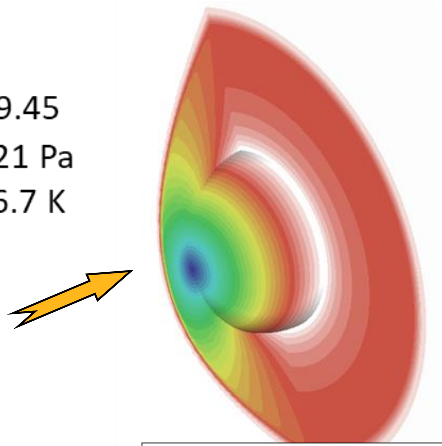
- Physics Models
  - Extension of built-in property models
    - NASA 9-coefficient thermodynamic property model for c_p
    - Eucken relation for k and Blottner for μ
  - Improvements in Species
    - Surface reactions (DBNS)
  - 2-temperature model combined with chemical reactions
  - External Ablation modeling with Vielles Law and Surface reactions. Include MDM at surface setup
- Current and planned R&D
  - External Ablation modeling CHT with MDM
  - Solid Rocket Fuel Ablation Modeling
    - Surface/Pyrolysis reactions
    - DPM injection
  - Improvements in Conjugate Heat Transfer (CHT) with DBNS solver

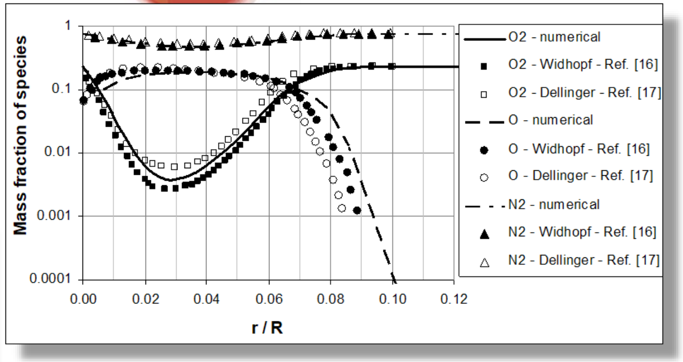
$$\frac{C_p^0(T)}{R} = a_0 T^{-2} + a_1 T^{-1} + a_2 + a_3 T + a_4 T^2 + a_5 T^3 + a_6 T^4$$

$$\frac{H^0(T)}{RT} = -a_0 T^{-2} + a_1 \frac{\ln T}{T} + a_2 + \frac{a_3}{2} T + \frac{a_4}{3} T^2 + \frac{a_5}{4} T^3 + \frac{a_6}{5} T^4 + \frac{a_7}{T}$$

$$\frac{s^0(T)}{R} = -\frac{a_0}{2} T^{-2} - a_1 T^{-1} + a_2 \ln T + a_3 T + \frac{a_4}{2} T^2 + \frac{a_5}{3} T^3 + \frac{a_6}{4} T^4 + a_8$$

Ma=29.45
P=12.21 Pa
T= 196.7 K



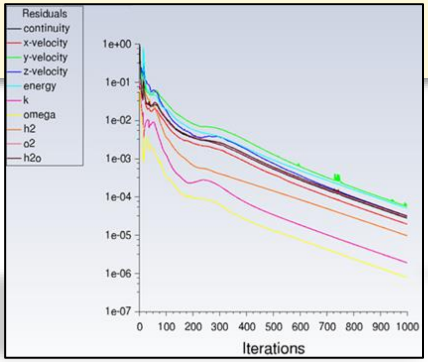


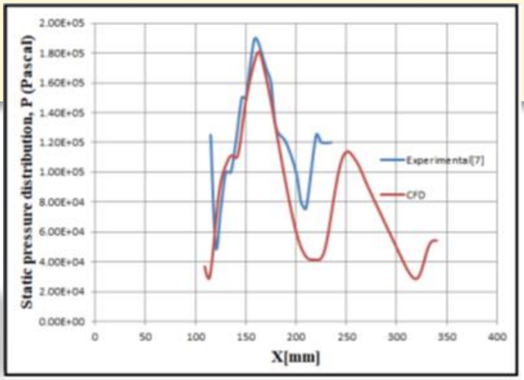
Distributions of normalized static temperature, density, and mass fraction of O_2, O and N_2 along the stagnation streamline

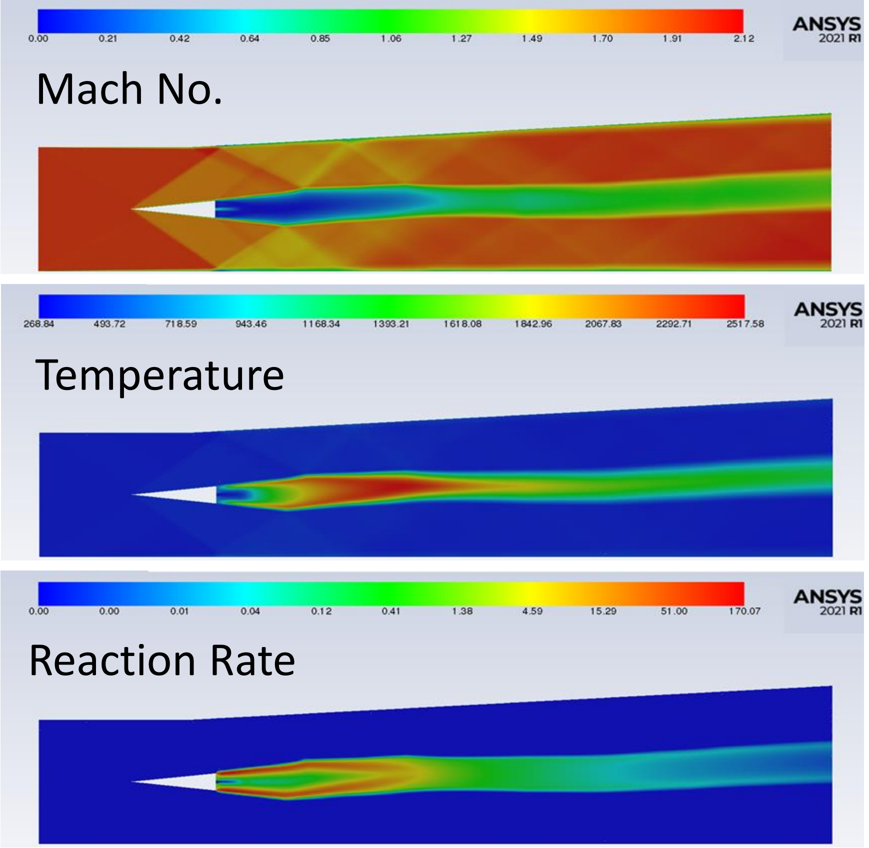
Ansys

Numerics: Enhancements for High-Speed Combustion/Reactions

- Recent key developments
  - Improvements with Species handling and Jacobian matrix for robust and faster convergence (DBNS)
  - Best Practices with Coupled Solvers setting in PBNS and DBNS
  - Initialization with viscous terms and species/reaction
- Current and planned R&D
  - Optimized numerics for finite rate chemistry
  - Chemical non-equilibrium and propulsion/combustion



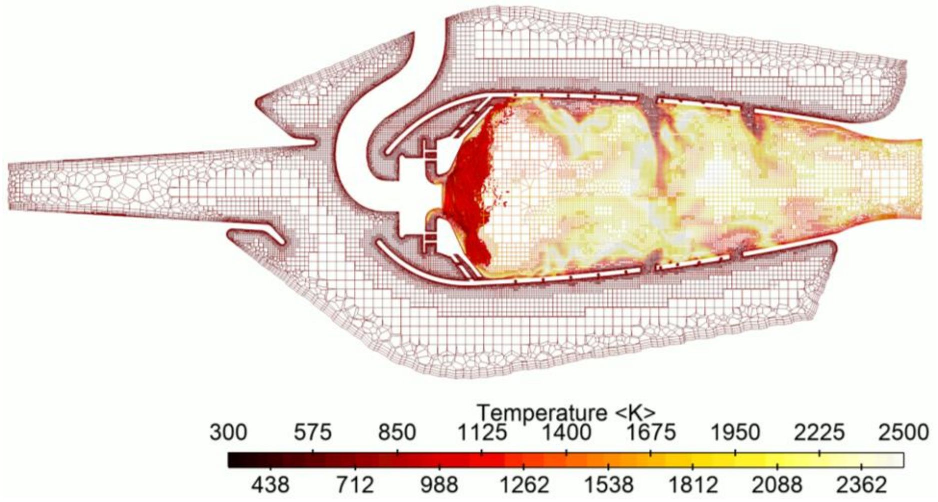




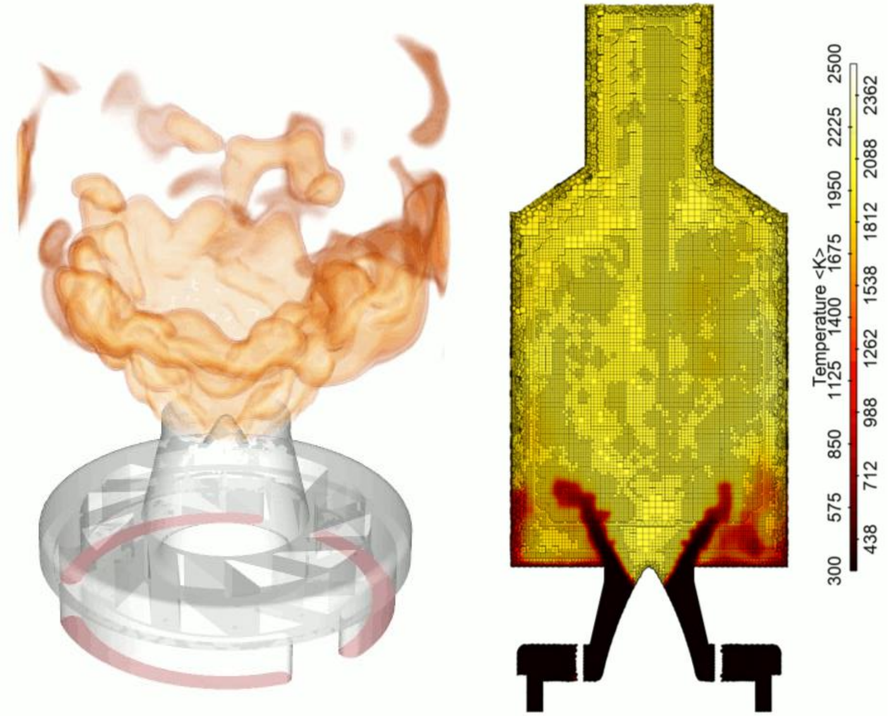
DLR SCRAMjet case testing and evaluation best practices

Mesh Adaption: High-Speed Combustion/Reacting Flows

- Recent key developments
  - Introduction of additional mesh adaption capabilities
    - Flame/Density/Shock-specific adaption criteria
    - Anisotropic adaption for polyhedral boundary layers (beta)
- Current and planned R&D
  - Anisotropic volume mesh adaption
  - Adaptation driven by estimate and reduction of solution error



Dynamic Mesh Adaption for GT Combustor



Polyhedral Unstructured Mesh Adaption (PUMA) based on new Shockwave Identification Parameter (SWIP) applied to Swirling Flame test case

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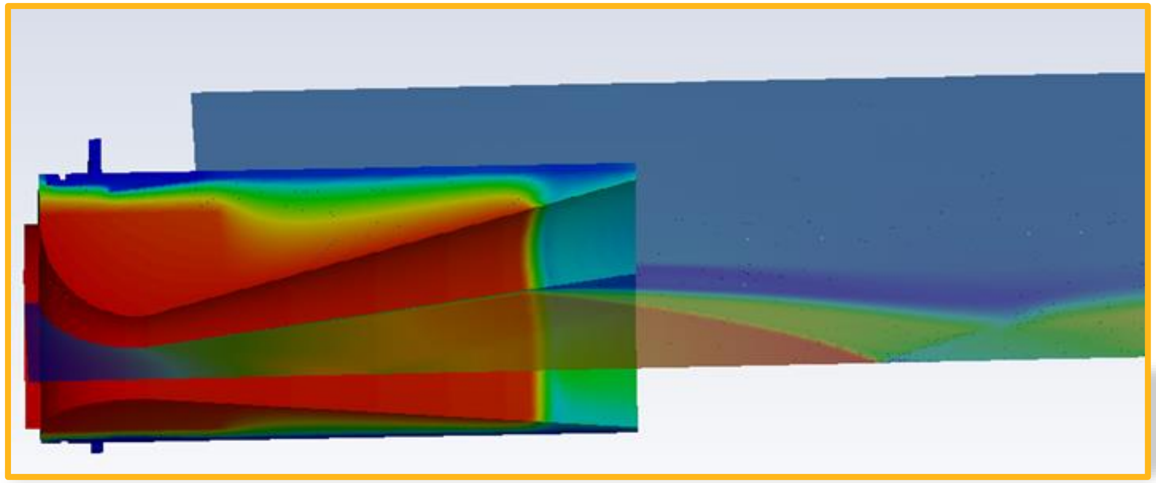

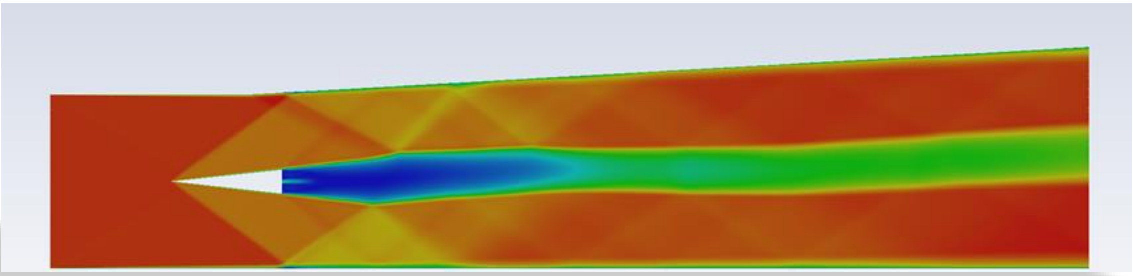

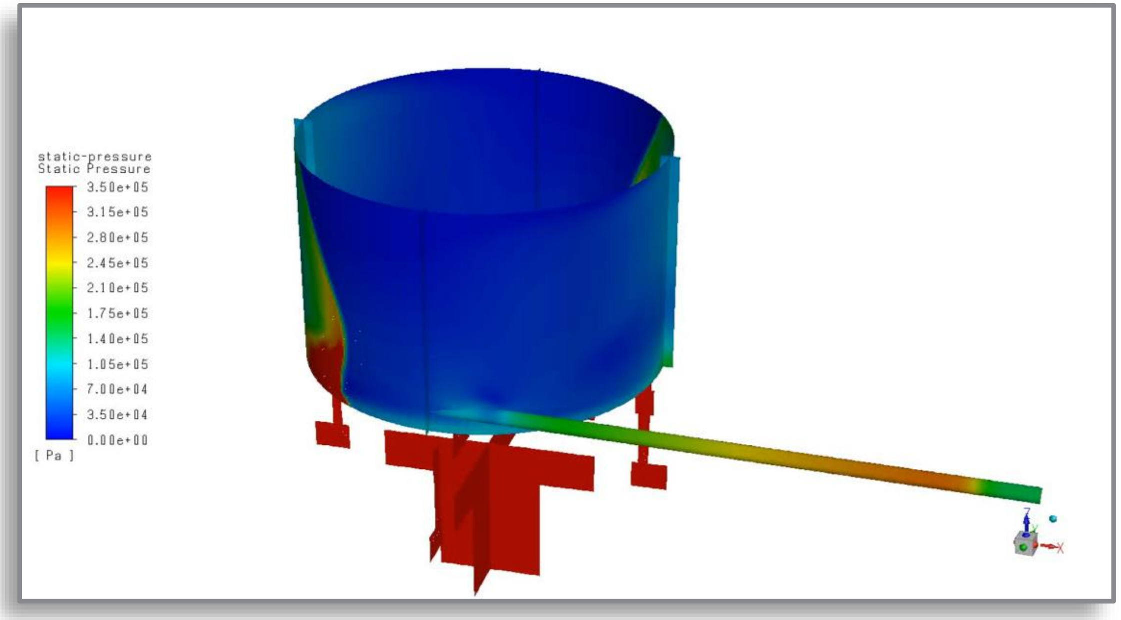

New Ansys R&D collaborations in hypersonics

- **University of Texas, Arlington**
  - Aerodynamic Research Lab (ARC): Director Prof Maddalena
  - The only US academic institution with arc-jet facility.
  - Inaugurated in summer 2019, with $1.5M funding from US Navy/DARPA
  - Cutting-edge experimental research in hypersonics (aerothermodynamics, SCRAMJET propulsion, ablation)
  - Currently working with AFRL/NRL/DARPA

- **Missouri Science and Technology, Rolla**
  - Aerodynamic Computational Lab led by Prof Hosder
  - Research sponsored by NASA and Missile Defense Agency:
    - Simulation technology for high-speed flows
    - Effect of particles on high-speed vehicles
    - Uncertainty Quantification
  - ARL has recently won an NSF grant for ~$2M to deploy a supercomputer dedicated to computer simulations.

- **University of Colorado, Boulder**
  - Collaboration with UC Boulder's Non-Equilibrium Gas and Plasma Dynamics Lab on hybrid coupling of CFD and DSMC methods for rarefied flows.

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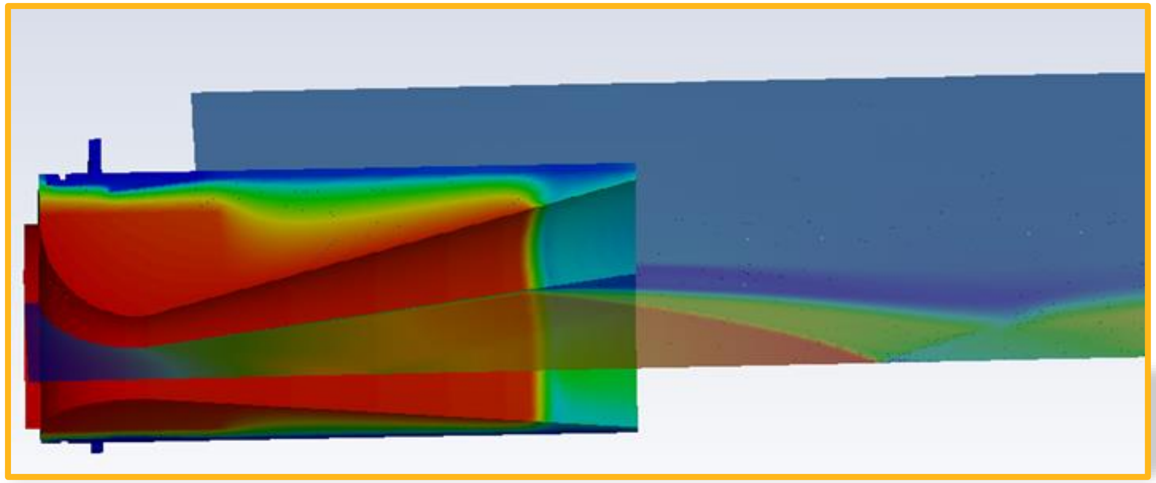
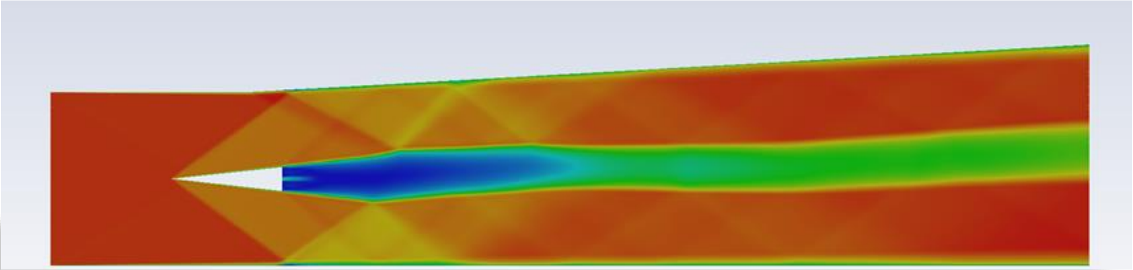
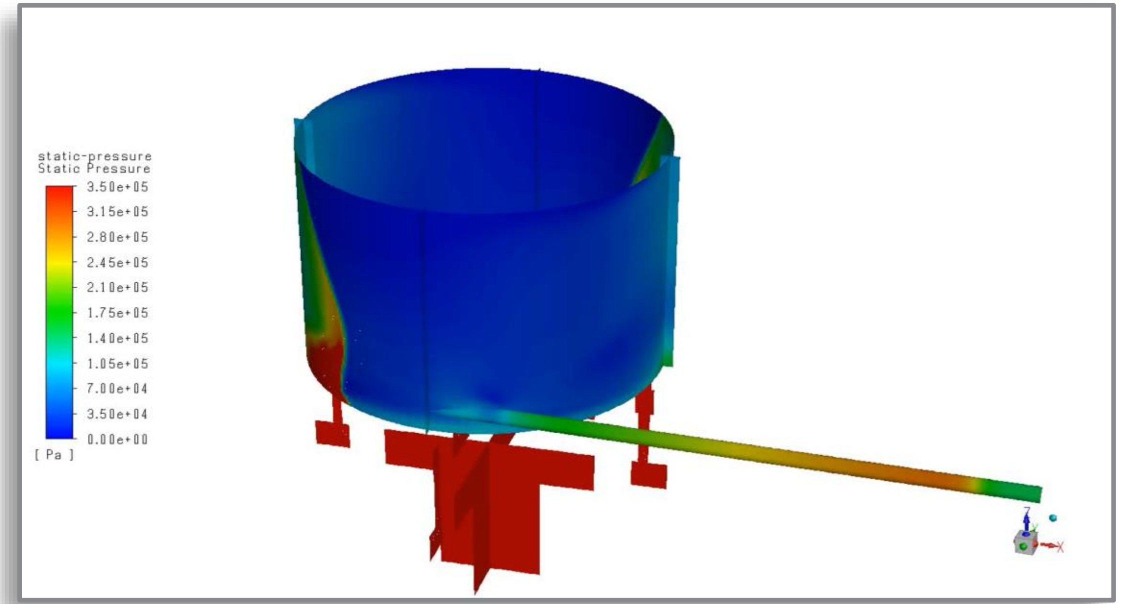






Validation: DLR scramjet validation and case study

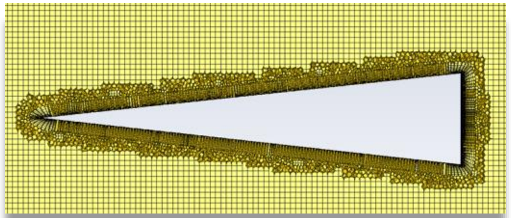
Full Evaluation/Validation of the DLR SCRAMjet case

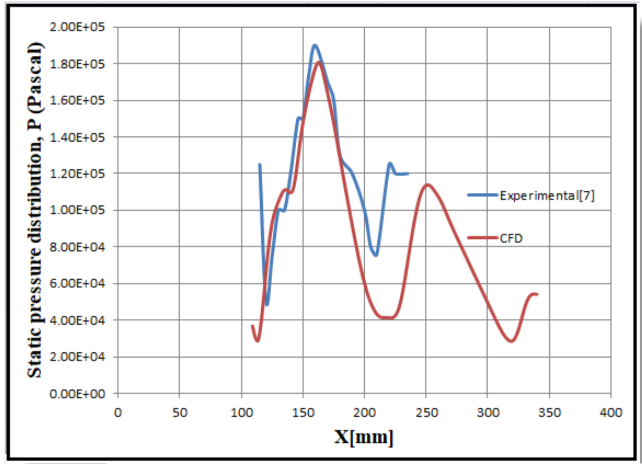
- Evaluating all Ansys mesh configuration: Hexcore, Poly, tetra, PolyHexcore, and SCIM Structure Meshing
- Testing both PBNS/DBNS Solvers
- Testing Finite Rate Chemistry (Fluent, CHEMKIN) and Equilibrium Solvers (RTE, Gibbs)
- Evaluating all TCI models (EDC,PaSR, etc)
- With PBNS, testing PDF, FGM models

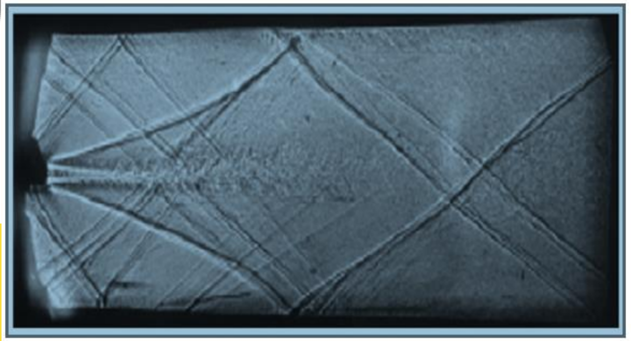
Outcome:

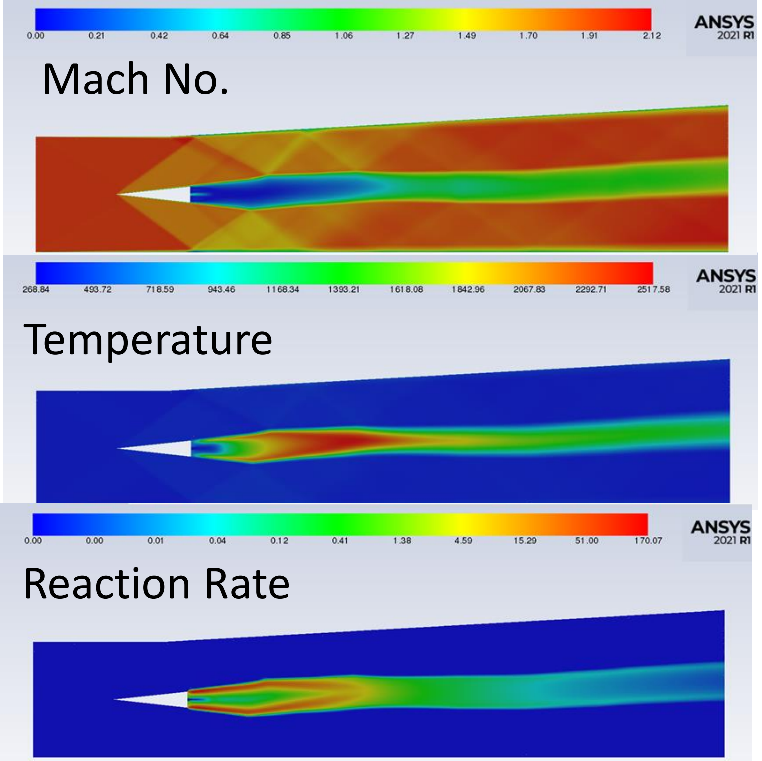
- improved solver convergence

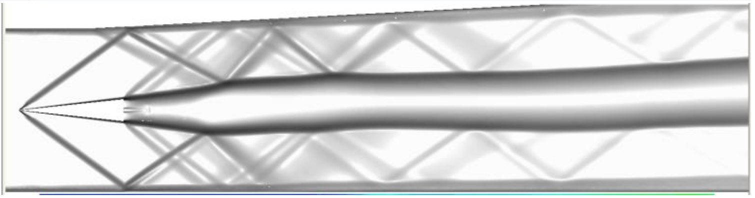
- developed best practices for SCRAMJETs







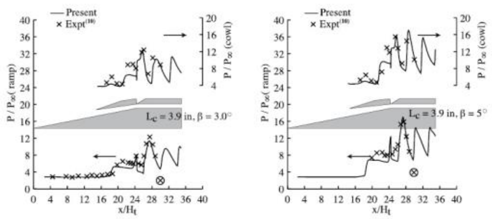




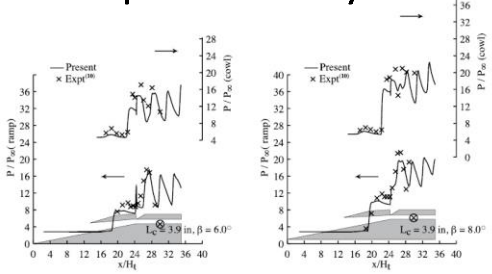
"CFD ANALYSIS OF THE EFFECT OF MACH NUMBER ONSCRAMJET COMBUSTION", G. SANTHANAM, C. SRINIVAS, CH. KHYATHI SREE & S. SRINIVAS PRASAD International Journal of Mechanical and Production Engineering Research and Development (IJMPERD) ISSN (P): 2249-6890; ISSN (E): 2249-8001 Vol. 9, Issue 4, Aug 2019, 393-402

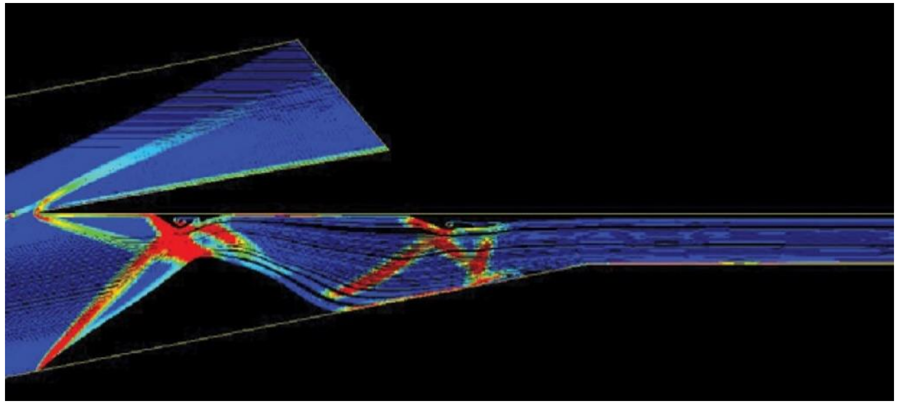
Babu’s Liquid JP4 SCRAMJET design for Mach 6.5 cruise

- Hypersonic technology demonstrator vehicle (HSTDV) tested and simulated at IIT Madras by Professor V. Babu
- Initial validation on scaled-down wind tunnel model
- After validation on scale model, move on full-scale design



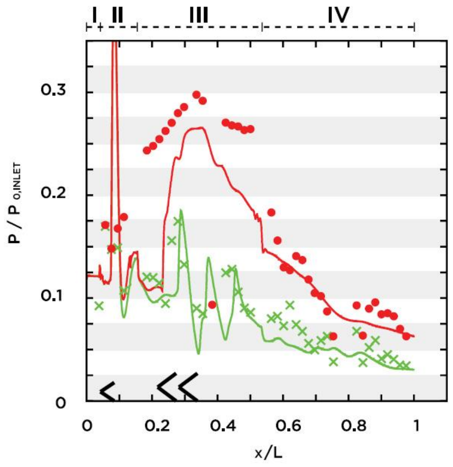
Validation of pressure recovery for 2 cowl angles



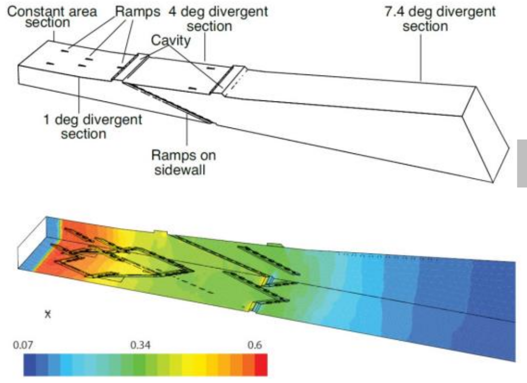


Side view of CFD results for scaled intake

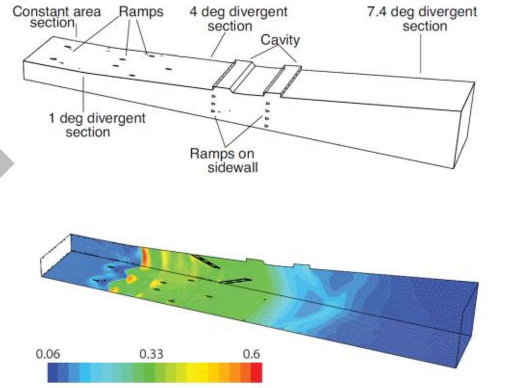
Pressure recovery of final design: experiment and CFD

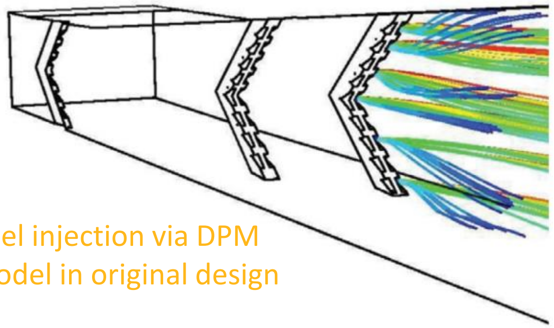


CFD simulation of original full-scale design



CFD simulation of modified full-scale design

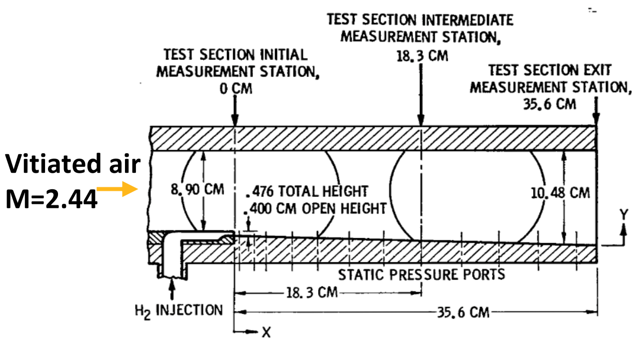


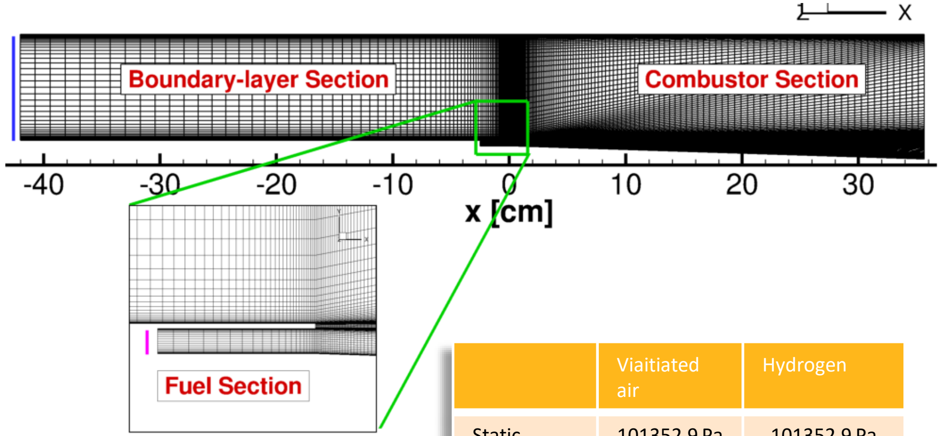


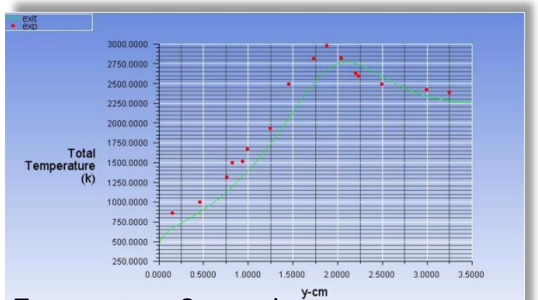
Fuel injection via DPM model in original design

Reference: V Babu, “Flight like the wind”, Ansys Advantage, Vol.8, 2014

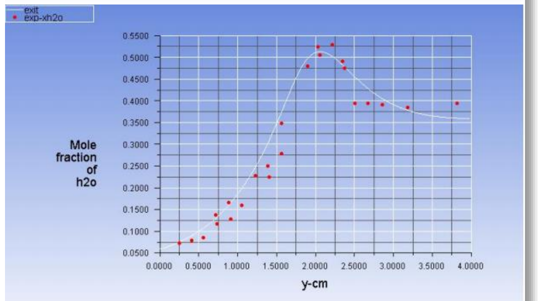
Validation: Burrows and Kurkov Supersonic Combustion test case





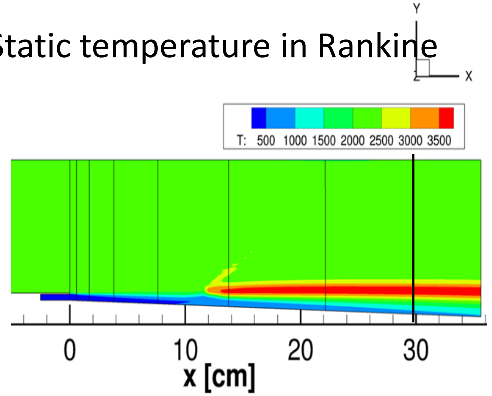


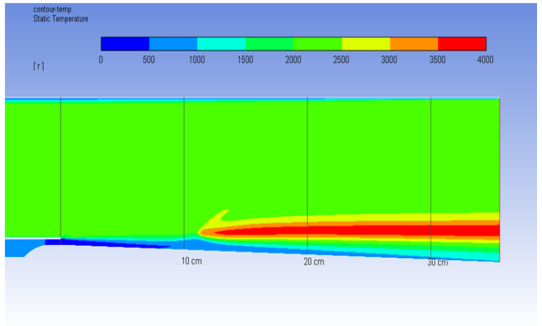
Temperature Comparison



H_2O mf Comparison

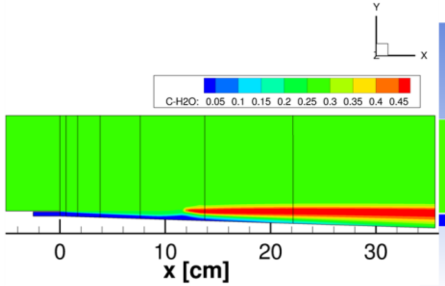
Static temperature in Rankine

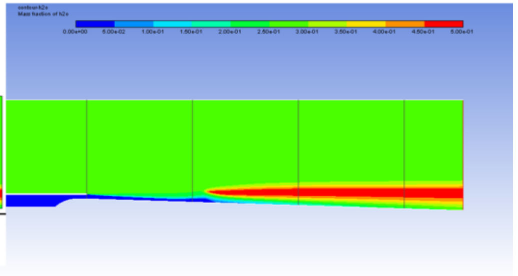




	Viaitiated air	Hydrogen
Static pressure	101352.9 Pa	101352.9 Pa @ nozzle
Mach number	2.44	1 @ nozzle
Static Temp	1270 K	254 K @ nozzle
X H2		1
X O2	0.203	
X H2O	0.359	
X N2	0.438	

- H2O mass fraction





Burrows, M. C. and Kurkov, A. P., "Analytical and Experimental Study of Supersonic Combustion of Hydrogen in a Vitiated Airstream," NASA-TM-X-2828, Sep. 1973.

https://www.grc.nasa.gov/WWW/wind/valid/bk/study02/bk2.html

Validation: NETL/AFRL Rotation Detonation Engine Validation

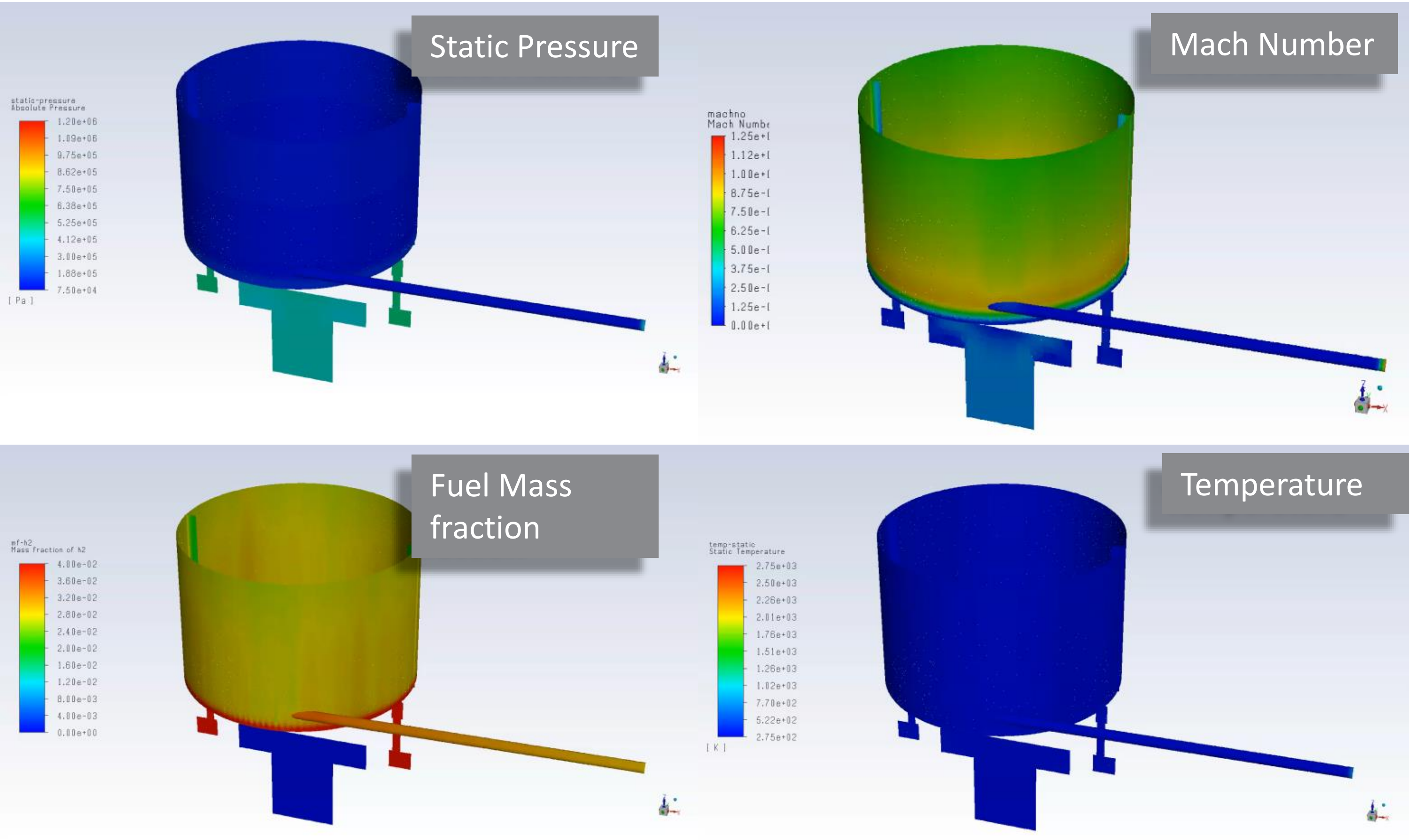
Validation Case of this RDE model with latest FLUENT solver

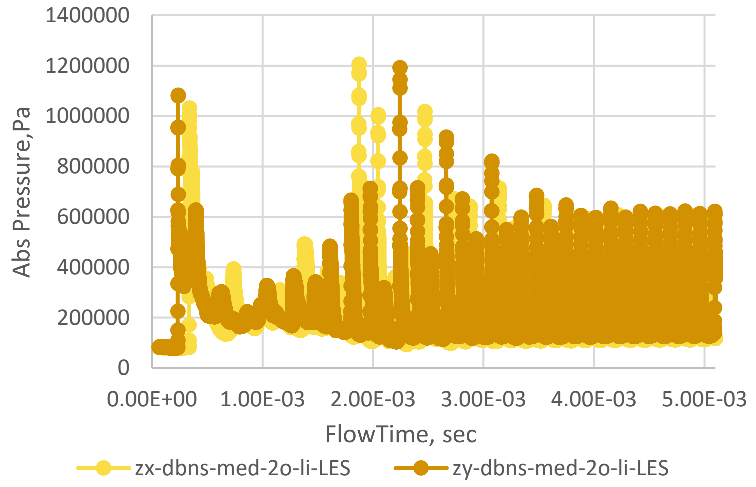
Rankin, Brent A., Fotia, Matthew, L., Paxson, Daniel E., Hoke, John L. and Schauer, Frederick R., "Experimental and Numerical Evaluation of Pressure Gain Combustion in a Rotating Detonation Engine", AIAA 2015-0877, 53rd AIAA Aerospace Sciences Meeting, Jan. 5-9, 2015, Kissimmee, FL.

Computationally Quantifying Loss Mechanisms in a Rotating Detonation Engine

Peter A. Strakey[1] and Donald H. Ferguson[2]
U.S. Department of Energy – National Energy Technology Laboratory, Morgantown, WV, 26505, USA

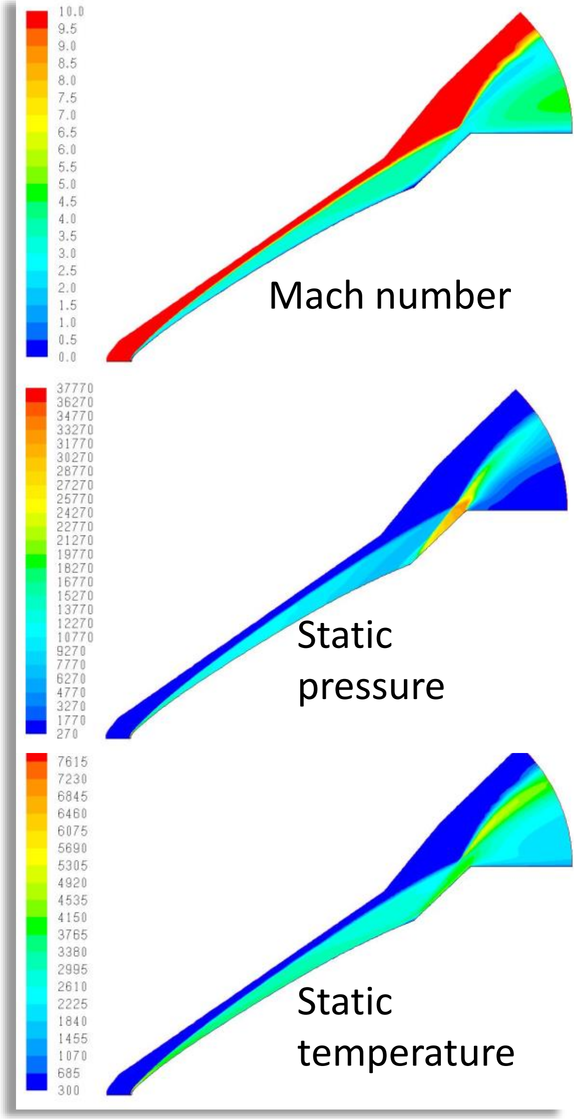
Andrew T. Sisler[3] and Andrew C. Nix[4]
West Virginia University, Morgantown, WV, 26505, USA





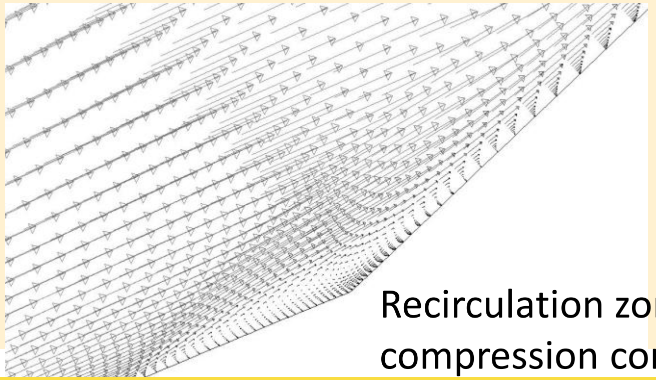
0.63 kg/s	Specific Thrust (N-s/kg)	Wave Freq (kHz)	Wave Speed (m/s)	Wave Speed (%CJ)	Air Plenum Pressure (kPa)	Fuel Plenum Pressure (kPa)	Annulus Pressure @ 2.54 cm (kPa)	Heat Loss (% sensible)	Unburnt fuel (% incoming)
Experiment	836	3.78	1740	88.0	431	503	213	N/A	N/A
Fluent Sim	984	3.64	1758	88.9	470	562	193	13.4%	19.3%
% Difference	+17.7	-3.7	+1.0	+1.0	+9.0	+11.7	-9.4		

Validation: Flow over Hyperboloid Flare at Mach 10



- Reacting dissociated mixture of five species (N_2, O_2, O, N, NO) in thermal and chemical non-equilibrium

$$O_2+M \Leftrightarrow 2O+M$$
$$N_2+M \Leftrightarrow 2N+M$$
$$NO+M \Leftrightarrow N+O+M$$
$$NO+O \Leftrightarrow O_2+N$$
$$N_2+O \Leftrightarrow NO+N$$

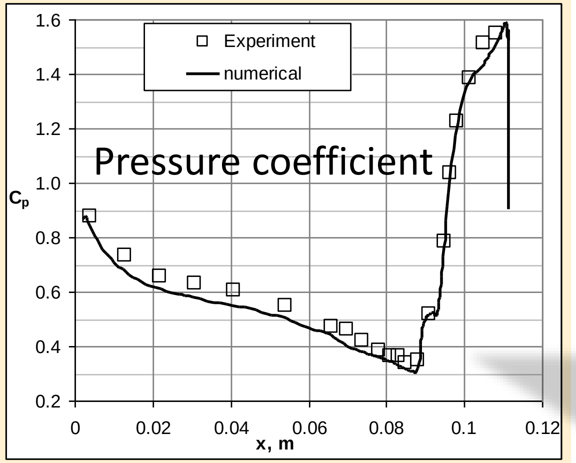


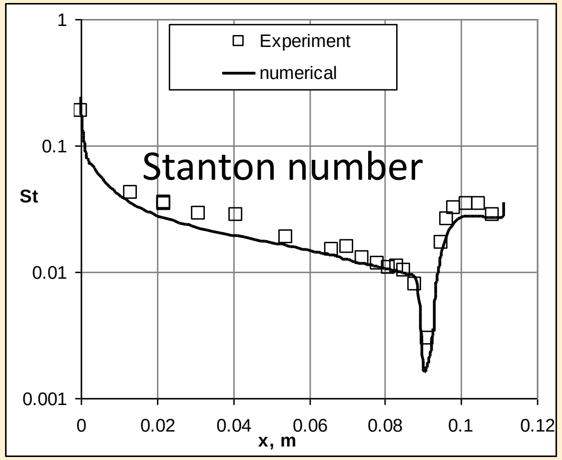
Recirculation zone at compression corner

References

1- Sagnier, Ph., Joly, V, and Marmignon, C., "Analysis of Nonequilibrium Flow Calculations and Experimental Results Around a Hyperboloid-flare Configuration", 2nd European Symposium on Aerodynamics for Space Vehicles, 1995.

2- Kurbatskii, K.A, Kumar, R., and Mann, D., "Simulation of External Hypersonic Problems Using Fluent 6.3 Density-Based Coupled Solver", 2nd European Conference for Aerospace Sciences





Validation: Doublet liquid fuel injection in rocket engine combustor

Inlet diameter: 1 mm

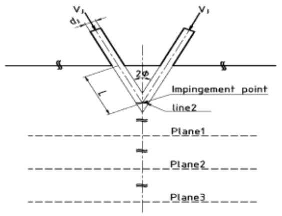
Liquid-Gas materials: Water – Air, 20 g/s

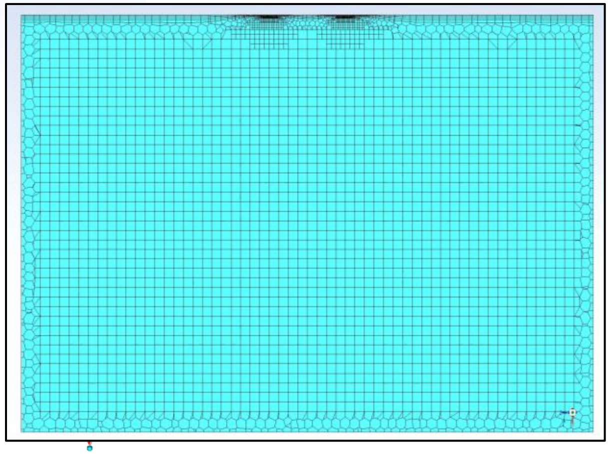
Inlet jet: Vj = 25.5 m/s, We = 9,029

Fluent setup:

Turbulence: Stress-Blended Eddy Simulation (SBES)

Multiphase models: VOF and DPM



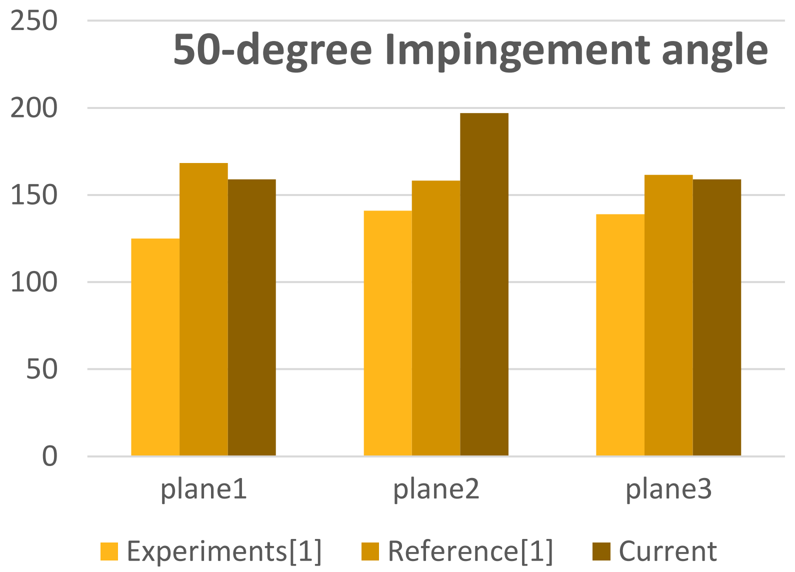


VOF-based mesh adaption

DPM Sampling Time : 1 ms

(from 4ms to 5ms simulation time)

Ref: Zheng et. al., 2015



Ref: Kumar, A., Kumar, V., Nakod, P., Rajan, A., Schütze, J., Multiscale Modelling of a Doublet Injector Using Hybrid VOF-DPM Method, AIAA 2020-2284, AIAA SciTech 2020, Orlando, FL, January 6-10th, 2020

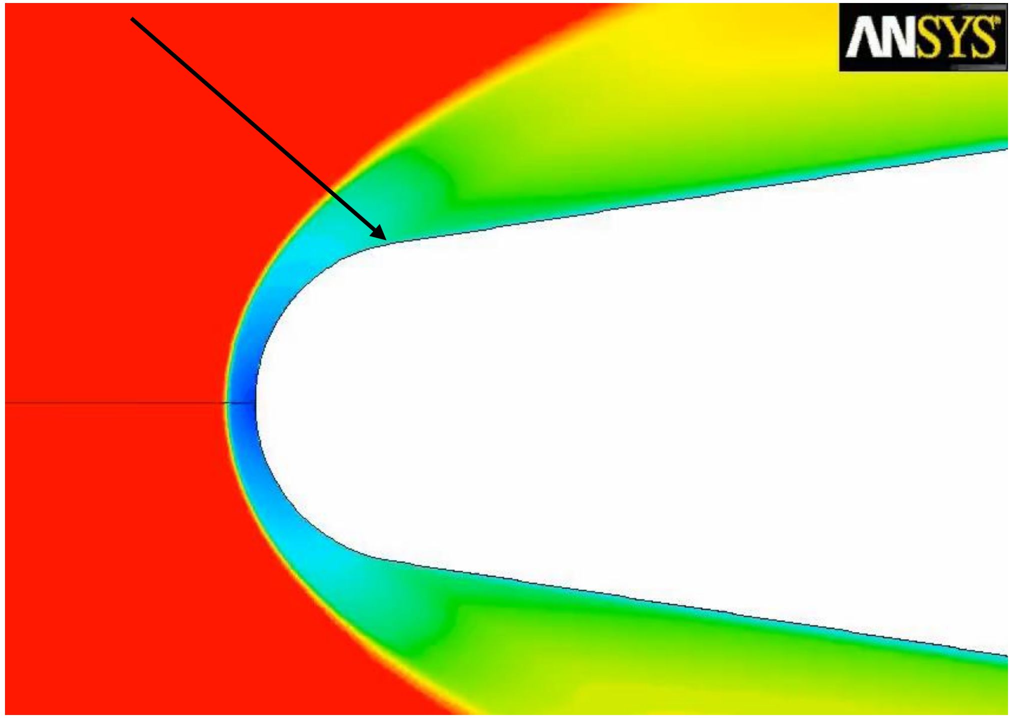
Ablation options in Ansys CFD

Reference: "Dynamic Simulation of Insulation Material Ablation Process in Solid Propellant Rocket Motor", Xu, Y. H., Hu, X., Yang, Y. X., Zeng Z. X., Hu, C. B., Journal of Aerospace Engineering, Issue 5, Vol. 28, October 2014.

- **Use built-in ablation module and moving-deforming wall (MDM) framework**
- **Specify recession rate using one of 4 methods:**

1. Use surface reaction rates, Arrhenius type
   - ✓ Includes chemistry and radiation
2. Use chosen empirical correlation, e.g. Vielle's law
   - ✓ E.g. Vielle's law, $\mathrm{r} = a \cdot p^n$ with a=f(T,…)
3. Conjugate heat transfer modeling capable
4. Use Fluent porous media to model ablating substrate
   - ✓ Use volumetric Arrhenius-type reaction rates (Pyrolysis)
5. Capability of coupling with ablation code
   - ✓ HERO, FIAT, others
   - ✓ Blowing effects including species and energy on BL will be modeled by loosely coupling Fluent with 3rd party software (HERO, FIAT) via input files for surface mass flux

r= Wall recession rate



- **Surface recession Limitation**
  - Work within erosion/mesh-smoothing framework
  - Use surface-reactions OR Viellie's law
  - No charring taken into account explicitly, just as a lump parameter inside Vielle's law, Can be added via injections and surface fluxes in 2022R1 and newer

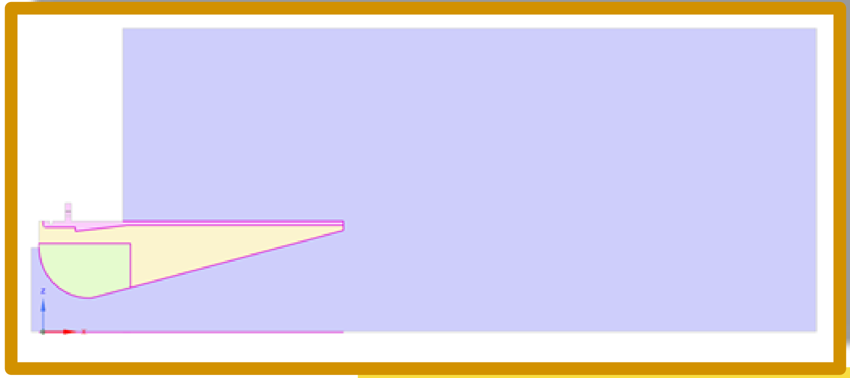
Case Study: Solid Rocket Motor

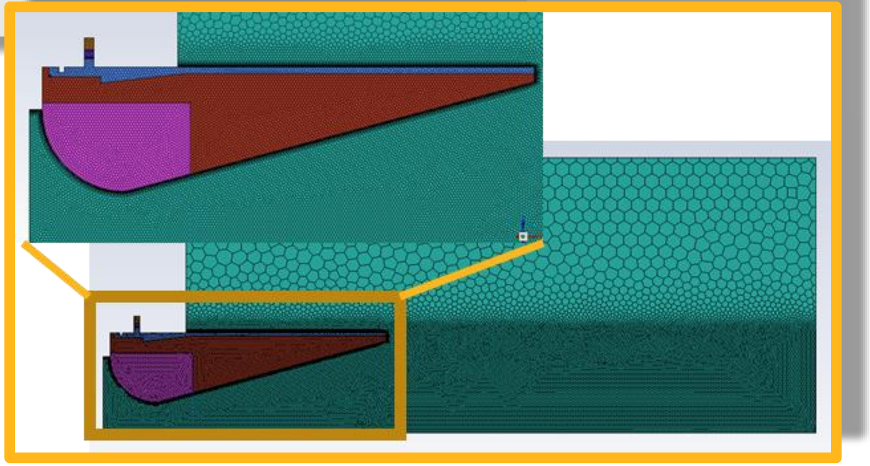
Generic Mach 3.0 Solid Rocket motor

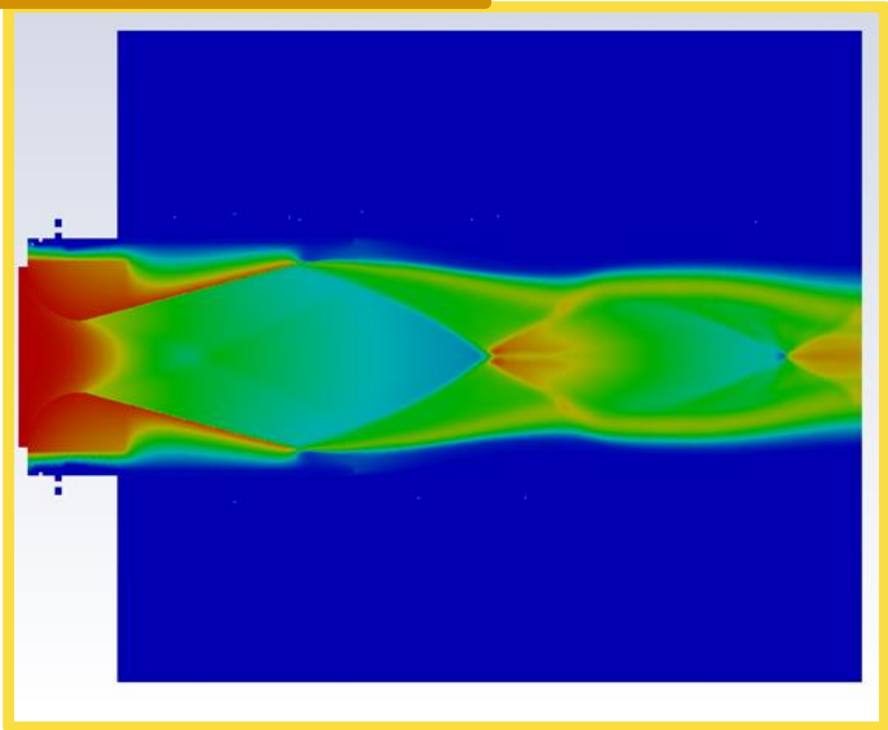
Demonstrate 3D Geometry to solution

- AP/HTPB/Al fuel combustion products flow through nozzle
- Conjugate Heat Transfer (CHT)
- DBNS Solver

Geometry to solution total time 3 hours



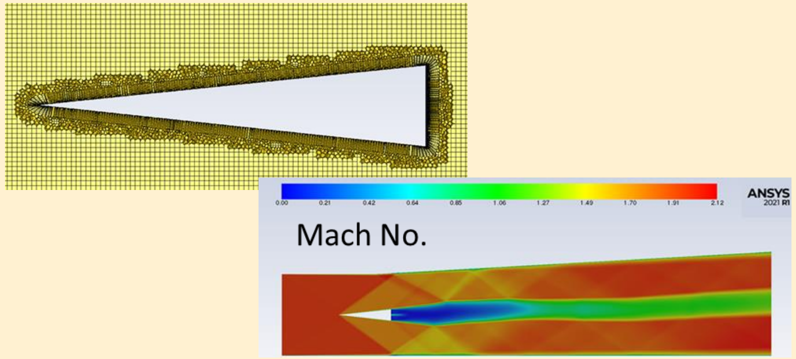




Advanced Training Class for High-Speed Combustion

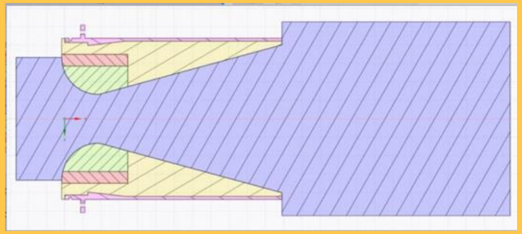
SCRAMjet Workshop

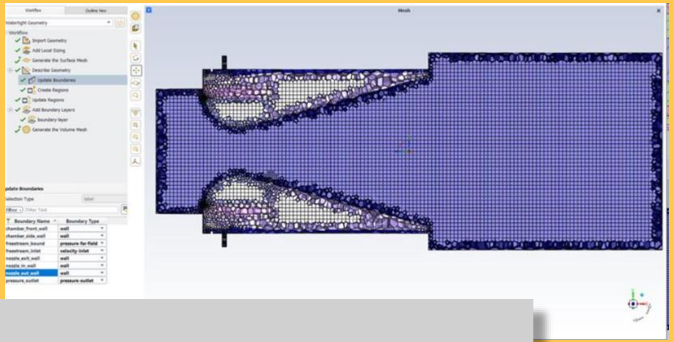
- Finite Rate Combustion model
- Moving Deforming Mesh (MDM)
- Turbulence modeling settings



Solid Fuel Rocket Workshop

- Nozzle Surface Ablation
  - Vielle's Law/Surface reaction
- Conjugate Heat Transfer (CHT)
- Radiation
- (Future) Solid Fuel recession
  - Surface reactions and recession, materials modeling (pyrolysis)





Liquid Fuel Rocket Workshop

- Real Gas EOS
- Finite rate Combustion
- Composition PDF Transport model

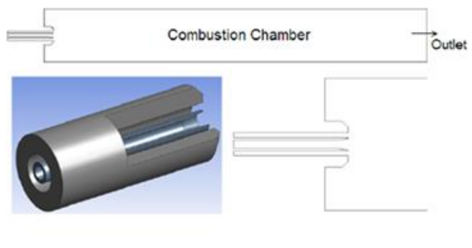
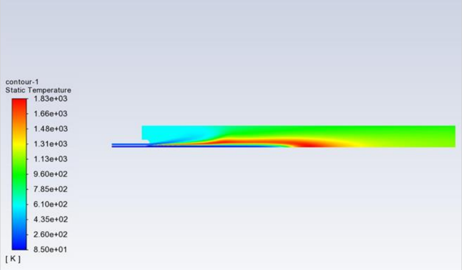
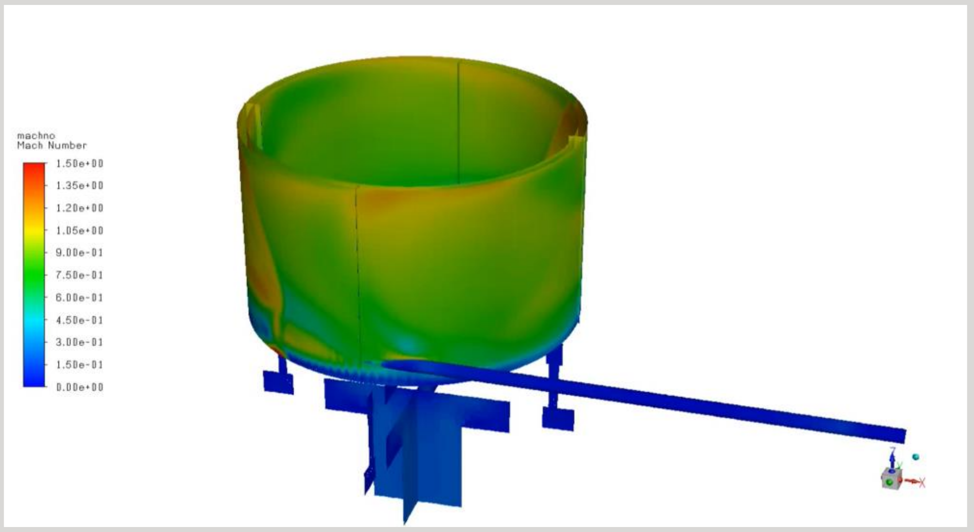


Figure 1: Details of MOSCOTTE Combustor



Summary

- Ansys is committed to advancing high-speed combustion/reacting flow simulation
  - Dedicated development and support teams
  - Extensive benchmarking and validation
  - Collaborative engagements with research institutes
- Increased focus on high-speed combustion/reacting flow simulation
  - Addition of required physical models
  - Improvements in solver robustness and efficiency
  - Streamlined workflow for greater user efficiency
- Ansys welcomes further collaboration
  - Validate current capabilities
  - Guide and shape development priorities
  - Support specific needs and requirements



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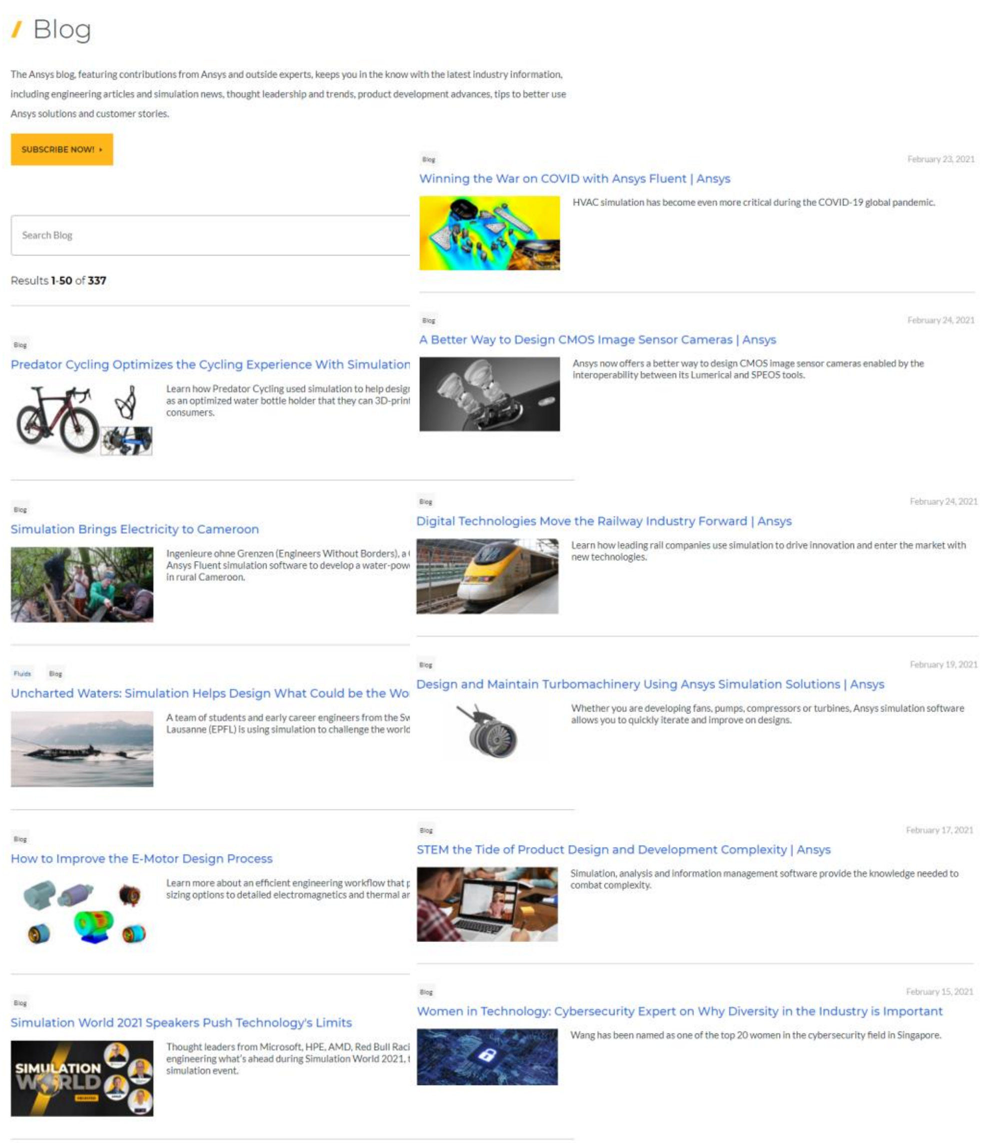

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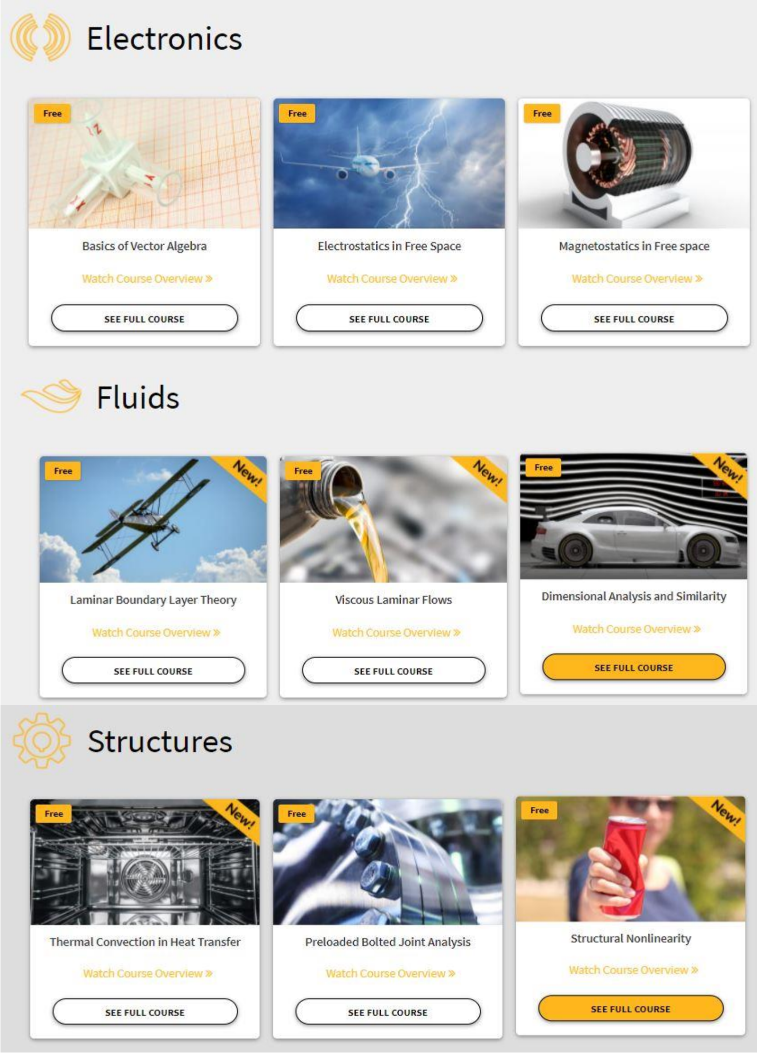
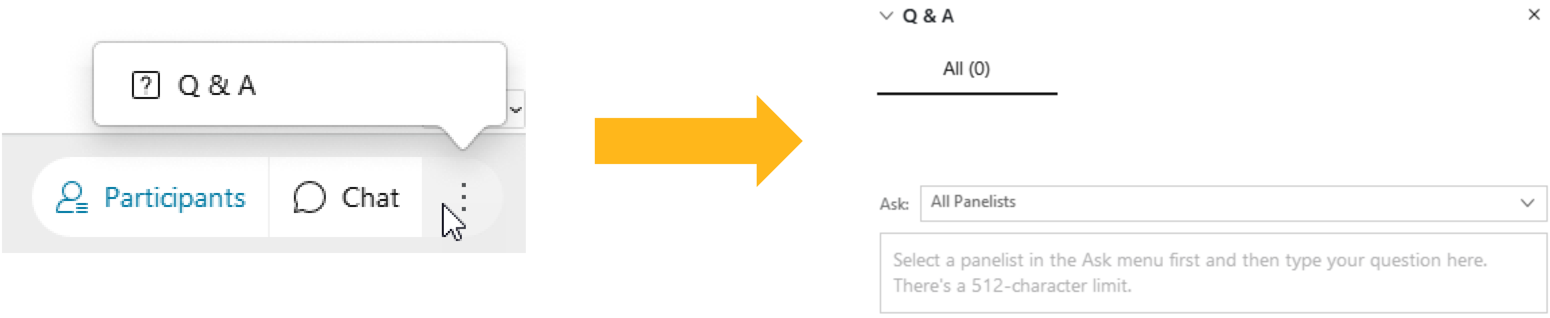


Questions?

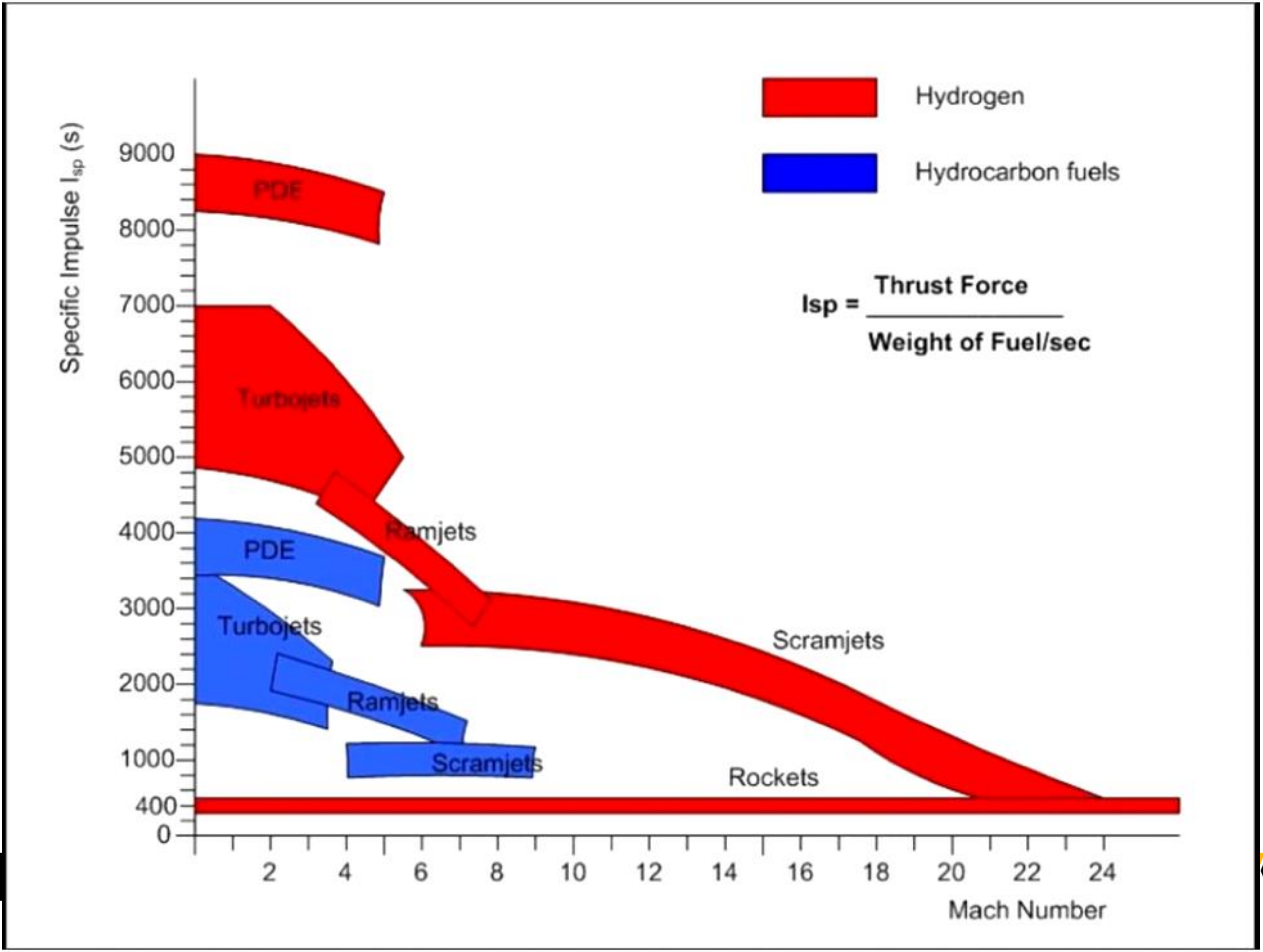
To ask a question, click on the Q&A button at the bottom of the screen to display the Q&A window:



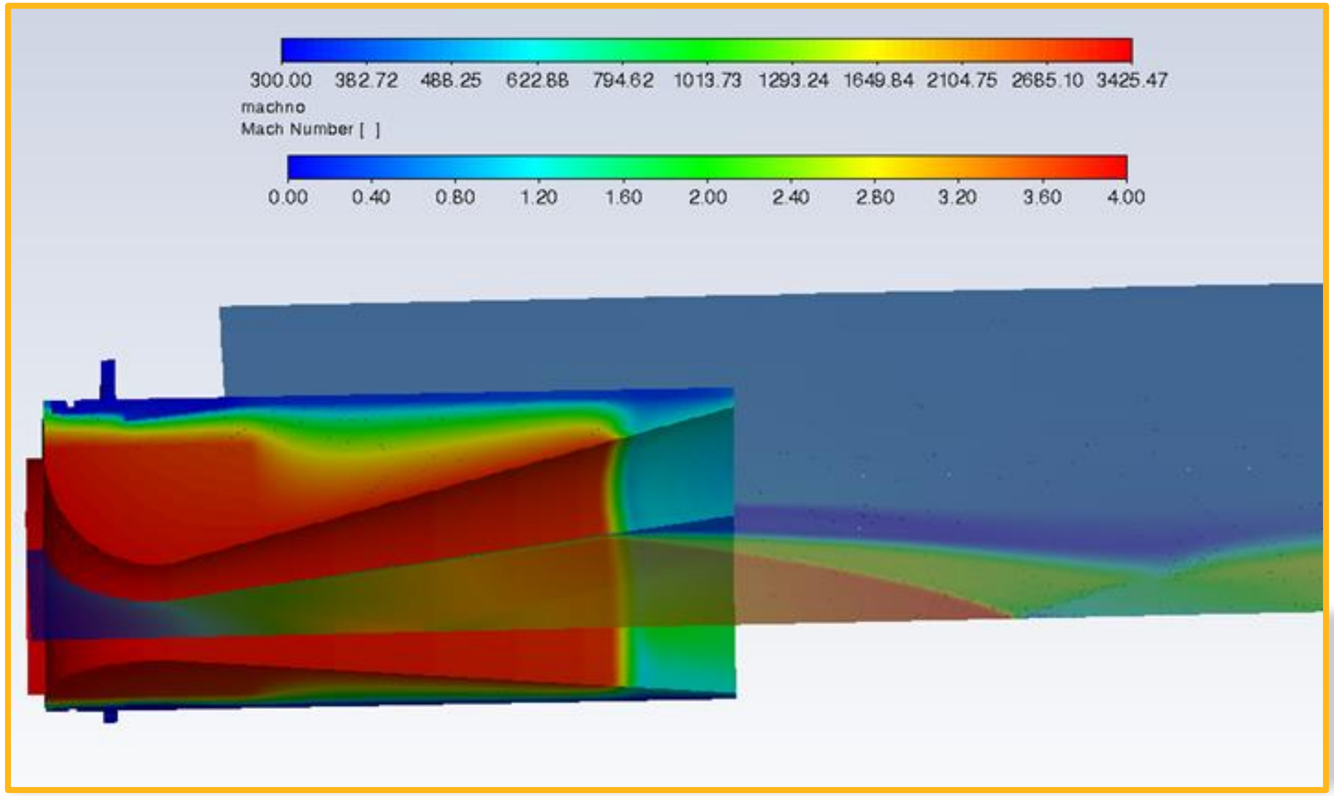
The recording will be available in about one week on the Ansys resource center:

ansys.com/resource-center

Ansys



Hydrogen
Hydrocarbon fuels
Isp = Thrust Force / Weight of Fuel/sec
Specific Impulse Isp (s)
9000
8000
7000
6000
5000
4000
3000
2000
1000
400
0
PDE
Turbojets
Ramjets
Scramjets
Rockets
2
4
6
8
10
12
14
16
18
20
22
24
Mach Number

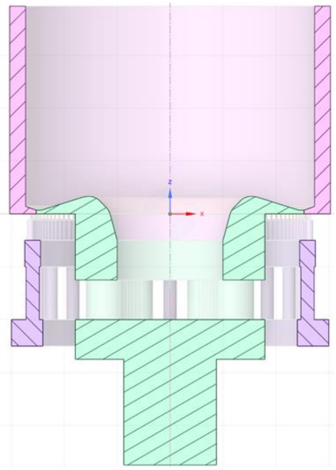


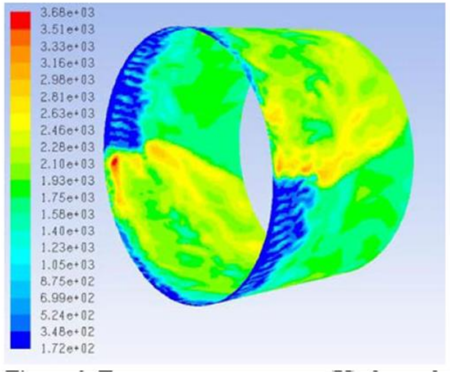
300.00 382.72 488.25 622.88 794.62 1013.73 1293.24 1649.84 2104.75 2685.10 3425.47
machno
Mach Number [ ]
0.00 0.40 0.80 1.20 1.60 2.00 2.40 2.80 3.20 3.60 4.00

Validation and Industrial Testing on High-Speed Combustion cases

- Combined efforts of Ansys development and technical support organization (Ansys Customer Excellence (ACE))
  - Internal development test cases and external publications
- Validation cases examples:
  - DLR Scramjet
  - Burrows and Kurkov Supersonic Combustion test case
  - AFRL/NETL Rotation Detonation Engine (RDE) Workshop/ Validation
  - AFRL Scramjet

AFRL RDE





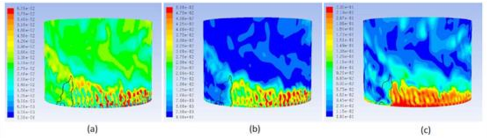
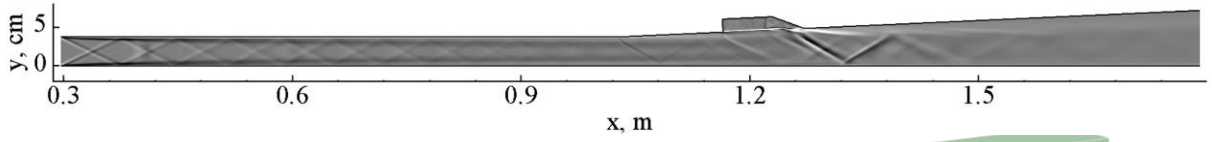


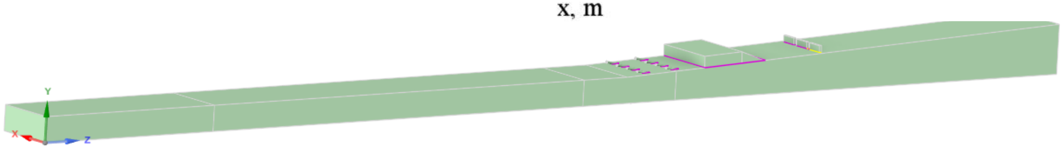
Figure 6. Mixture fraction contours (a), hydrogen mass fraction (b), and oxygen mass fraction (c). NETL geometry, with inlet, 1 kg/s air, ϕ=1.

Computationally Quantifying Loss Mechanisms in a Rotating Detonation Engine Peter A. Strakey1 and Donald H. Ferguson2 U.S. Department of Energy – National Energy Technology Laboratory, Morgantown, WV, 26505, UA Andrew T. Sisler3 and Andrew C. Nix4 West Virginia University, Morgantown, WV, 26505, USA

Rankin, Brent A., Fotia, Matthew, L., Paxson, Daniel E., Hoke, John L. and Schauer, Frederick R., "Experimental and Numerical Evaluation of Pressure Gain Combustion in a Rotating Detonation Engine", AIAA 2015-0877, 53rd AIAA Aerospace Sciences Meeting, Jan. 5-9, 2015, Kissimmee, FL.

AFRL SCRAMjet





CASE Study: Solid Rocket Motor