Aerothermal Modeling Challenges for Entry, Descent and Landing Missions

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Modeling is Critical Path for EDL Aerosciences

- **Direct Simulation Monte Carlo analysis used for aerobraking missions, low ballistic coefficient entries**
- **CFD predictions define aerothermal environments, aerodynamic performance & stability**
- **Material response, coupled to CFD, defines TPS thickness and design**

Can’t we retire all uncertainties via testing? – No!

- No ground test can simultaneously reproduce all aspects of the flight environment. A good understanding of the underlying physics is *required* to trace ground test results to flight; extrapolation without a good understanding of the relevant physics can have catastrophic results.
- All NASA EDL missions are reliant on modeling and simulation to predict flight performance of what is typically a single point failure system.

> *“For complex missions that cannot be fully tested on Earth, we rely on computer models to convince ourselves that the integrated system will work in its intended environment. We have no other way to do this. Detailed subsystem hardware and software testing help us validate that each of these models do a good job of representing reality.”*
>
> **-- Rob Manning (JPL), Former Mars Program Chief Engineer**

Two (Opposite) Directions of Research

- **We need to better understand our problems at the microscale level**
  - Modeling gas-kinetic, fluid dynamic and gas-surface processes at the atomistic level enables a much deeper understanding of the behavior
  - We need more physics in the simulations

- **We need to model EDL at the system level**
  - Full 3D CFD simulations have long been the standard in the discipline
  - Models informed by microscale data to include maximum fidelity at an engineering level of design
  - Careful UQ/sensitivity analyses to ensure that we insert sufficient fidelity to accurately predict quantities of interest, but not so much that our engineering efficiency is compromised

Validation data are required at both ends of the spectrum!

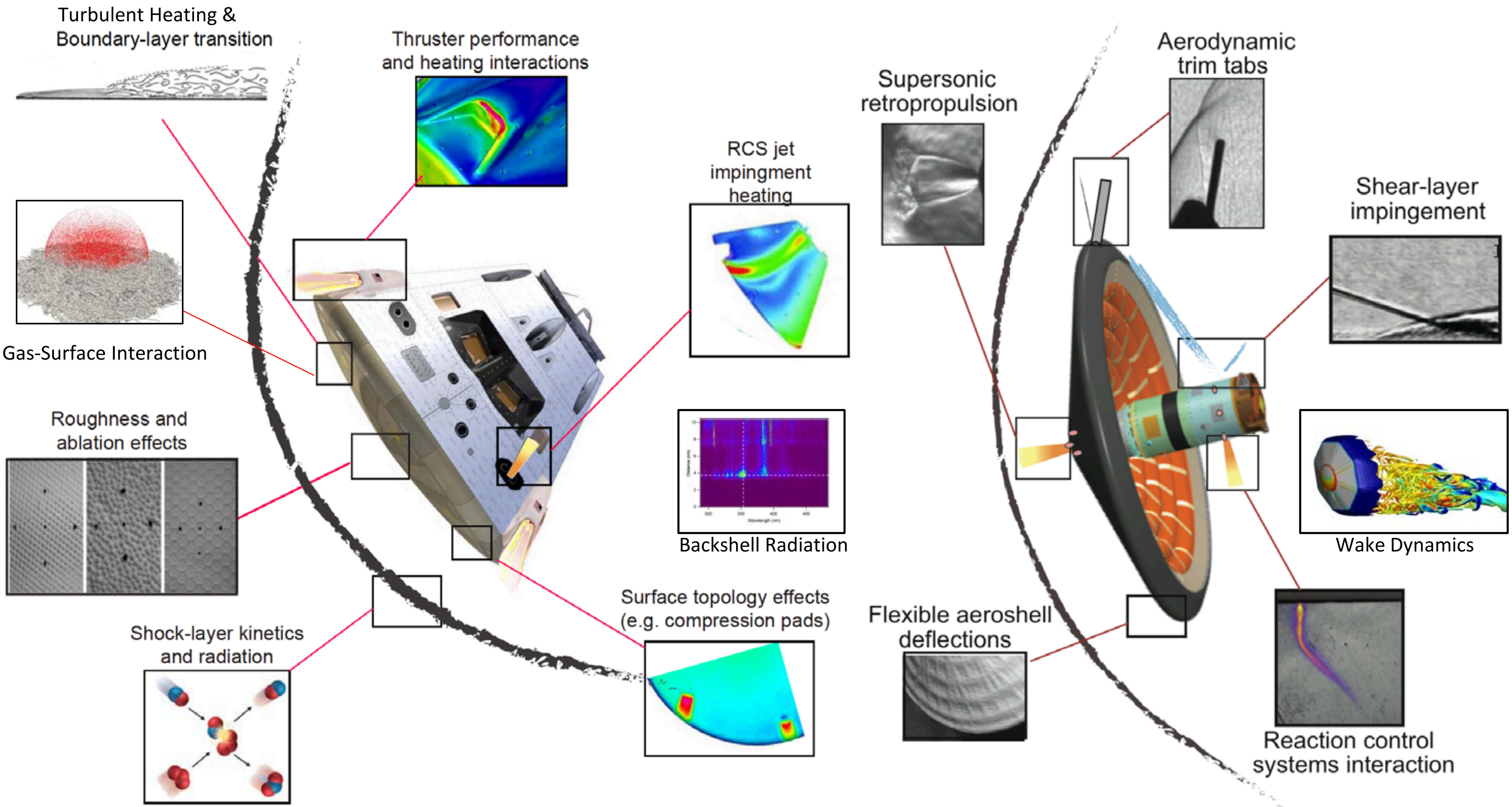
The Scope of This Talk

- **Models are critical across all speed regimes in multiple disciplines**

- **This talk will focus on EDL (as opposed to hypersonics), and constrain itself to high-speed / high-enthalpy aerosciences**
  - Many of the underlying physical problems are relevant in hypersonics as well, however EDL brings a unique “spin,” including the importance of shock layer radiation and non-air gas mixtures

- **This talk will <u>not</u> focus on architecture-specific challenges (e.g. flaps, deformable structures**
  - Three generic vehicle classes (blunt, deployable and lifting) are confronted with many of the same challenges at the level of the underlying physics

Our Challenges in a Nutshell



Turbulent Heating & Boundary-layer transition

Thruster performance and heating interactions

Gas-Surface Interaction

Roughness and ablation effects

Shock-layer kinetics and radiation

RCS jet impingment heating

Backshell Radiation

Surface topology effects (e.g. compression pads)

Supersonic retropropulsion

Aerodynamic trim tabs

Shear-layer impingement

Wake Dynamics

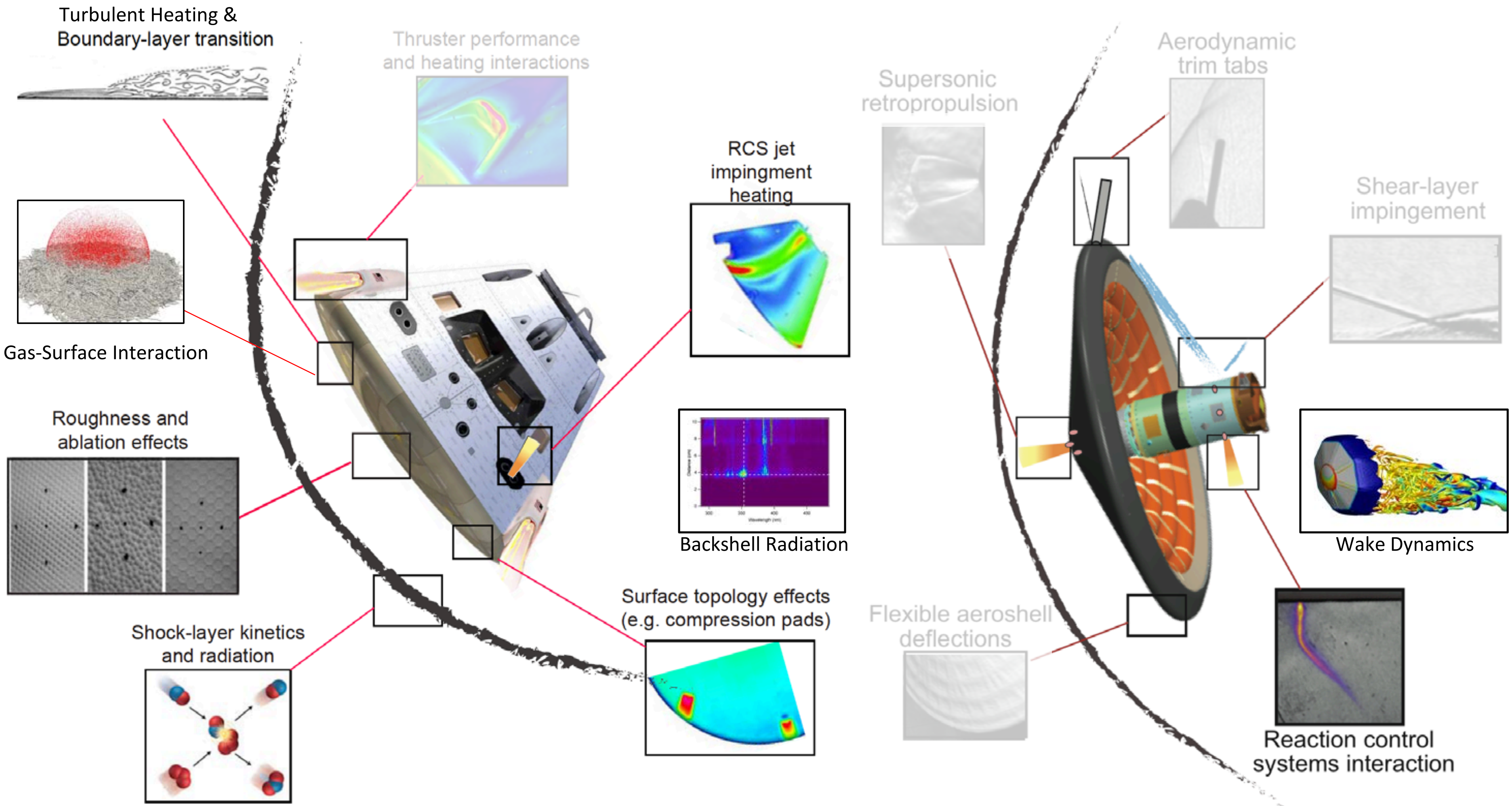
Flexible aeroshell deflections

Reaction control systems interaction

Facility characterization

Image Credit: Hollis

Focus Areas for Today



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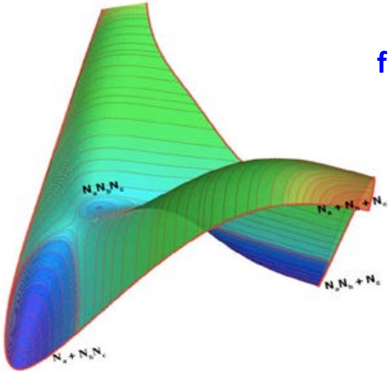
- **Shock layer radiation & gas-phase kinetics**
- Gas-surface interactions
- Roughness effects on transition and turbulence
- Wake dynamics with or without RCS
- Facility characterization

Shock Layer Radiation : The Problem

- **Shock layer radiation remains the largest source for aerothermal uncertainty (and TPS margin) across multiple NASA missions**
  - Orion: 37% heatshield
  - Mars2020: ~50% on heatshield and backshell
  - InSight/OSIRIS-Rex/Venus: 70% on backshell
  - Saturn (estimate): 300% heatshield and backshell
  - Titan (estimate): 100% heatshield and backshell
- **Recent advancements have led to tremendous improvements in our understanding of shock layer radiation from air in equilibrium**
- **Nevertheless, considerable aspects remain unquantified or unknown**
  - CO_2 mid-IR radiation accounts for up to 30% of heating in the stagnation region of MSL; completely unknown during design
  - Minimal validation of kinetic or radiation models in expanding flow (backshell)
  - Prediction of non-equilibrium radiation is very sensitive to input rates
  - Little work has been done for gas/ice giants or Titan
- **Improved knowledge of gas-phase kinetics and transport in the shock layer underpins our ability to model convective and radiative aeroheating**

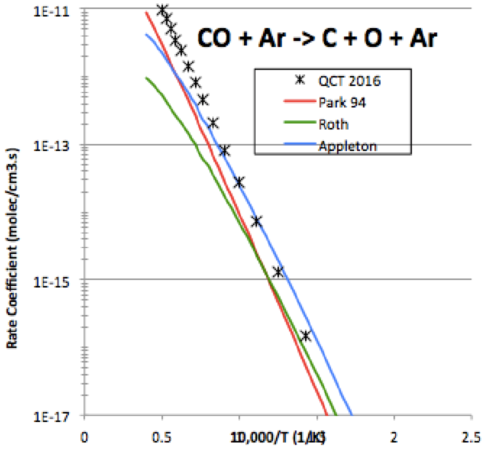
Foundational Analysis

- **Computational chemistry and direct molecular simulation can provide detailed data for reaction rates and other thermodynamic data *based purely on first-principles***

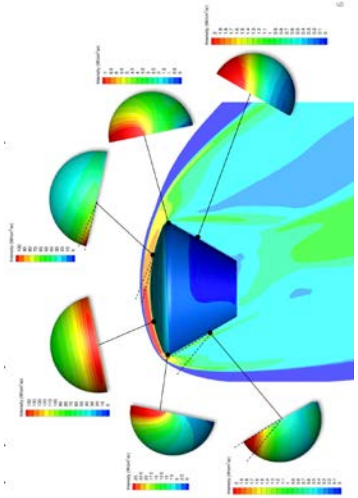


Compute potential energy surfaces from quantum mechanics. Apply QCT or DMS analysis to directly infer reaction rates.

Credit: Jaffe et al.

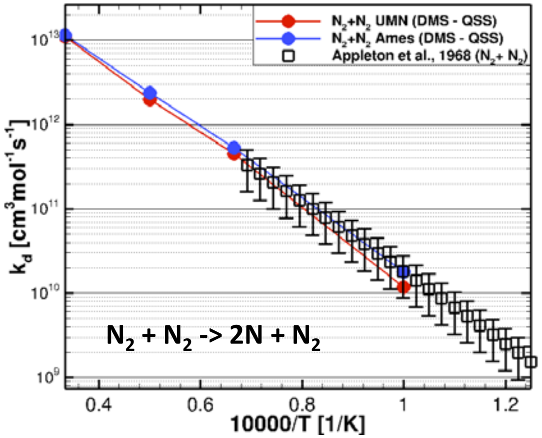


- **Once the most sensitive reaction rates are determined, experimental data can be analyzed more accurately**
- **Maximize confidence in our assessment of non-equilibrium models and choices for spectroscopic data**
- **DMS in particular is poised to have game-changing impact on the field**
  - New validation data are required



Reaction rates are fundamental inputs to CFD. Same data are also mined for thermodynamic and transport properties.

Credit: Schwartzentruber et al.

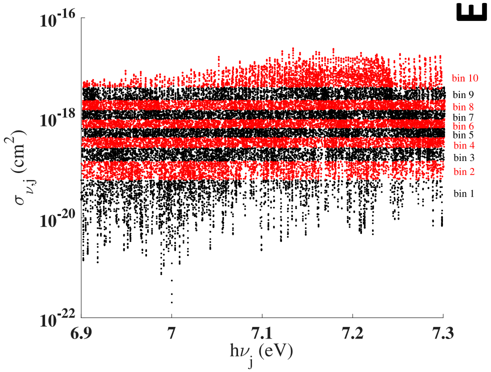


Applied Modeling

- **Build a new generation of *physics-based tools for aerothermodynamic analysis and design***
  - Phase 1: Self-consistent kinetic models for non-equilibrium radiation – Reduce uncertainty for immediate application
  - Phase 2: Fully-coupled, 3-D radiative transport

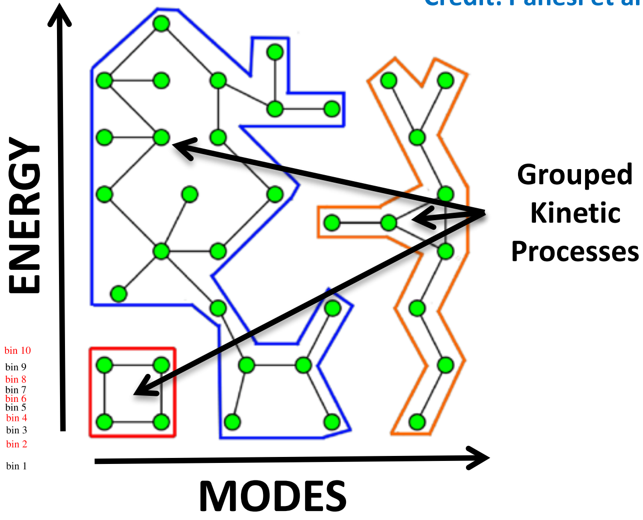
MBOB Approach

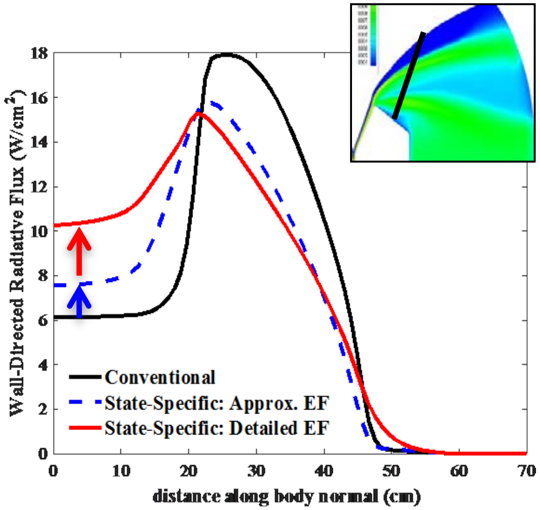
Credit: Johnston et al.



- **Investments in state-to-state models are demonstrating promise for dramatically improving SOA**
  - Grouped kinetic models & multiband opacity binning resolve the microscopic level at a modest cost
  - Critical for resolving non-equilibrium processes, particularly the backshell environment where traditional methods are demonstrably non-conservative

Credit: Panesi et al.

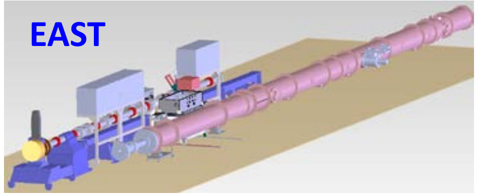


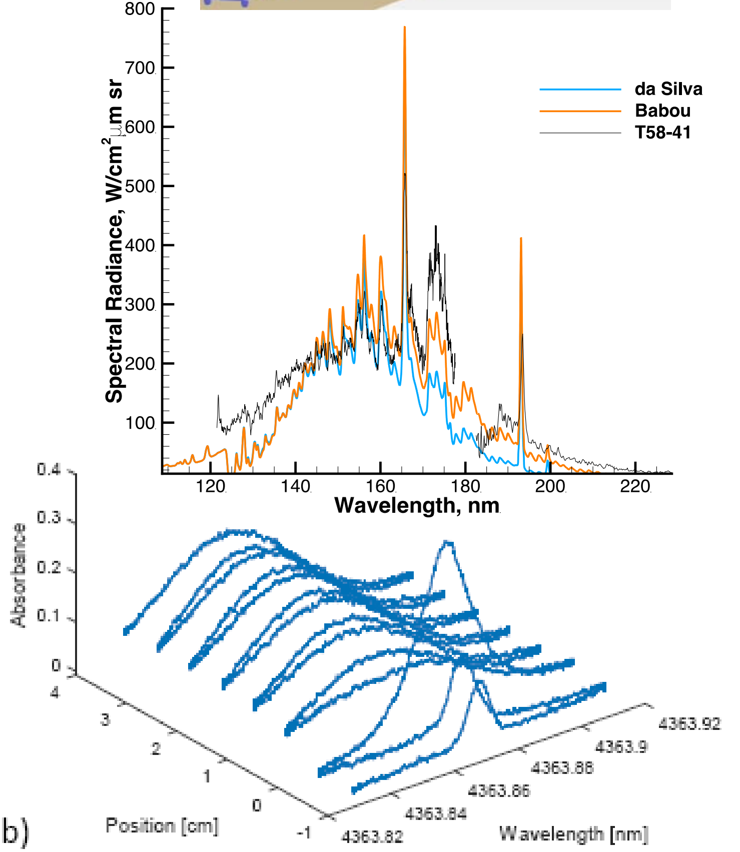


(TOP) Reduced-order models provide microscopic detail at conventional cost. (BOTTOM) Applied to Mars Pathfinder backshell, traditional approach is *non-conservative*

Experimental Validation

- **Experimental validation is crucial for establishing quantified uncertainties and informing margin policy**
- **Critical phenomena lack sufficient data**
  - Kinetic data largely from 1960’s
  - Extremely limited data for expanding flows (backshell)
  - CO_2 database (Mars &Venus) is in its adolescence
  - Outer planet and Titan databases are nearly non-existent
  - Earth return above 12 km/s
  - Highly ionized flows in general
- **Shock Tubes (such as EAST) are the premier source of spectroscopic & kinetic data for entry vehicles**





(TOP) First ever experimental resolution of CO vUV spectrum as compared to existing models. (BOTTOM) First ever application of TDLAS to CO ground state in shock tube

Credits: Cruden et al., McDonald et al.

What is Needed

- **Equilibrium data for CO 4th Positive in VUV (Mars)**
- **CO_2 2.7μm MWIR data (Mars)**
- **Carbon bound-free in the VUV (Venus)**
- **Data for these reactions:**
  - Earth: $N + N \leftrightarrow N_2^+ + e$; $N^+ + 2e \rightarrow N + e$; $N + NO^+ \rightarrow N^+ + NO$ (Earth)
  - Ro-vibrational energy transfer and dissociation in CO_2+CO_2, CO_2+CO & CO+CO (Mars)
  - $N_2 + C \rightarrow CN + N$ (Titan)
  - Excited state reactions including those involving $N(^2D)$ and $O(^1D)$ and molecules (Earth, Mars)
  - Heavy particle quenching rates of excited CO, N2, NO, C, N and O at elevated T (Earth, Mars)
- **Transport property extensions to 20,000K (all destinations)**
- **High resolution spectral data for better line shapes for atomic lines in VUV**
- **Reaction rates/absorption coefficients of ablation products (e.g. C_2H, C_2H_2)**
- **Kinetic & emission data for V > 25 km/s H_2/H/He (Giant Planets)**
- **Direct measurements of electron kinetics in non-weakly ionized flow**

- Shock layer radiation & gas-phase kinetics
- **Gas-surface interactions**
- Roughness effects on transition and turbulence
- Wake dynamics with or without RCS
- Facility characterization

Gas-Surface Interactions:
The Problem

- **Wall reactions are a primary source of aeroheating for planetary EDL**

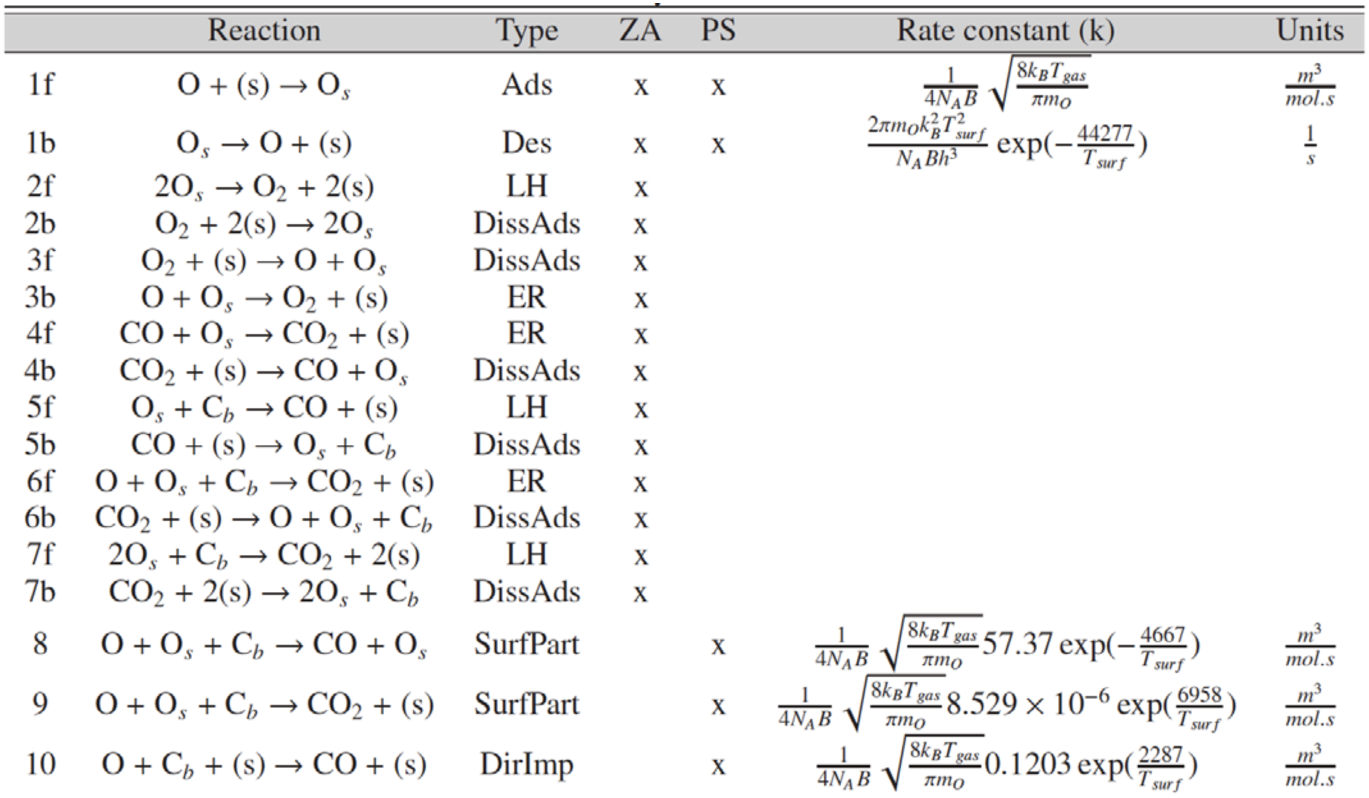
$$q_w = k\nabla T_w + \sum_k k_k \nabla T_{k,w} + \sum_s J_{s,w} b_s h_s$$

- **Two reaction classes can occur simultaneously during entry: catalytic & participatory**
- **Early models for catalysis simplified the problem to the flux of reactants to the surface and "catalytic efficiency" factor γ. Energy accommodation (β) was generally assumed to be perfect**
  - Validation typically via arc jet (measured heat flux to the surface), or diffusion tube (measured reactant depletion and/or product formation)
  - Validation approaches dealt inconsistently with γ vs β
- **Models for participatory reactions typically assume surface equilibrium**
  - Perhaps a good assumption at DoD ballistic entry conditions, less so for NASA
- **Flight data returned from MSL, EFT-1, Galileo clearly demonstrate that current models are inadequate, and in some cases non-conservative**

Finite-Rate Models

Carbon Oxidation on PICA

Credit: Borner, et. al

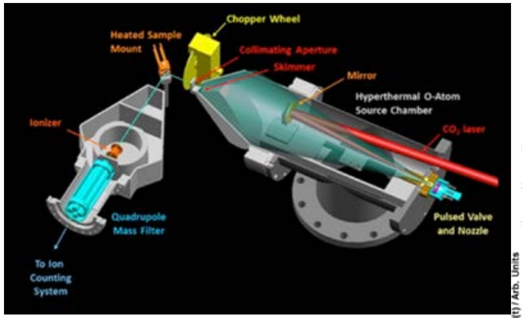


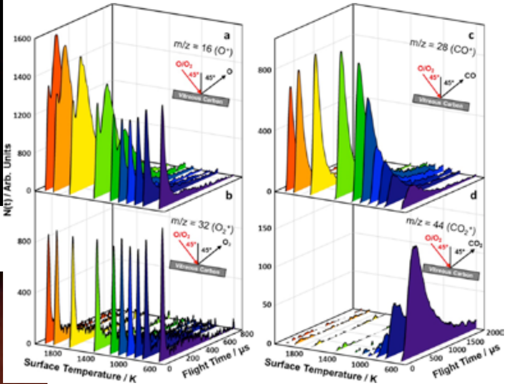
	Reaction	Type	ZA	PS	Rate constant (k)	Units
1f	$O + (s) \rightarrow O_s$	Ads	x	x	$\frac{1}{4N_A B}\sqrt{\frac{8k_B T_{gas}}{\pi m_O}}$	$\frac{m^3}{mol.s}$
1b	$O_s \rightarrow O + (s)$	Des	x	x	$\frac{2\pi m_O k_B^2 T_{surf}^2}{N_A B h^3}\exp(-\frac{44277}{T_{surf}})$	$\frac{1}{s}$
2f	$2O_s \rightarrow O_2 + 2(s)$	LH	x			
2b	$O_2 + 2(s) \rightarrow 2O_s$	DissAds	x			
3f	$O_2 + (s) \rightarrow O + O_s$	DissAds	x			
3b	$O + O_s \rightarrow O_2 + (s)$	ER	x			
4f	$CO + O_s \rightarrow CO_2 + (s)$	ER	x			
4b	$CO_2 + (s) \rightarrow CO + O_s$	DissAds	x			
5f	$O_s + C_b \rightarrow CO + (s)$	LH	x			
5b	$CO + (s) \rightarrow O_s + C_b$	DissAds	x			
6f	$O + O_s + C_b \rightarrow CO_2 + (s)$	ER	x			
6b	$CO_2 + (s) \rightarrow O + O_s + C_b$	DissAds	x			
7f	$2O_s + C_b \rightarrow CO_2 + 2(s)$	LH	x			
7b	$CO_2 + 2(s) \rightarrow 2O_s + C_b$	DissAds	x			
8	$O + O_s + C_b \rightarrow CO + O_s$	SurfPart		x	$\frac{1}{4N_A B}\sqrt{\frac{8k_B T_{gas}}{\pi m_O}}57.37\exp(-\frac{4667}{T_{surf}})$	$\frac{m^3}{mol.s}$
9	$O + O_s + C_b \rightarrow CO_2 + (s)$	SurfPart		x	$\frac{1}{4N_A B}\sqrt{\frac{8k_B T_{gas}}{\pi m_O}}8.529 \times 10^{-6}\exp(\frac{6958}{T_{surf}})$	$\frac{m^3}{mol.s}$
10	$O + C_b + (s) \rightarrow CO + (s)$	DirImp		x	$\frac{1}{4N_A B}\sqrt{\frac{8k_B T_{gas}}{\pi m_O}}0.1203\exp(\frac{2287}{T_{surf}})$	$\frac{m^3}{mol.s}$

- **Newer models take much more of the physics into account**
    - Adsorption/desorption, site hopping, etc.
- **However, more equations means more parameters to measure (avoid GIGO)**
- **Surface morphology plays a critical role**

Approach

Molecular beam testing





Credit: Minton, et. al

ICP Testing

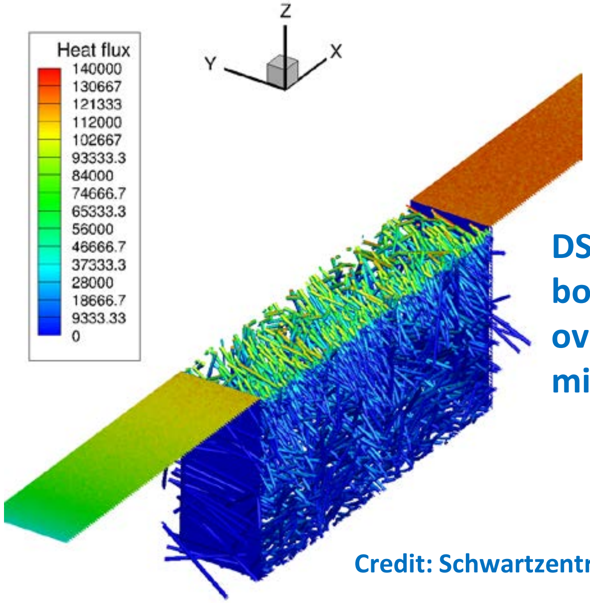
Credit: Fletcher & Meyers et al.

- **Detailed validation experiments (molecular beam, diffusion tube, ICP) to evaluate not only rates of reaction, but also the energetics of reaction**

- **Detailed simulations (DSMC, DMS, MD) of key gas-surface processes**

Molecular beam simulation in PuMA

Credit: Ferguson, et. al



DSMC – resolved boundary layer flow over real TPS microstructure

Credit: Schwartzentruber, et. al

What is Needed

- **Experimental data on REAL materials with flight-relevant morphology (including defects & damage)**
  - Virgin and charred ablators (PICA, HEEET, Avcoat)
  - Metals used in calorimetry and/or surface instrumentation (copper, platinum, silver, beryllium)
  - Surface coatings
- **Reaction rates for key gas-surface processes, including important low lying excited states**
  - Improved understanding of the impact of morphology; is carbon carbon?
- **Associated energetics for each process; how much energy is deposited on surface vs carried away by product; what is the internal state of the products**
- **Gas-phase kinetics: ablation product boundary layer interactions**
- **Mechanism reduction and up-scaling into a form suitable for CFD/Material Response analysis**

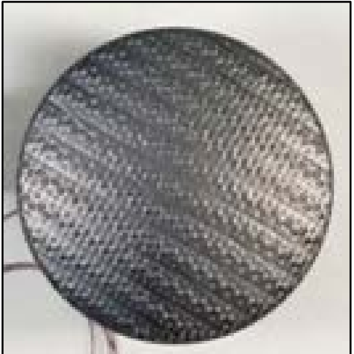
- Shock layer radiation & gas-phase kinetics
- Gas-surface interactions
- **Roughness effects on transition and turbulence**
- Wake dynamics with or without RCS
- Facility characterization

Roughness:
The Problem

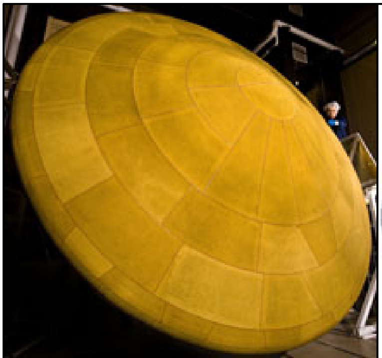
- **NASA missions encompass multiple types of surface roughness**
  - Ablation induced roughness (e.g. sandgrain, woven fibers, hexcomb)
  - Discrete roughness from gaps, seams, flexible TPS substructure
  - Discrete roughness from surface features (e.g. compression pads, penetrations)
- **We know that the presence of roughness not only accelerates transition to turbulence, but can cause substantial augmentation to surface heating as compared to a smooth surface**
- **Current models for roughness-induced transition and heating augmentation are largely based on semi-empirical correlation to experimental data**
  - Deeper understanding of the underlying physics is required

Sand-grain
Ablated PICA on Stardust

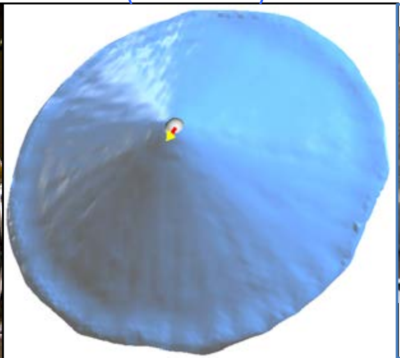
Wavy
Woven TPS (arc-jet sample)



Discrete
Block TPS panels on MSL



Scalloped
HIAD Flexible TPS (scan data)

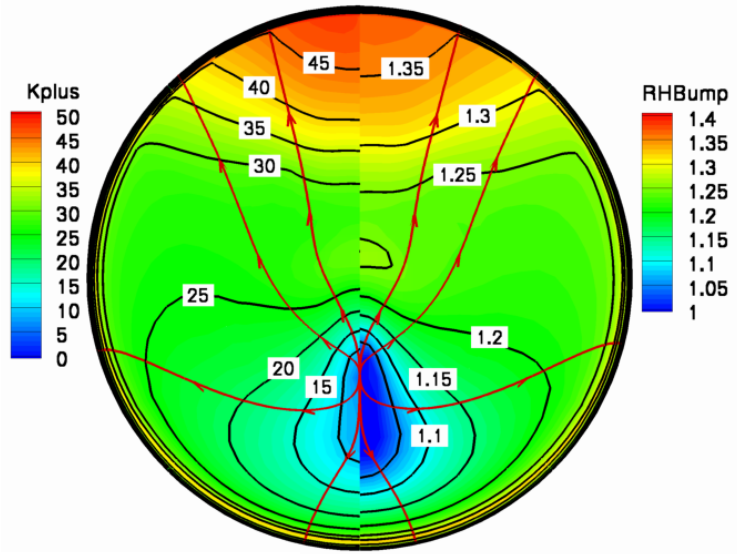


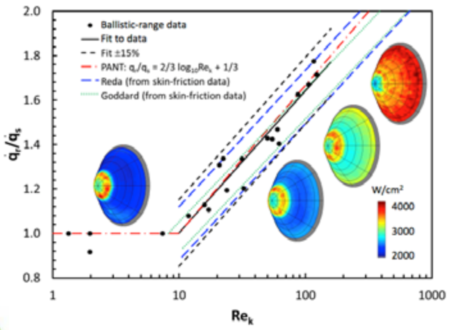
Feature
Orion EFT-1 Compression Pads

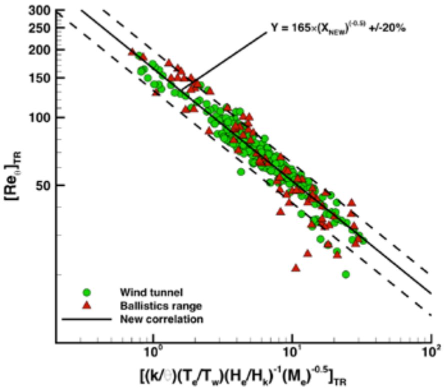
Distributed Roughness

- **Ablators develop a roughness pattern**
  - Roughness is known to augment convective heating and shear stress
  - Factors correlated to a wide range of historical data, from water channels to hypersonic flows
- **Unknowns:**
  - What is the characteristic roughness developed by a given ablator?
  - How does the actual roughness map to equivalent roughness used in the correlations?
  - Under what conditions does an ablator have a propensity to form "pattern roughness"?
  - What is the ground-to-flight traceability of current correlations and test data?

MSL Prediction
1mm sand grain roughness

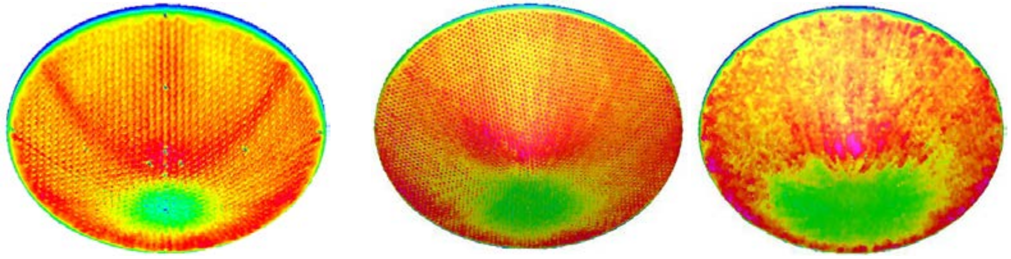






Data correlations from Wilder (top) and Hollis (right)

LaRC Mach 6 Testing of Augmented Heating on 70° Sphere Cone



Ablated Hexcomb

Hemispheres

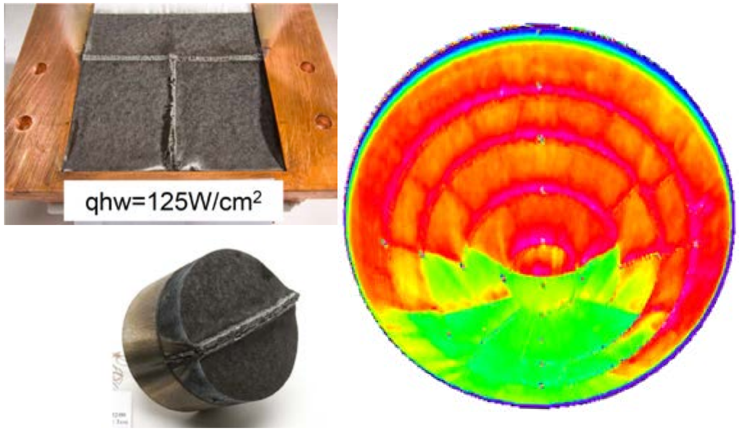
Sandgrain

Credit: Hollis et al.

Discrete Roughness

- **Discrete roughness has a very different impact**
  - $k/\delta \gg 1$
  - Localized heating and shear
  - Transition “trip”
- **Equivalent correlations have minimal value**
  - Models must be developed for the specific type of roughness encountered
  - This can be done purely experimentally (e.g. Orion), but:
    - Very high cost
    - Residual risk of extrapolation to flight
  - CFD models still require experimental validation
- **When does distributed roughness become discrete (what is the relevant length scale)?**

MSL Gap Filler Protrusion:
Arc jet coupons (left) and LAL M6 test (right)



Thermal image of Orbiter windside during STS-119

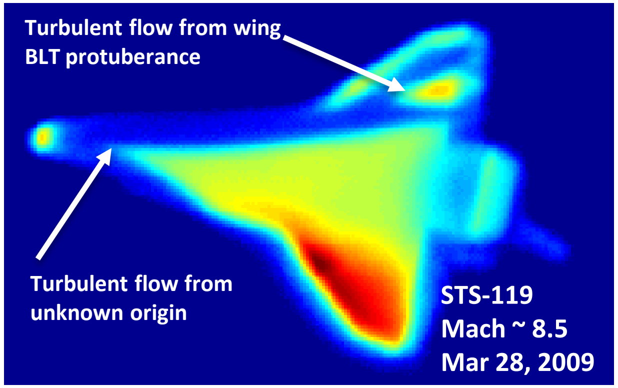
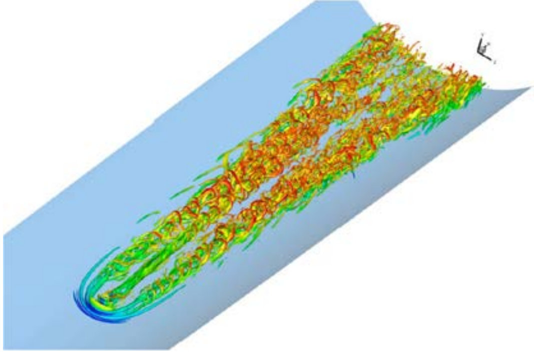


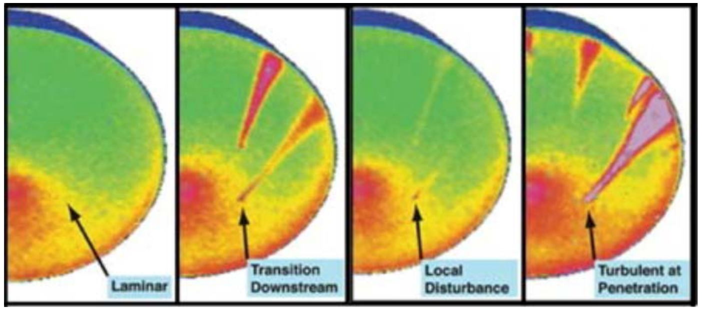
Image Credit Horvath, et al.

CFD simulation of disturbances downstream of discrete roughness at Mach 6



Credit Candler, et al.

LAL Mach 6 testing of proposed MSL HS compression pads



Credit Hollis, et al.

What is Needed?

- **Short-term: generalized correlation based approach**
  - Recognize that there are multiple types of “roughness” and each type of TPS will have it’s own correlation space.
  - Transition correlations are workable as engineering for most type of roughness, need to develop heating augmentation correlations/models

- **Long-term: physics-based modeling approach**
  - Detailed simulations over realistic microstructure
  - Thermal/structural models for response of TPS to heating/shear and formation of roughness/ablation
  - Direct evaluation of heating & shear augmentation, as well as ablation/blowing

- **Validation data (applicable for both short and long term)**
  - TPS response data (arc jets) on development of roughness
  - Measurements of surface heating/temperature to determine transition & heating augmentation
  - Off-body flowfield diagnostics to measure BL flow properties near surface

- Shock layer radiation & gas-phase kinetics

- Gas-surface interactions

- Roughness effects on transition and turbulence

- **Wake dynamics with or without RCS**

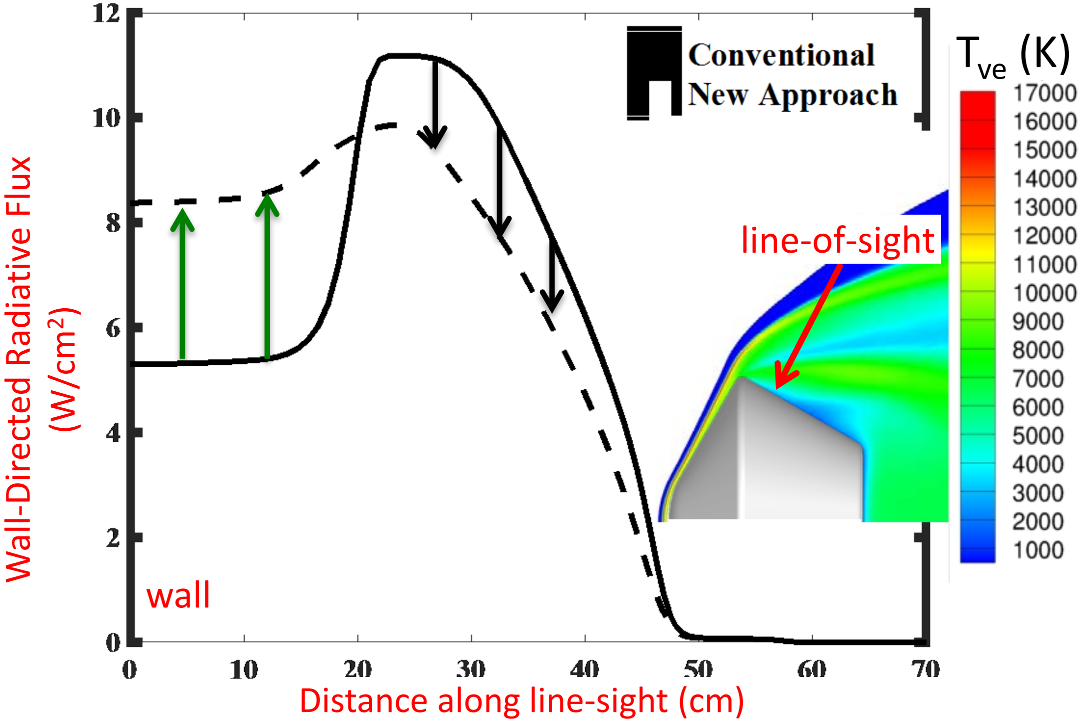
- Facility characterization

Wake Dynamics: Aerothermal Environments

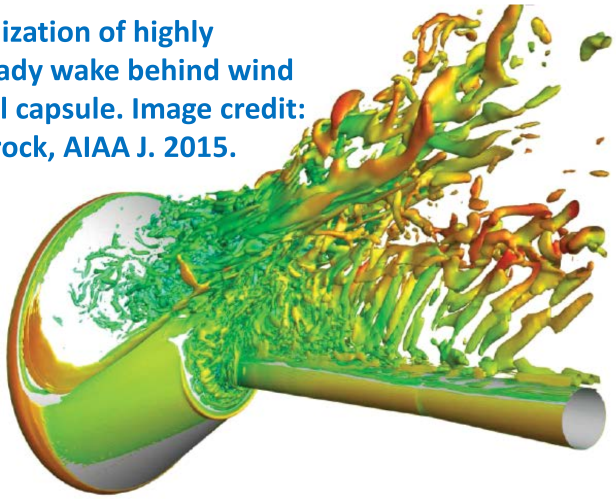
Wake dynamics drive aftbody environments

- Turbulent convective heating
- Thermal state and gas chemistry in presence of expansion/mixing define radiation to body
- Unsteady interactions from separation events

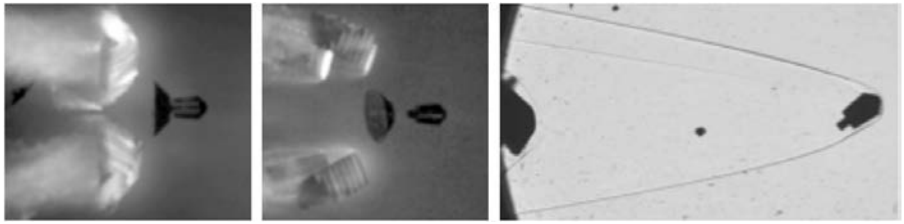
Modern CFD still largely dependent on quasi-steady RANS models with limited validation



State-specific radiation models needed for accuracy but dependent on accurate prediction of state of the gas. Image credit: Chris Johnston.

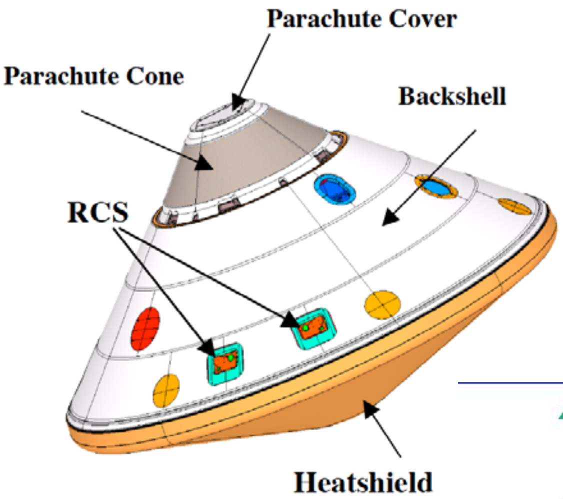


Visualization of highly unsteady wake behind wind tunnel capsule. Image credit: Joe Brock, AIAA J. 2015.

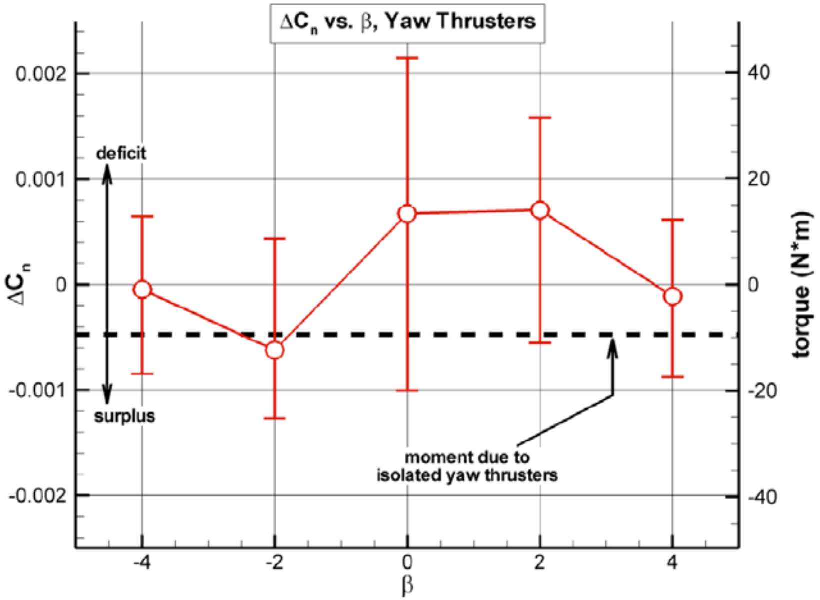


Ballistic range separation test. Image credit: Nelessen, IPPW 2018.

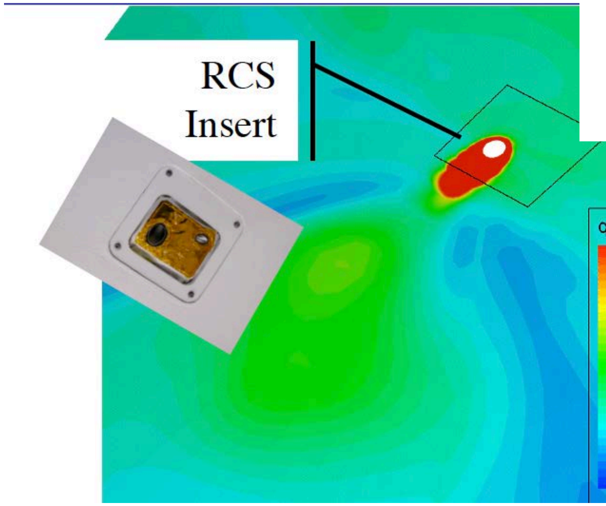
Wake Dynamics: Phoenix RCS



***Problem*: RCS Undersized for Mission Requirements**



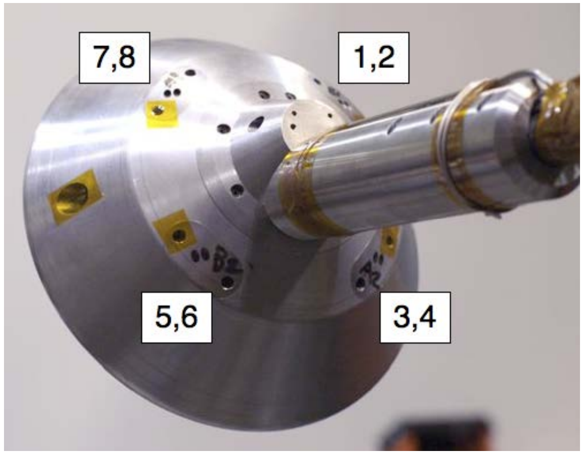
***Approach*: CFD Simulations using best available methods to guide mission response**



***Result*: Two day TIM in July 2007; CFD results had large error bars and often gave conflicting results.**

***Conclusion*: ‘deadband’ RCS thrusters; enter as a knuckleball.**

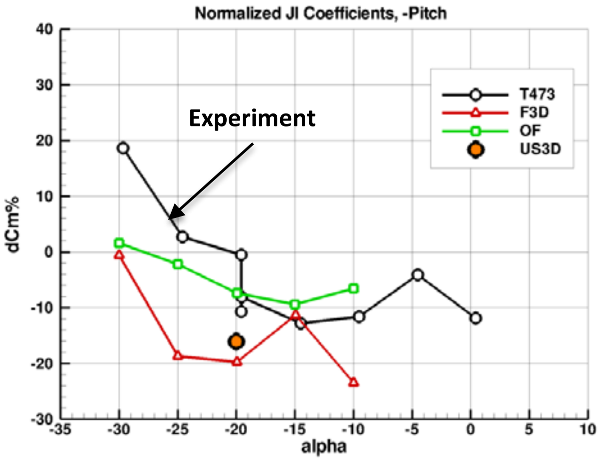
Wake Dynamics:
RCS/Aerodynamic Interaction



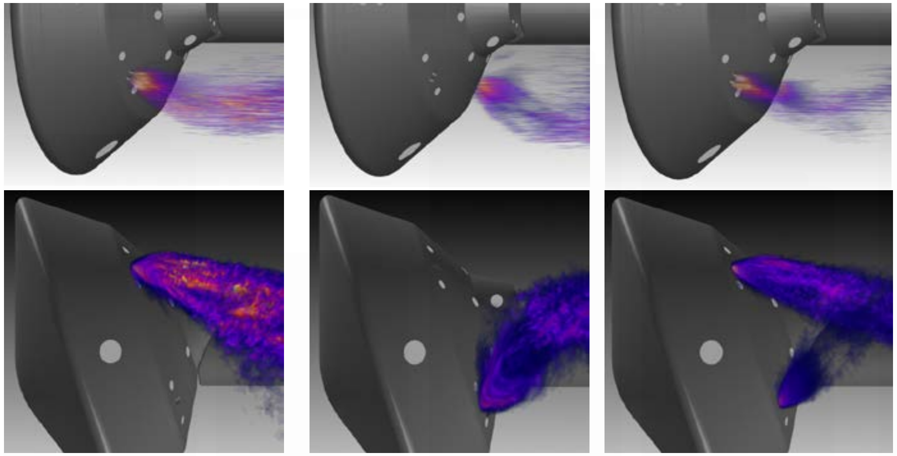
Cold-gas RCS model in Langley Mach 10 tunnel

MSL faced similar uncertainty concerning control authority of the RCS

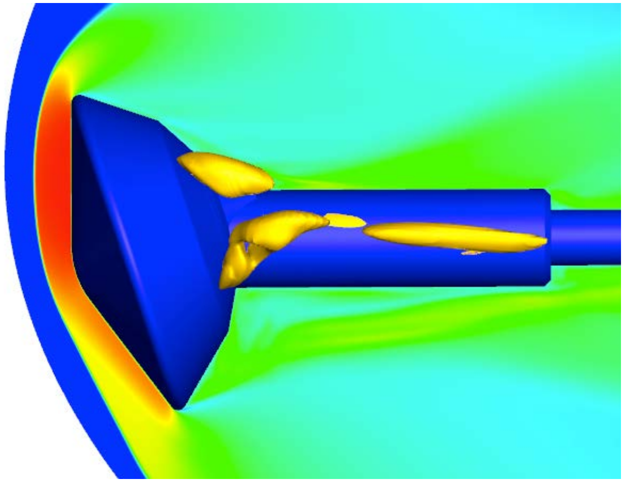
Experiments bounded uncertainty but computational validation was inconsistent



Measured vs. simulated jet interaction coefficients for pitch maneuver



NO PLIF visualization of RCS plumes



Simulated visualization of RCS plumes

POC: *Mark Schoenenberger (LaRC)*

Wake Dynamics: What Is Needed

- **Wake Structure**
  - Velocity, temperature, pressure fields
  - Flow separation and reattachment
  - Measurements on stingless / free flying models a priority

- **Gas Composition and Spectroscopy**

- **Surface Measurements**
  - Pressure, temperature, heat flux (convective and radiative)

- **More Data on Plume/Aerodynamic Interactions**

- **More Data on Multi-body Separations**

Advances to the state of the art in wake flow modeling, with and without plumes, is critical to future mission design. Impacts to RCS, SRP and terminal descent.

- Shock layer radiation & gas-phase kinetics

- Gas-surface interactions

- Roughness effects on transition and turbulence

- Wake dynamics with or without RCS

- **Facility characterization**

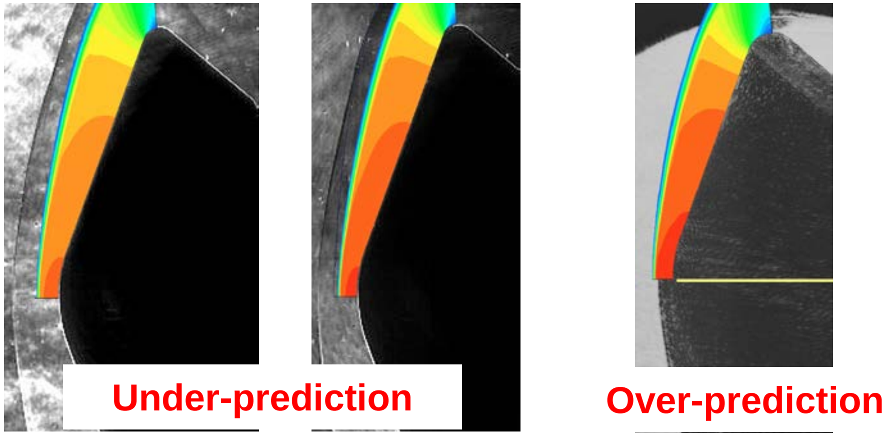
Facility Characterization: The Problem

- **Ground test environments are not a good match to flight environments**
  - Typically matching 1 or 2 of the identified key parameters for flight
- **Our ability to understand test conditions DIRECTLY impacts our ability to extrapolate ground test results to flight environment**
  - Transition to turbulence
  - Aeroheating
  - Gas-surface properties
  - Many more…
- **In high enthalpy facilities, the test environment is frequently more complex than the associated flight environment**
  - The “bruised gas” problem
  - Fundamental question: how much energy should be expended on high-fidelity facility models that are not flight relevant?

Canonical Example in EDL

- **Testing in two domestic shock tunnels in support of MSL produced conflicting, and non-flight like, results**
  - Multiple theories (and published papers) in attempt to explain data – still active today!
  - Likely due at least in part to non-flight like state of freestream
  - Later testing in expansion tunnels (LENS-XX, HET) produced better agreement with predictions, but several questions remain
- **My Conclusion:**
  - We lack a well characterized test facility for high-enthalpy aerothermodynamics validation
  - Problem is worse in CO_2 than in air, but challenges persist in both cases

MSL Era CO_2 Shock Tunnel Testing



LENS-1, Series-2, Shot 8
H0-Hw =5.6 MJ/kg

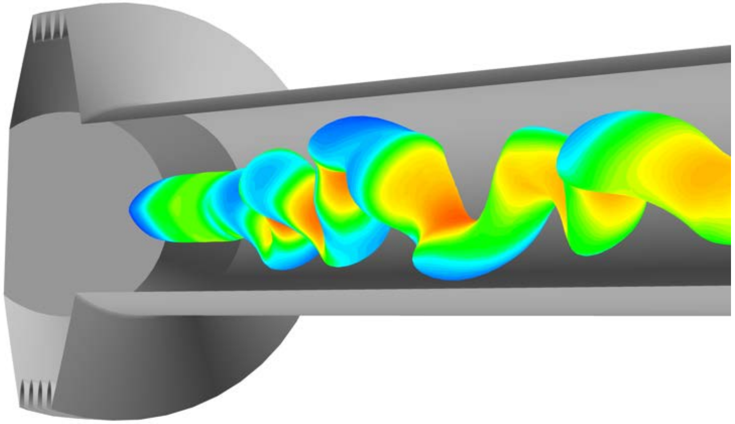
LENS-1, Series-2, Shot 13
H0-Hw =8.6 MJ/kg

Caltech T5, Shot 2255
H0-Hw =11.3 MJ/kg

Credit: Hollis et al.

The Grand Challenge: Arc Jets

- **Our only truly hypervelocity high enthalpy long duration test facilities**
  - Current use largely restricted to “TPS cookers”
  - Why? The environment that the models are subjected to is largely uncharacterized
- **Approach**
  - Green-field model of arc jet column, including FD, Radiation, Kinetics and MHD, coupled to existing models for flow from throat to test article
- **Validation**
  - Need a multitude of data ranging from throat and freestream to data taken in the arc column itself



Instantaneous current iso-surface in arc column

Credit: Mansour et al.

Arc attachment instability

What is Needed

- Accurate determination of fluid dynamic properties: velocity, pressure, density as well as their distribution and temporal variation across the test section
- Improved understanding of throat conditions
- Flow uniformity, turbulence, noise
- Kinetic state of the gas; composition, dissociation/ionization level, internal energy distribution, radiation
  - Complete understanding of flow enthalpy and the contribution of all components
- Improved direct measurement of surface quantities with sufficient temporal & spatial resolution: pressure, temperature, heat flux, incident radiation
- Improved understanding of “upstream” processes - how is the enthalpy getting into the flow?
- Reference calorimeters with known catalytic properties

My Answer: The value of a given facility as a validation tool is directly proportional to how well that facility is characterized. Increased emphasis on experimental characterization, and development of models for facility operation, will have ongoing benefit to all future testing.

Conclusions, or Are We There Yet?

- **Aerosciences and material response models, have largely undefined uncertainty levels for many problems (limited validation)**
  - Without well defined uncertainty levels, it is difficult to assess system risk and to trade risk with other subsystems. The consequence is typically (but not automatically) overdesign
- **Missions get more ambitious with time**
  - Tighter mass, performance and reliability requirements (MSR-EEV)
  - More challenging EDL conditions require that models evolve
- **Even reflights benefit from improvement**
  - Reflights are never truly reflights; changing system performance requires new analysis, introduces new constraints
  - ‘New physics’ still rears its head in the discipline
- **Some of the most challenging problems have the “worst” models**
  - Separation/wake dynamics, TPS failure modes, backshell radiation, facility characterization

Addressing these challenges requires focused investment in Modeling and Simulation, carefully guided by ground-based validation testing.

Backup