Tutorial on Ablative TPS Entry Convective Heating (CFD)

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21 August 2004

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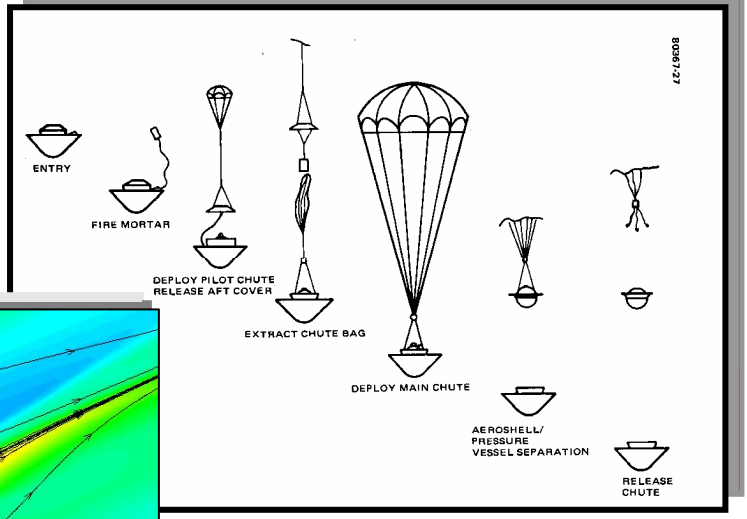
Outline

- Introduction
- Basic Equations and Kinetics
- Transport Modeling
- Turbulent Heating and Transition
- Afterbody Modeling
- Radiation/Flowfield/Ablation Coupling
- Uncertainties and Sensitivities
- Validation and Verification

Introduction

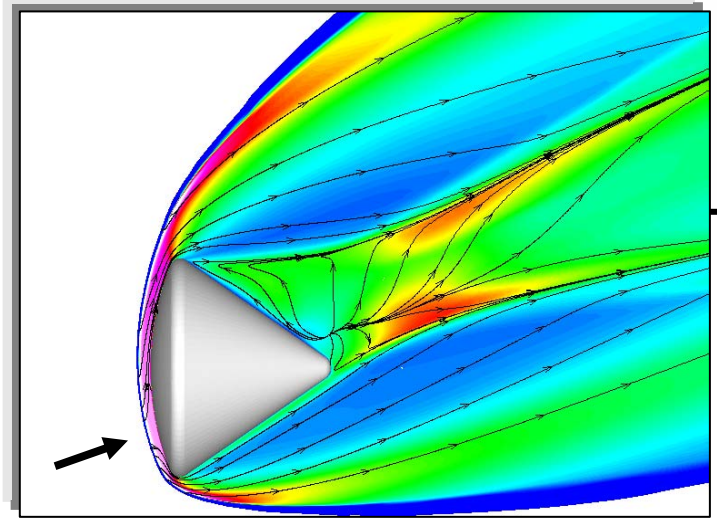
- Purpose is to give a general overview of the important physical phenomena that must be modeled for planetary entry probe aeroheating
- Key physical parameters will be discussed, and examples given to demonstrate their importance as well as our current ability to simulate
- Each section includes references for further reading
- Emphasis is on the continuum regime - no discussion of non-continuum (DSMC) or hybrid methods
- No discussion of the details of the computational methods, grid generation, or other elements of the CFD process

Introduction (cont.)
Hypervelocity Flow



Typical Entry and Descent

CFD simulation at a trajectory point in time



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Extended Navier-Stokes Equations for Reacting Flows

- **Species Continuity (*ns* equations):**

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho_s u_j + \rho_s v_{sj}\right) = \dot{w}_s$$

- **Momentum (3 equations)**

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}\left(\rho_s u_i u_j + p\delta_{ij}\right) + \frac{\partial \tau_{ij}}{\partial x_j} = 0$$

- **Total Energy Conservation (1 equation)**

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left((E+p)u_j\right) + \frac{\partial}{\partial x_j}\left(q_j + \sum_k q_{kj}\right) + \frac{\partial}{\partial x_j}\left(u_i \tau_{ij}\right) + \sum_s \frac{\partial}{\partial x_j}\left(v_{sj} h_s\right) = 0$$

- **Species Energy (*ne* equations)**

$$\frac{\partial}{\partial t}(\rho e_k) + \frac{\partial}{\partial x_j}\left(\rho e_k u_j + \rho e_k v_{sj}\right) + \frac{\partial q_{kj}}{\partial x_j} = \dot{Q}_k$$

Types of Terms in N-S Equations

- **Time derivatives (integrate equations to steady state)** $\frac{\partial \rho_s}{\partial t} \to 0$
- **Euler (convective) terms** $\frac{\partial}{\partial x_j}\left(\rho_s u_j\right)$
  - for supersonic flows these terms are typically upwinded by one of many numerical methods
- **Viscous terms** $\frac{\partial}{\partial x_j}\left(\rho_s \nu_{sj}\right)$
  - diffusive in nature, generally central differenced
- **Source terms** $\dot{w}_s, \quad \dot{Q}_k$
  - usually pointwise; exact form and discretization is specific to nature of term

Closure and Species Thermodynamics

- **Additional closure relation is the equation of state:** $p = \sum \rho_s R_s T$

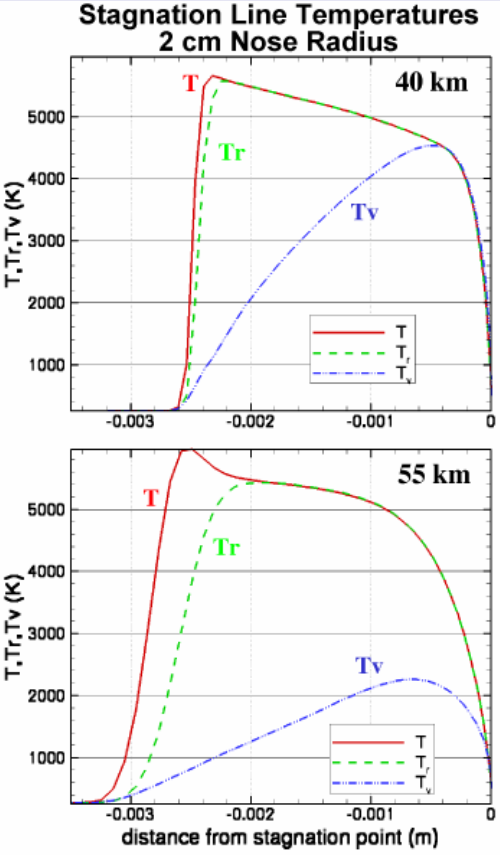
- **Species thermodynamic properties required to compute total and internal energies**
  - have been tabulated in many sources

- **Curve fits for *Cp, H, S* can be constructed for high temperature air components and used to determine thermodynamic properties of gas mixtures**
  - thermal nonequilibrium accounted for by subtracting out energy modes not in equilibrium with translational and modeling separately

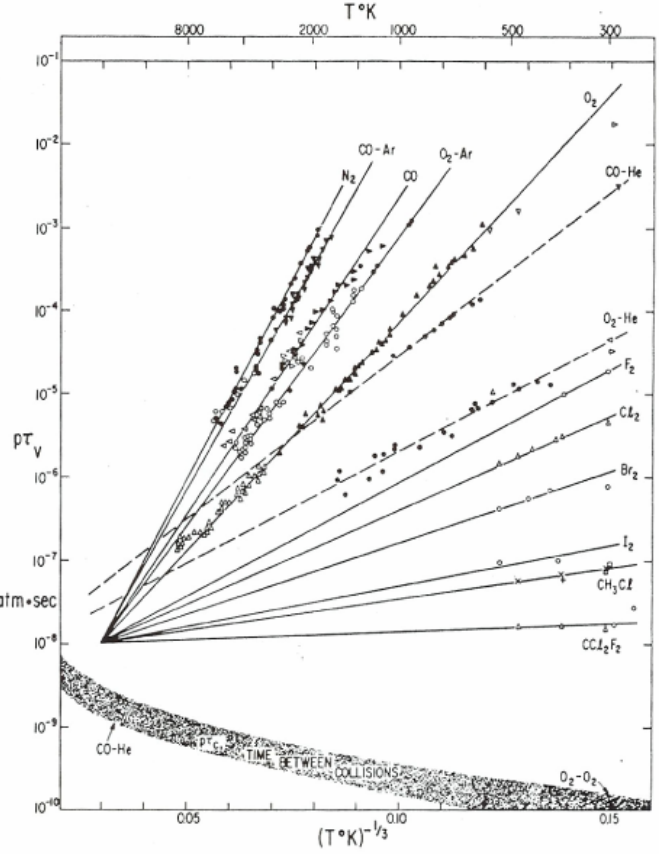
- **Equilibrium constants can also be determined by computing change in Gibbs free energy**
  - assumes K_{eq} is a function only of temperature -- valid for only a limited regime, which fortunately encompasses most problems of interest

Internal Energy Relaxation

- **For most problems of interest significant non-equilibrium exists behind shock wave**
- **Simplest approach to such cases is to solve multiple internal energy equations**
  - Assume energy modes are governed by multiple temperatures (each mode in a Boltzmann distribution)
  - Lump multiple modes together to reduce the number of energy equations to be computed
- **Commonly used models**
  - Two temperature (T-T_{ve}) developed for N_2 dominated flows due to well known resonance
  - Three and four temperature models assume rotational (T_r) and/or electronic (T_e) modes are separate
  - Detailed model include temperatures for every species vibrational (T_{vs}), rotational (T_{rs}) mode
  - State-specific models have been developed to eliminate Boltzmann requirement
- **Problem becomes modeling all of the source terms that are required**



Vibrational Relaxation



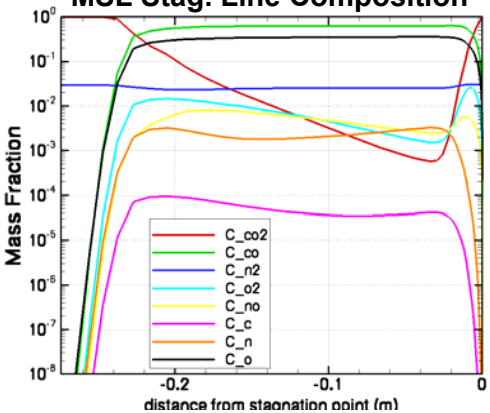
- Millikan and White have shown that VT relaxation times versus temperature can fit in a straight line
- Simple expression for relaxation time as a function of binary properties works well for many species
- Corrections required for certain molecules (e.g. CO_2)
- High temperature corrections also required to prevent relaxation time from becoming shorter than collision time
- Similar models can be constructed for other energy relaxation mechanisms

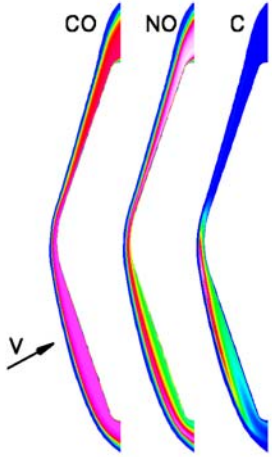
Ref: *Journal of Chemical Physics*, Vol. 39, No. 12

Chemical Kinetics

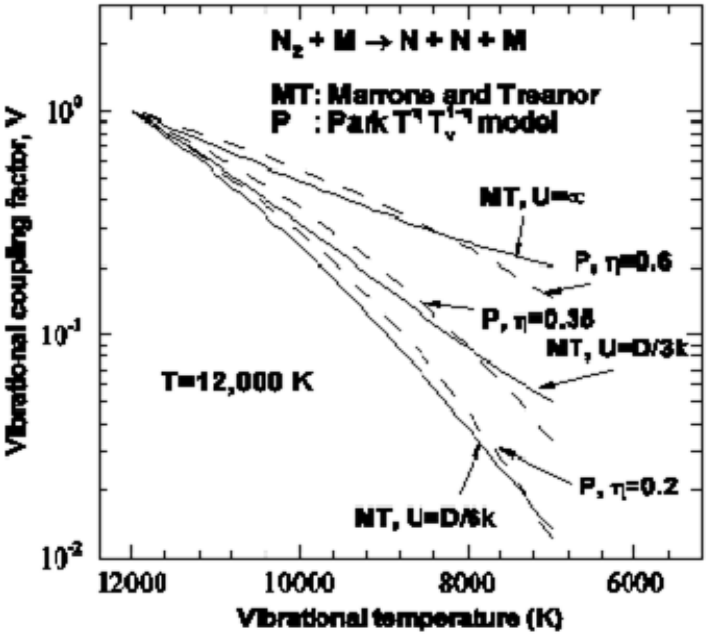
- **Thermal reaction rates are available in literature for most common reactions of interest**
  - kinetic mechanisms have been published for Earth, Mars, Titan, outer planet entries
- **Extrapolation to reentry conditions is usually required**
- **Most experimental sources do not account for effects of thermal nonequilibrium on reaction rates**
  - must be modeled in the simulation
- **Equilibrium constants can be computed via a Gibbs free energy approach using thermodynamic properties**

MSL Stag. Line Composition





Vibration-Dissociation Coupling



$$V = k(T,T_v)/k(T)$$

- The effect of thermal nonequilibrium on chemical reaction rates is uncertain
- In many engineering models Park's $T^{\eta}T_v^{1-\eta}$ is used with $\eta = 0.5$, i.e. the "effective" reaction temperature is an average of translation and vibrational temperatures
- More advanced models exist, such as Marrone and Treanor, which account for preferential dissociation from exited vibrational states
- For cases with strong thermal nonequilibrium Park's model can significantly underpredict reaction rate (in Park's model the rate tends to zero as $T_v << T$)

Ionization

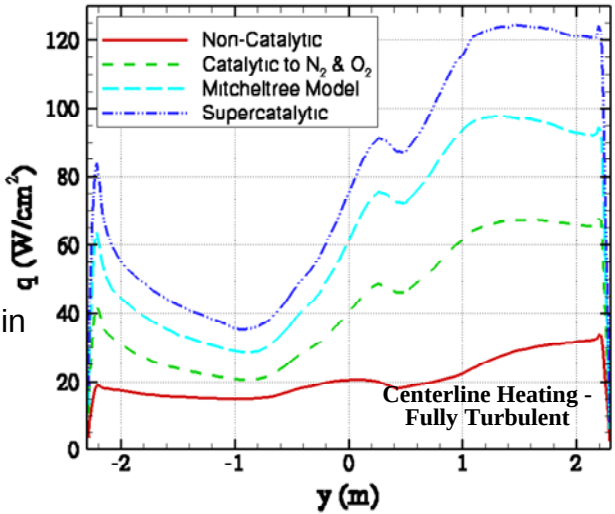
- **Weakly Ionized flows (<1%) can be modeled with only a few changes to basic equations**
  - transport properties are affected (to be discussed in next section)
  - electron impact rate processes must be accounted for
  - free electron temperature must be modeled
- **As ionization levels increase, problem complexity grows**
  - additional terms are required in momentum, energy equations due to electron pressure work
  - fluxes become non-homogeneous as electron energy must be solved as a separate equation
- **Applied electromagnetic fields also greatly complicate problem**
  - becomes a solution of the MHD equations, which is beyond the current scope

Surface Kinetics

Types of Surface Reactions

- **Catalysis -- recombination of incident species**
  - increases heat transfer to surface
  - material specific behavior; low-catalytic coatings exist
  - models exist for Earth; less fidelity for Mars/planetary applications
- **Oxidation/Nitridation -- incident atoms react with the surface**
  - material specific; e.g. carbon is extremely reactive in the presence of O atoms
  - models are under development
- **Sublimation -- solid goes directly to gas phase**
  - decreases net heat transfer; energy is carried away
  - will be discussed as part of material modeling

Mars Science Laboratory - Impact of Catalysis Model on Heating



⇒ **Models are required for all of the processes to accurately predict net heat transfer**

Surface Energy Balance

- **Net heat transfer consists of several components:**
  - **Inbound components**
    - convective, catalytic, and radiative heating
  - **Rejected components**
    - reradiation, pyrolysis, ablation
  - **Conduction into the surface**

- **Typically for design we first assume radiative equilibrium**
  - **Inbound heating is balanced by reradiation:** $\dot{q}_w = \varepsilon \sigma T_w^4$
    - conservative initial assumption
  - **Remaining components modeled via material response analysis**
    - either uncoupled or coupled to the CFD

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Governing Equations and Energy Relaxation

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Navier-Stokes Terms
For Reacting Flows

- **Mass :** $J_i = -\rho v_i = -\rho D_i \nabla X_i$ ← Ordinary Diffusion
- **Momentum :** $\tau_{ij} = \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\mu\nabla \bullet V$
- **Energy :** $q = \kappa\nabla T + \sum_s J_s h_s + \sum_i \kappa_i^* \nabla e_i$

Energy Conduction

Chemical Enthalpy Diffusion

Internal Energy Conduction

- **Models are required for each of these transport coefficients (μ, κ, κ_i, D)**

Theory

- **Expressions for the required transport coefficients can be derived from kinetic theory via Sonine polynomial expansions**

- **In general for mixtures an accurate representation of the transport coefficients requires solving systems of linear equations**

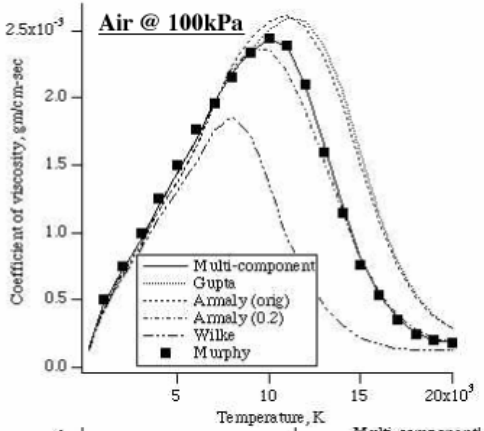
- **It has been shown that for most reentry flows of interest a 1st - order expansion is sufficient (note that thermal diffusion is zero in a 1st -order expansion)**
  - One exception is electron transport properties, which converge slowly and require a higher order expansion
- **All expansions require knowledge of binary interaction parameters (collision integrals) for each interaction**
  - Three quantities required for 1st order expansion: diffusion ($\Omega^{1,1}$), viscosity ($\Omega^{2,2}$), and a dimensionless ratio B^*

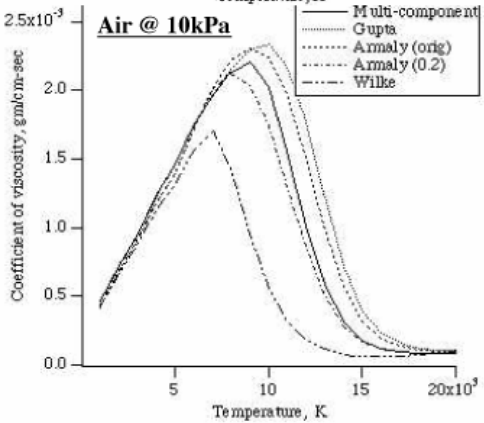
Collision Integrals

- **General types: neutral-neutral, ion-neutral, ion-ion, electron-neutral**
- **Collision integrals are obtained via a variety of methods:**
  - Experimentally (property measurements, beam experiments, discharge tubes)
  - Computationally (quantum mechanical *ab initio* calculations)
  - Analytic potentials
- **Commonly a simplified form of the interaction potential is assumed for which analytical expressions for collision integrals are available**
  - Lennard-Jones, exponential repulsion, polarizability
  - Ion-ion and ion-electron assumed to behave as shielded coulomb interaction
  - No simple approximation possible for electron-neutral interactions; must be obtained via integration of cross sections
- **Tabulated collision integral data are available for most common interactions of interest to planetary entries**

Viscosity

- 1st-order expression for pure species: $\mu_i = \dfrac{5k_bT}{\Omega_{ii}^{2,2}}$
- For mixtures the individual binary components must be properly accounted for. The resulting expression includes $\Omega^{1,1}$ and $\Omega^{2,2}$
  - System of *ns* equations which much be solved to determine μ
- Many simplifications appear in literature that eliminate necessity for equation solver (Blottner-Wilke, Gupta-Yos, Armaly-Sutton)
  - Utility for reacting flows reviewed *JTHT* v17 n2 (2003)
- Results show that Blottner-Wilke is good only for low *T* (below ~6000 K) and that the Armaly-Sutton mixing rule is a good approximation for air and H_2-He flows across temperature range

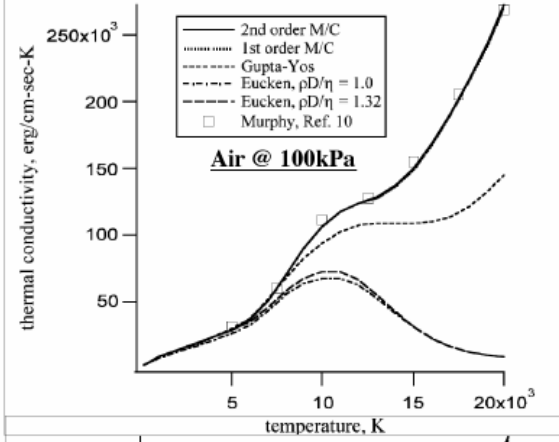


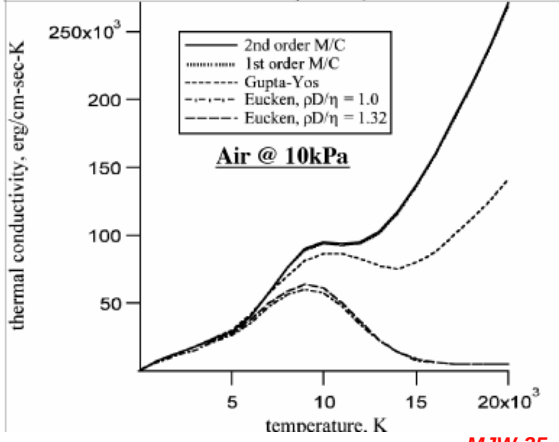


Ref: *JTHT*, Vol. 17, No. 2

Thermal Conductivity

- **Thermal conductivity separated into translational and (for molecules) internal components due to energy relaxation**
- **For mixtures the binary components must be properly accounted for**
  - The resulting expression for translational component includes $\Omega^{1,1}$, $\Omega^{2,2}$, and B^*
  - Expressions for internal components are diffusional and include only $\Omega^{1,1}$
  - System of *ns* equations which much be solved to determine κ
- **Again, simplifications can eliminate necessity for equation solver**
  - Utility for reacting flows reviewed in *AIAA Paper No. 2003-3913*
- **Results show that Eucken relation is good only for low *T* (below ~6000 K) and that full multicomponent method should be used at higher temperatures**





Ref: AIAA Paper No. 2003-3913

Diffusion

- **Diffusion coefficients (D_i) are required for each species in mixture**
- **Expressions for binary diffusion coefficients (D_{ij}) are straightforward functions of $\Omega^{1,1}$**
- **Simply mixing D_{ij} to form D_i violates mass conservation, which requires that the diffusion velocities ($J_i = -\rho v_i = -\rho D_i \nabla X_i$)sum to zero**
- **Rigorous calculation requires solution of Stefan-Maxwell equations, which can be time consuming (equations are ill conditioned since diagonal is small -- no self diffusion)**
- **Simplest approximation is to assume that all D_i are equal and related to either μ (constant Schmidt number *Sc*) or κ (constant Lewis number *Le*)**
  - Can be reasonable in weakly reacting flows, but does not capture the true physics, as D_i does not have the same functional form as either μ or κ
  - Does not account for differences in diffusion rate (light species diffuse faster than heavy species) and different particle types (ions and electrons behave very differently than neutrals

Diffusion, cont.

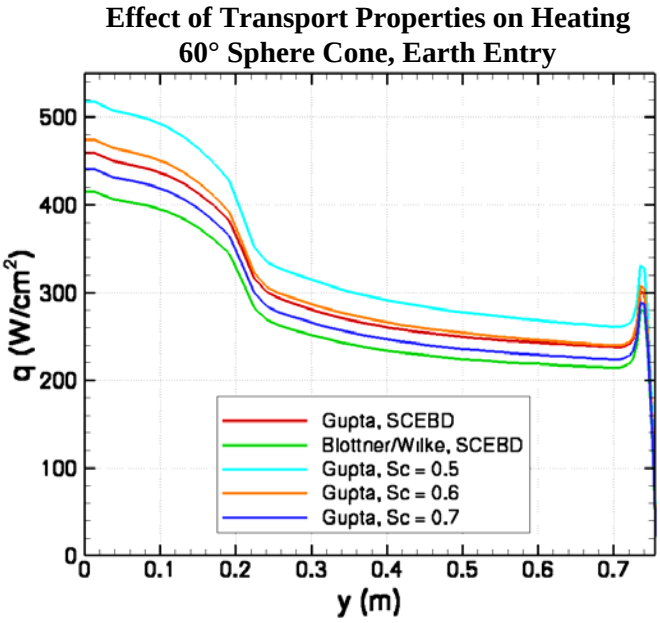
- **SCEBD method avoids difficulties by redistributing mass conservation error to all species**
  - Independently proposed by Ramshaw (1990) and Sutton & Gnoffo (1998)

$$J_i^0 = -\rho D_i \nabla X_i \quad ; \quad J_i = J_i^0 - \frac{\rho_i}{\rho} \sum J_i^0$$

- **Correction is seemingly arbitrary, but physical justification is sound**
- **Resulting expression shown to be in excellent agreement with Stefan-Maxwell solutions**
- **For ionized flows correction is required for ambipolar diffusion**
  - Simple approximation ($D_a = 2D$) accurate only for single ion
  - Better to enforce charge neutrality: $\sum J_i z_i = 0$
  - Compute ion diffusion normally and then set electron diffusion to be as necessary to enforce charge neutrality
- **Extensions demonstrated for cases where thermal and/or pressure diffusion are non-negligible**

Impact on Aeroheating

- **Different models for transport properties can change predicted aeroheating by ±15% at Earth and by more than ±25% at Mars**
  - larger differences at Mars due to large disparity in molecular weights leading to breakdown of "binary gas" assumption
- **If the "right" answer is known a constant Schmidt number can be chosen that approximates multi-component diffusion**
  - becomes harder for ionized flows, since charged particle interactions are very different than neutral interactions
- **Since using a Schmidt number relates diffusion to viscosity, the model used to compute the viscosity is closely coupled to the model used for diffusion**



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Outline

- Basic Equations and Kinetics
- Transport Modeling
- **Turbulent Heating and Transition**
- Afterbody Modeling
- Radiation/Flowfield/Ablation Coupling
- Uncertainties and Sensitivities
- Validation and Verification

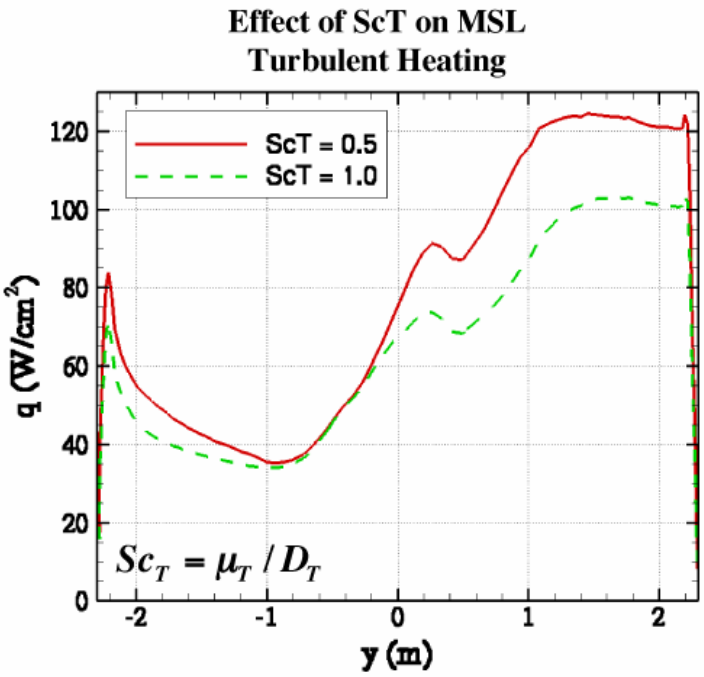
Turbulence Models

- **Many models exist in literature**
  - Most are Reynolds-averaged Navier-Stokes (RANS) methods developed for incompressible turbulence
- **Models classed by the number of additional conservation equations**
  - Zero equation models (e.g. Baldwin-Lomax and Cebeci-Smith) solve an algebraic equation for turbulent viscosity, which is then added to laminar value
  - One-equation models (e.g. Spalart-Allmaras) solve a field equation for turbulent eddy viscosity
  - Two-equation models (e.g. k-ε, k-ω, SST) solve equations for turbulent kinetic energy and some form of turbulent dissipation
- **Newer models, such as Detached Eddy Simulation (DES) and Large Eddy Simulation (LES) bridge the gap between RANS models and Direct Numerical Simulation (DNS)**
- **Corrections to the basic models are generally required to account for compressibility effects**
  - Historically these corrections have been somewhat ad-hoc, but recently DNS data have been used to assess necessary corrections numerically

Turbulence Models

Reacting Flows

- **For chemically reacting flows, an additional correction is required to model turbulent mixing impact on diffusion**
  - turbulent Schmidt number (Sc_T) is generally employed
  - value ranges from 0.5-1.0 in boundary layers, free shear layers
  - value chosen can significantly impact predicted surface heating if catalysis is important (higher Sc_T = lower heating)

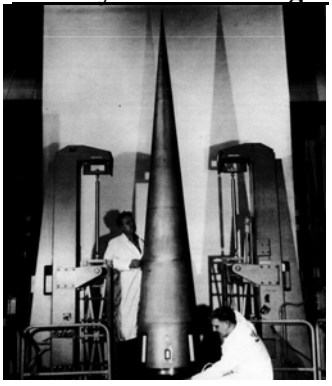


Turbulence Models

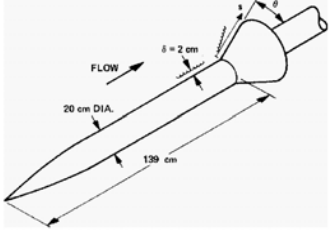
Model Validation

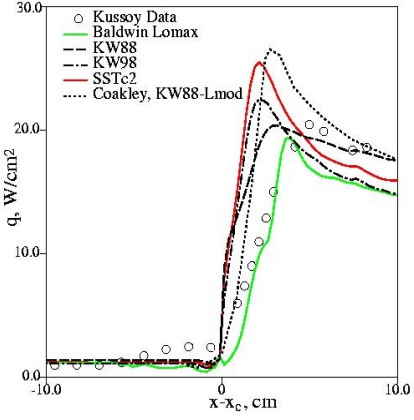
- **Comparisons with test data have shown that most models do a reasonable job of predicting fully turbulent heating on flat plates and blunt geometries in a zero or favorable pressure gradient**
- **Compressible Baldwin-Lomax generally employed for design purposes since it gives reasonable results with minimal performance penalty**
- **One or two equation models may be required for separated or adverse pressure gradient flows**

Reentry-F Prior to Flight

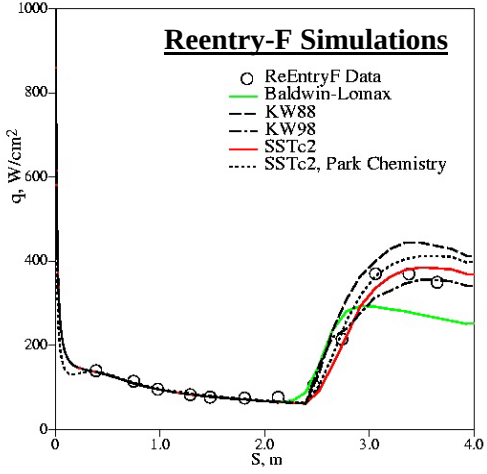


Kussoy Compression Corner





Reentry-F Simulations

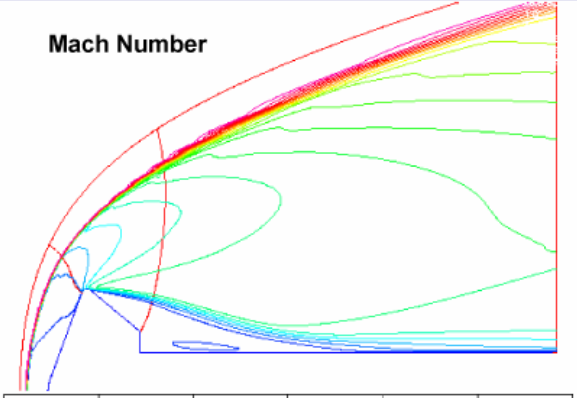


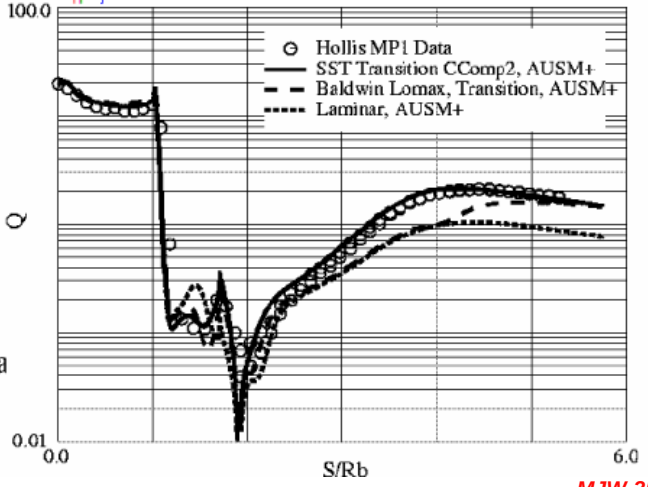
Ref: AIAA Paper 2002-3308

Hypersonic Turbulence

Model Validation, Cont.

- **Goal**: Determine best available turbulence model for hypersonic flow simulations
- Validation cases included M10 boundary-layer, compression corner, sphere/cone cases, base flows
- Best overall performer is SST with modified Wilcox compressibility correction
- Example case:
  - Hollis "Mars Pathfinder" experiment
  - Mach 10 70° sphere-cone, sting-mounted
  - Transition specified at shoulder





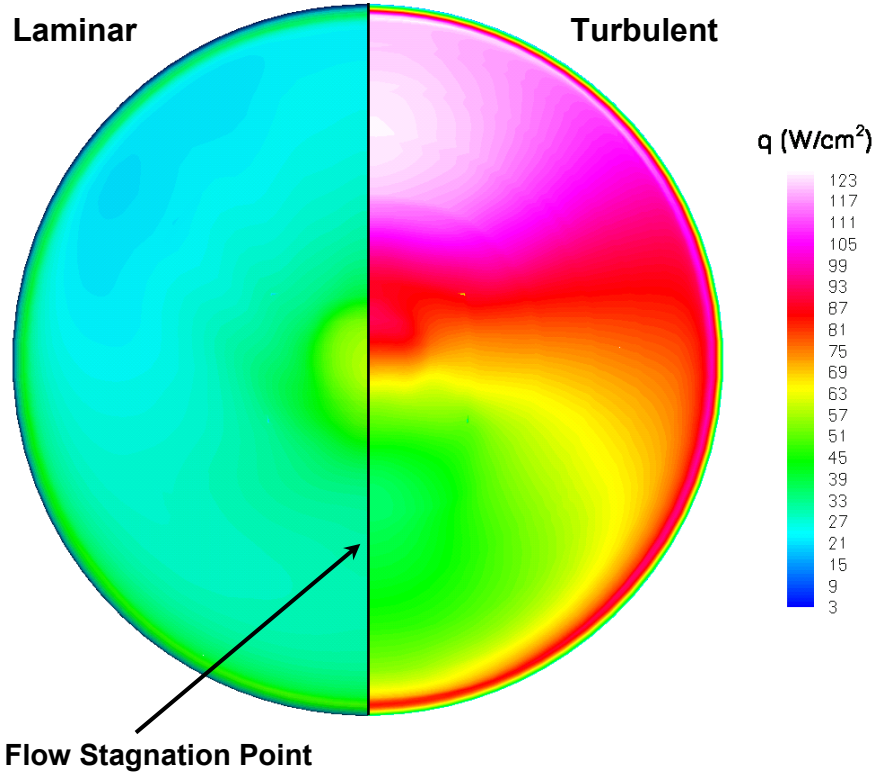
⇒ **Conclusions:**

- **Current standard (Baldwin-Lomax) reasonable & conservative for unseparated flows**
- **SST model is robust and provides most accurate hea transfer predictions for separated flows**

Ref: AIAA Paper 2002-3308

Mars Science Laboratory:
Turbulent Heating on Lifting Capsules

MSL Peak Heating (α = 16°)

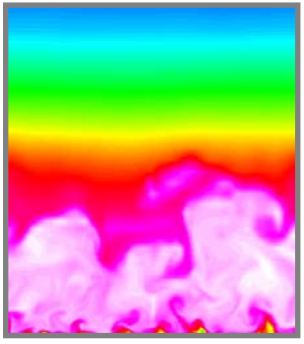


- 70° sphere-cone flying at angle of attack
- Leeside turbulent heating levels dominate aeroheating environment - design to stagnation point heating would not be conservative
- High heating levels drive TPS material selection and thickness
- Testing in shock tunnels at CalTech and CUBRC to understand turbulent augmentation factors and enable validation of CFD at flight enthalpy

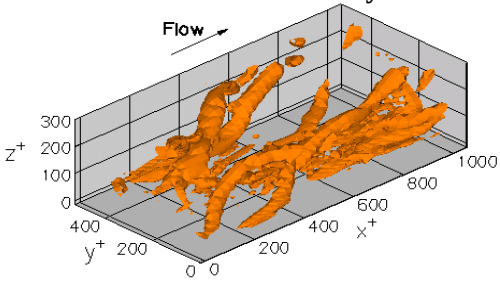
Direct Numerical Simulation
of Turbulent Boundary Layers

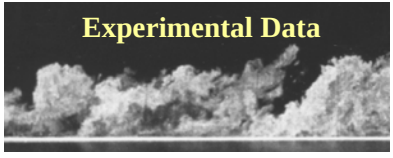
- **Direct solution of all relevant length scales of the problem**
  - extremely computationally intensive
  - has been done only for isotropic turbulence and limited boundary layer simulations
  - utility will grow as computers become faster

DNS Simulation
Mach 4 Boundary Layer

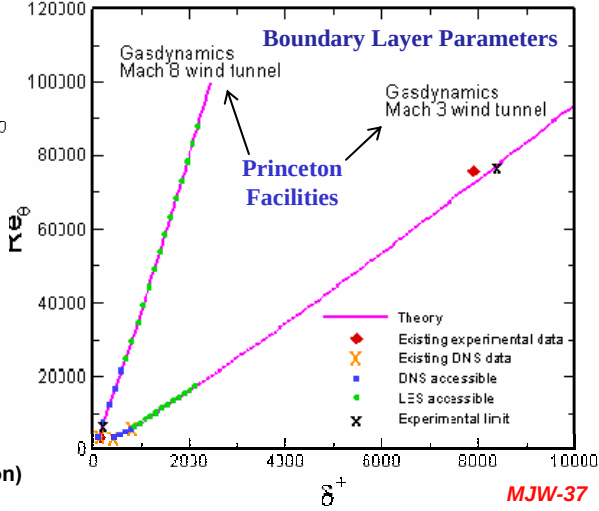


Vorticity





Accessibility of Experimental Conditions Using DNS and LES Methods



Ref: Dr. Martin (Princeton)

Turbulent Transition

- **Current ability to predict transition is very limited**
  - most turbulence models "force" turbulence when used and cannot be employed in a predictive manner
  - some progress has been made using linear and parabolized stability theory
  - additional models, such as the k-ζ (enstrophy) model, have shown promise for limited classes of problem
- **Many transition models exist in literature**
  - one of the most commonly used is Re_θ/M_e = const., where the value depends on the problem class and is typically in the range of 150-350.
  - developed based on Shuttle data, frequently applied as a smooth wall transition criterion

Turbulent Transition

Impact of Roughness

All ablators form a distributed surface roughness pattern as a result of charring

Roughness can drive transition process

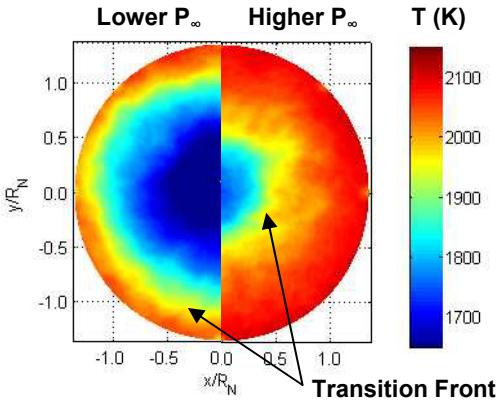
Roughness-dominated transition is configuration dependent

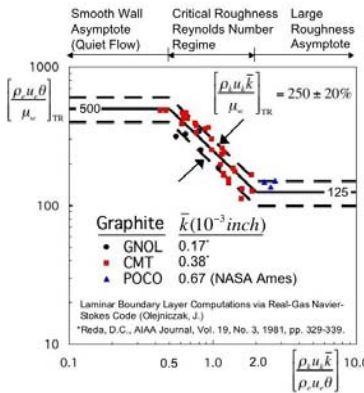
- roughness must be characterized for material of interest

Roughness-dominated transition model exists for hemispherical shapes at hypersonic speeds

→No roughness-dominated transition model exists for blunt, large-angle cones typical of planetary entry vehicles

70° Sphere-Cone
Hypersonic Flight in Ballistic Range





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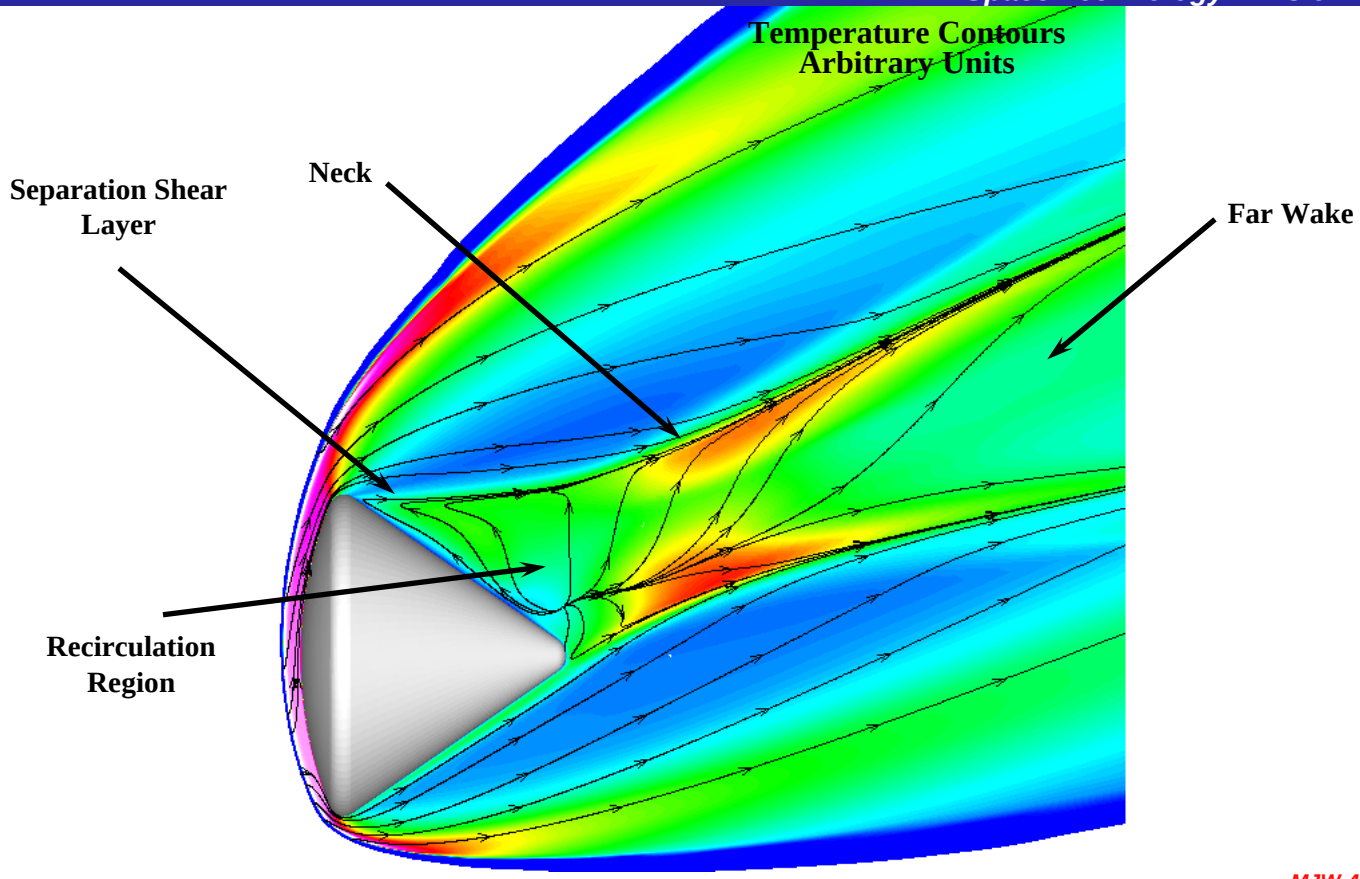
Afterbody Flow Topology



Recent Status

- **Large design uncertainties**
  - 300% uncertainty used for Mars Pathfinder design
- **Many reasons for large uncertainty levels**
  - complexity of flowfield physics
  - lack of flight data for validation
  - minimal code validation with existing flight data
- **It is fair to say that until recently the actual uncertainty in our ability to predict afterbody aeroheating was not large, it was <u>unknown</u>**
- **Recent progress and available flight data will be summarized in a talk at this workshop**

Issues with Modeling

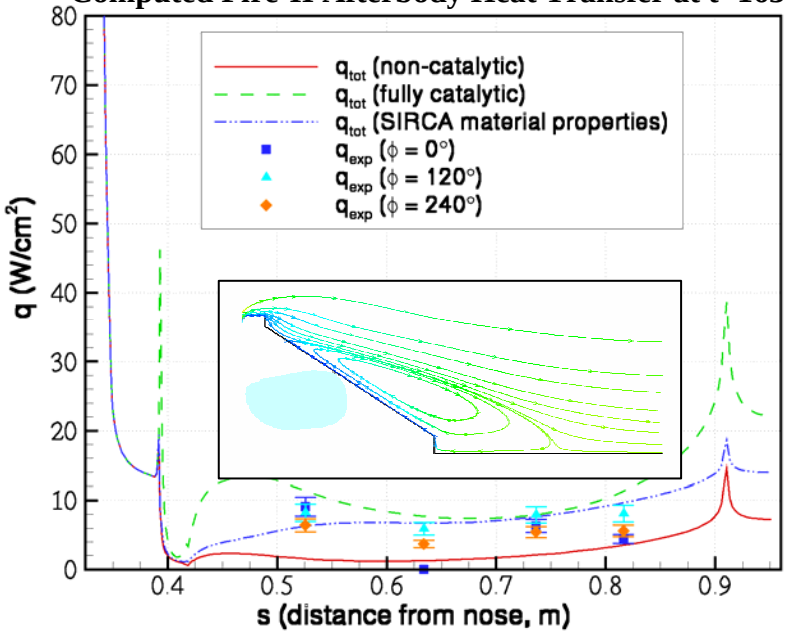
Afterbody Aeroheating

- **Disparity in time scales**
  - rapid expansion into base region freezes out slow processes, leading to a highly nonequilibrium flow state
- **Disparity in length scales**
  - smallest scale vortical features must be resolved to accurately predict base heating
- **Flow unsteadiness**
  - as Reynolds number increases flow will become unsteady
  - 3D simulations may be required to capture nature of unsteadiness
- **Computational grid design/topology**
  - wake features are sensitive to volume grid quality, which must have sufficient points to capture features and must be tailored to resolve separation point and shear layer
- **Flow evolution time**
  - large subsonic recirculation region naturally converges slowly, and many more iterations are typically required to reach a steady state solution
- **Non-continuum effects**
  - portions of flowfield can be continuum and while others are rarified
- **Turbulent transition**
  - turbulence models for separated flows are not well validated

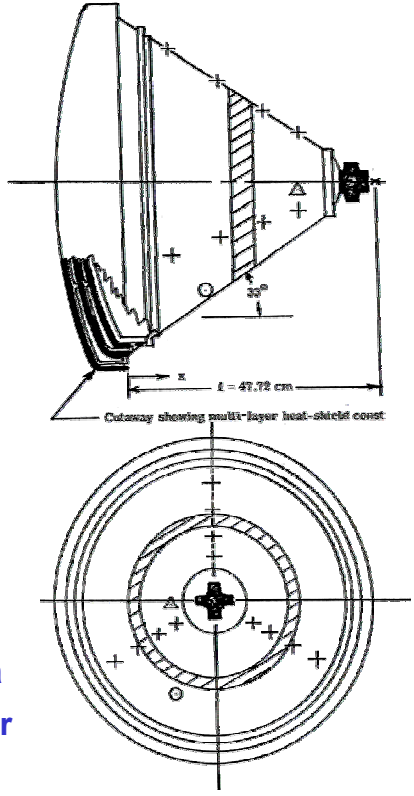
Afterbody Aeroheating

Validation with Fire-II Flight Data

Computed Fire-II Afterbody Heat Transfer at t=1634s



Fire-II Instrumentation

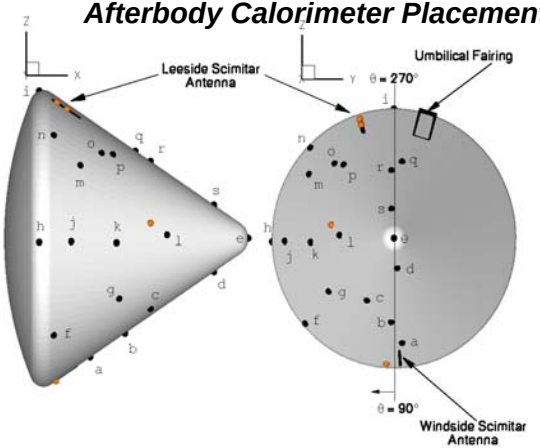


- **Goal: reduce uncertainty levels by validation with flight data**
- **Excellent agreement between CFD and flight data for laminar flows without afterbody TPS blowing**

Ref: *JTHT*, Vol 17, No 2, 2003

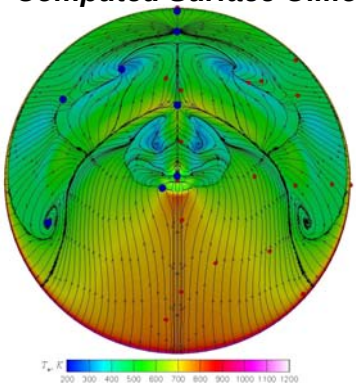
Afterbody Aeroheating
Validation with Apollo Flight Data

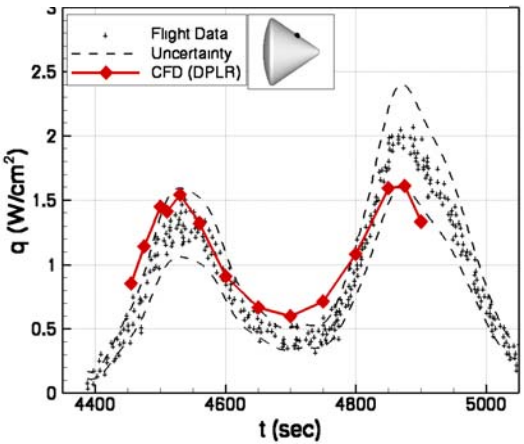
Afterbody Calorimeter Placement

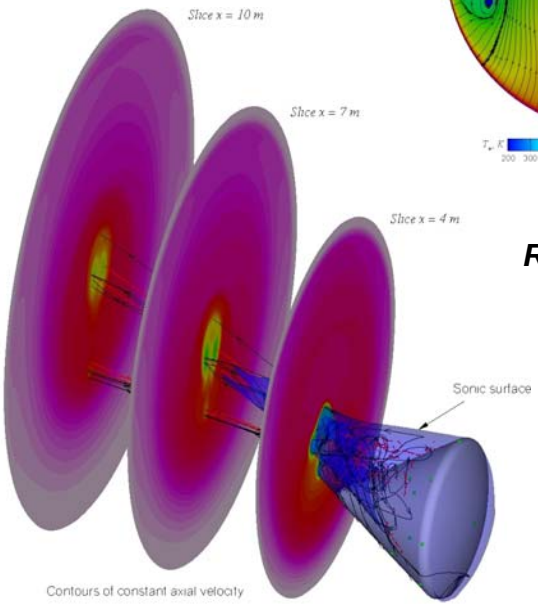


DPLR computations generally agree with flight data to within ±20% uncertainty at 15 of 19 calorimeter locations.

Computed Surface Oilflow







t= 4900 s,
$Re_D = 7.6\times10^5$

Ref: AIAA 2004-2456

Afterbody Aeroheating

Future Work

- **Current ability to predict laminar aeroheating on non-ablating materials is good**
- **Additional validation required for turbulent flows, ablating walls**
  - Apollo flight data is a good validation resource
- **Gas chemistry effects on afterbody aeroheating not as well understood**
  - Vast majority of available flight data is Earth entry

For Further Reading:
Afterbody Modeling

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Importance of Coupling

- **Traditional design approaches neglect coupling**
  - incident aeroheating is assumed to be the sum of computed convective heating plus the radiative heating determined by post-processing the CFD solution
  - net heating is then computed by computing the material response of the TPS based on the input aeroheating values
- **This approach can be very conservative for high energy entries**
- **May also neglect important physical phenomena that can alter the distribution or timing of the net heating**

Radiation Flowfield Coupling

- **Radiation/flowfield coupling must be addressed when Goulard number (Γ - ratio of radiative energy flux to total energy flux) is large**

$$\Gamma = 2q_{rad} / (\tfrac{1}{2}\rho_\infty V_\infty^3)$$

  – Γ >0.4 at peak heating for Titan aerocapture, ~.01 for Fire-II and ~.10 for Galileo

- **Engineering estimates of coupling impact to radiative heating (Tauber & Wakefield, 1971):**

$$q_{coup} / q_{unc} = 1/(1 + \upsilon\Gamma^{0.7})$$

Approaches to Radiation Coupling

Uncoupled

- **Radiation computed as a post-processing step; does not impact flow**

Loosely Coupled

- **Iterate between flowfield and radiation solutions**
- **Demonstrated for weak to moderate coupling (Stardust, Fire-II)**
- **Becomes expensive for strong coupling (many iterations required)**

Tightly Coupled

- **In general this requires simultaneous solution of fluid dynamic and radiative transport equations (integro-differential equation set)**
  - prohibitively expensive for full 3D calculations
  - attempts have been made in literature for 1D, 2D and 3D flows
- **BUT Titan is an exception; optically thin shock layer**
  - radiation computation becomes pointwise; radiation either intersects surface or leaves computational domain
  - exact treatment of radiation coupling is possible

Impacts of Radiation Coupling

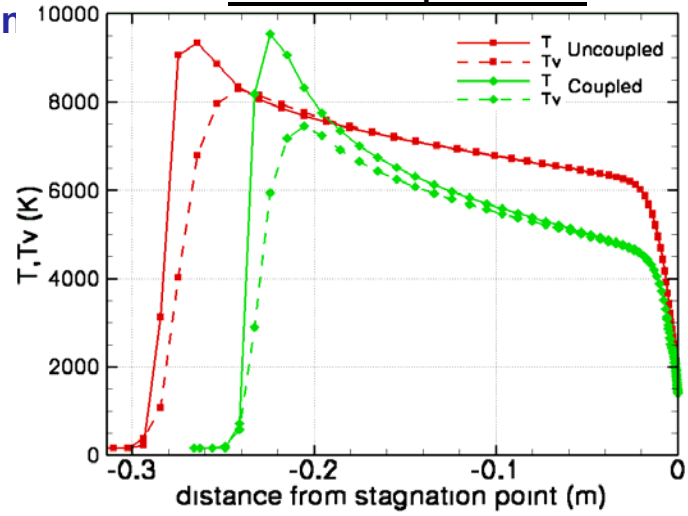
- **Non-adiabatic (volumetric) effects**
  - **Radiation acts as a sink of energy as it leaves a cell, and as a source when it is absorbed within a cell**

- **Surface energy balance effects**
  - **Radiative heating to surface affects energy balance:**

$$q_{conv} + q_{rad} = \varepsilon \sigma T_w^4$$

  - **Will increase wall temperature and impact boundary layer profiles**
  - **Should <u>slightly</u> reduce convective heating rate**

<u>Titan Aerocapture Case</u>



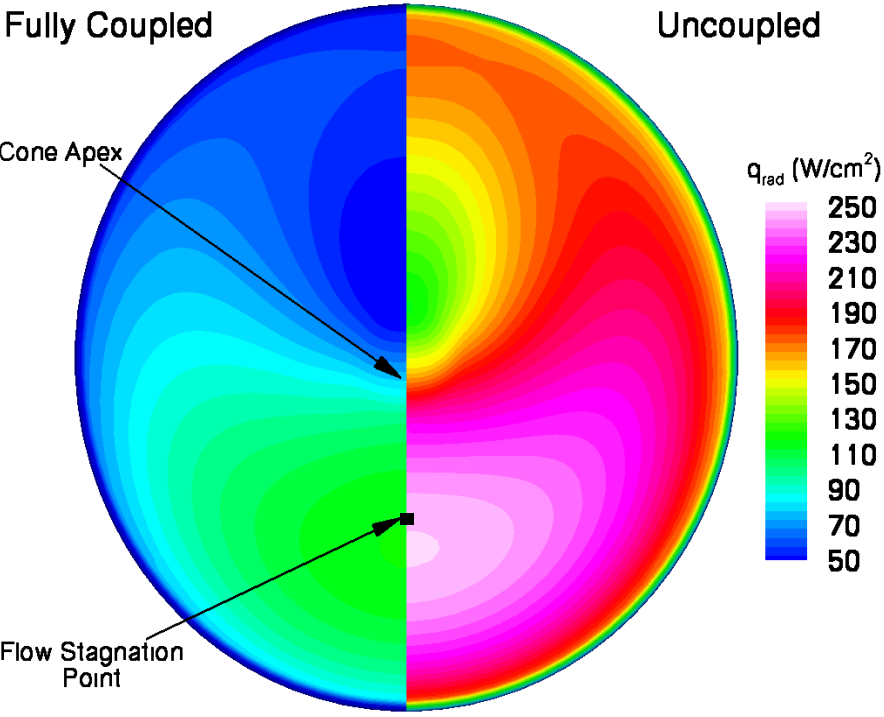
⇨ **Shock standoff distance and post-shock temperature significantly reduced by non-adiabatic effects**

Ref: AIAA-2004-0484

Radiation-Flowfield Coupling

Titan Aerocapture

t = 253s, 6.5 km/s lift up min. atmosphere



- **Radiative heating dominates convective**
- **ARC-developed fully coupled methodology enables accurate assessment of radiative heating**
- **Coupled radiative heating less than half of uncoupled levels!**
- **Radiation coupling also reduces convective heating by ~30%**
- **Net result is more than a factor of two reduction in predicted heat load**

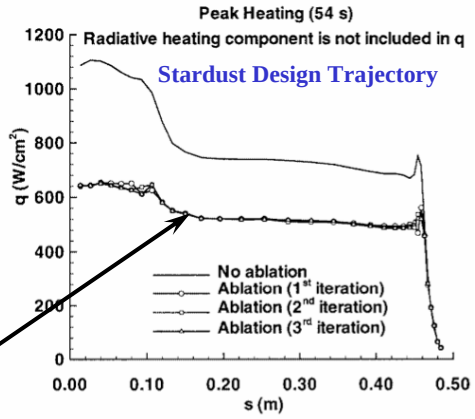
➔ **For this environment, coupled solutions are required to obtain reasonable aeroheating predictions and to make informed TPS decisions**

Ref: AIAA-2004-0484

Ablation-Flowfield Coupling

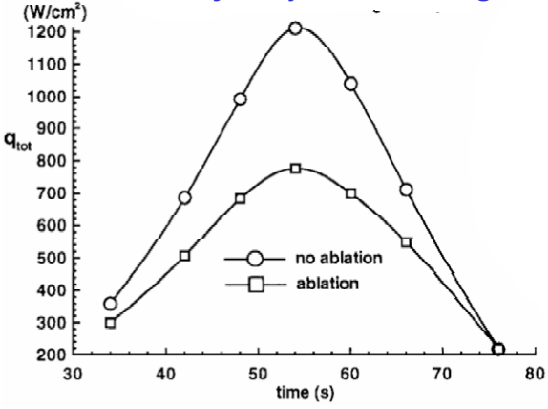
Stardust Sample Return

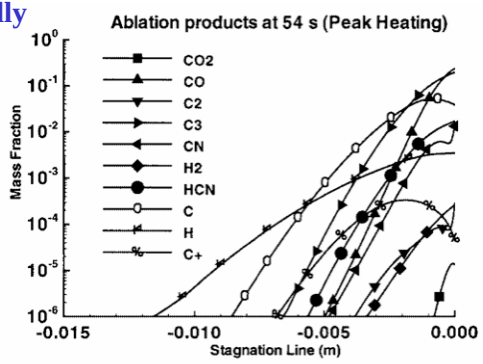
- Loose coupling was demonstrated for Stardust design
- Iterate between CFD and material response solver
- Must include gas-phase models for ablation product - boundary layer interactions, and absorption models for ablation product - radiation interactions
- Gas-surface interaction modeling requires special treatment



Iterative loosely coupled approach converges rapidly

Stardust Trajectory Based Heating



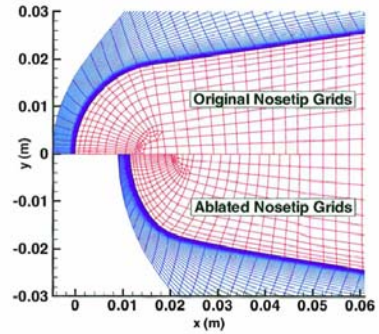


Ref: *Journal of Spacecraft and Rockets*, Vol. 36, No. 3

Recession-Flowfield Coupling

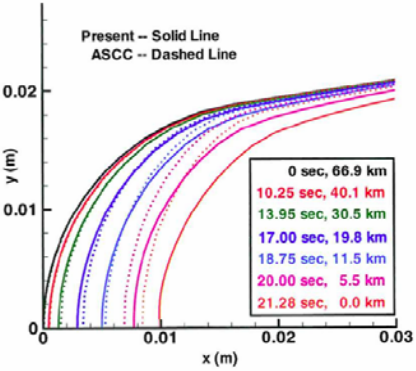
- For cases with significant ablation shape change during entry will be significant and must be accounted for
- Shape change will affect both heating and aerodynamics of entering vehicle
- Loosely coupled simulations accounting for shape change have been demonstrated by Kuntz et al. (2001)

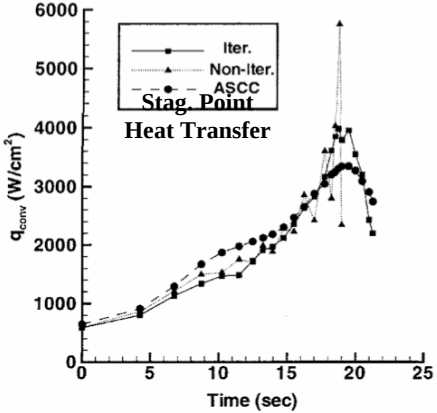
Initial and Final Computational Grids



IRV Vehicle

Recession Time History





Ref: JTHT Vol. 15, No. 2

Ablation-Flowfield Coupling

Gas-Surface Interaction

- **Simplest approach is to assume thermochemical equilibrium at the surface**
  - Not valid for conditions of most planetary entries of interest
- **Higher fidelity models require finite rate mechanisms for possible gas-surface reactions**
  - Catalysis, oxidation, nitridation, sublimation
- **Work has been done for certain special cases**
  - Carbon-carbon, graphite (Park, Havstad et al., Zhuluktov et al.)
  - Carbon-phenolic (Chen et al.)
- **Much more work is required to understand the appropriate mechanisms and to determine the required rates**

For Further Reading:
Flowfield-Radiation Coupling

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- Tauber, M. and Wakefield, R., "Heating Environment and Protection During Jupiter Entry," *Journal of Spacecraft and Rockets*, Vol. 8, No. 3, 1971, pp. 630-636.
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- Hartung, L., Mitcheltree, R., and Gnoffo, P., "Coupled Radiation Effects in Thermochemical Nonequilibrium Shock Capturing Flowfield Calculation," AIAA Paper No. 92-2868, Jul. 1992.
- Olynick, D., Henline, W., Hartung-Chambers, L., and Candler, G., "Comparison of Coupled Radiative Flow Solutions with Project Fire II Flight Data," *Journal of Thermophysics and Heat Transfer*, Vol. 9, No. 4, 1995, pp. 586-594.
- Sakai, T., Tsuru, T., and Sawada, K., "Computation of Hypersonic Radiating Flowfield over a Blunt Body," *Journal of Thermophysics and Heat Transfer*, Vol. 15, No. 1, 2001, pp. 91-98.
- Matsuyama, S., Sakai, T., Sasoh, A., and Sawada, K., "Parallel Computation of Fully Coupled Hypersonic Radiating Flowfield Using Multiband Model," *Journal of Thermophysics and Heat Transfer*, Vol. 17, No. 1, 2003, pp. 21-28.
- Wright, M., Bose, D., and Olejniczak, J., "The Impact of Flowfield-Radiation Coupling on Aeroheating for Titan Aerocapture," AIAA Paper No. 2004-0484, Jan. 2004.

For Further Reading:
Ablation-Flowfield Coupling

- Bartlett, E., Kendal, R., and Rindal, R., "An Analysis of the Coupled Chemically Reacting Boundary Layer and Charring Ablator," Parts I-VI, NASA CR-1063, Jun. 1968.
- Wilson, K., "Stagnation Point Analysis of Coupled Viscous Radiating Flow with Massive Blowing," NASA CR-1548, Jun. 1970.
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- Moss, J., "Advancements in Aerothermodynamics in Support of the Galileo Probe," *Proceedings of the 13th International Symposium on Space Technology and Science*, Tokyo, 1982, pp. 613-624.
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- Milos, F. and Chen, Y.-K., "Comprehensive Model for Multicomponent Ablation Thermochemistry," AIAA Paper No. 97-0141, Jan. 1997.
- Olynick, D., Chen, Y.-K., and Tauber, M., "Aerothermodynamics of the Stardust Sample Return Capsule," *Journal of Spacecraft and Rockets*, Vol. 36, No. 3, 1999, pp. 442-462.
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- Chen, Y.-K. and Milos, F., "Finite Rate Ablation Boundary Conditions for a Carbon-Phenolic Heat Shield," AIAA Paper No. 2004-2270, Jun. 2004.

Outline

- Basic Equations and Kinetics
- Transport Modeling
- Turbulent Heating and Transition
- Afterbody Modeling
- Radiation/Flowfield/Ablation Coupling
- **Uncertainties and Sensitivities**
- Validation and Verification

Why Uncertainty Analysis?

- **Evaluate uncertainties associated with heating predictions**
  - judge if the predictions have sufficient reliability
  - move toward day where error bars are placed on CFD
- **Identify target areas where research should be directed to achieve maximum payoff**
  - based on the uncertainty contributions, technology gaps can be prioritized
- **Experiment design, error analysis and data reduction**
  - if reliability is insufficient, targeted experiments can be designed
  - in order to reduce model uncertainties, the required level of experimental precision can be specified
- **Probabilistic design and risk analysis**
  - a deterministic aerothermal prediction has unknown reliability
  - as designs become more critical, the practice of designing to all unfavorable events occurring simultaneously may produce unacceptable weight.
  - a probabilistic analysis can be used to determine a realistic factor of safety corresponding to a desired level of TPS risk tolerance.

Types of Uncertainty

Parametric Uncertainties:

- Reaction rate coefficients
- Thermal relaxation rates
- Vibration-chemistry coupling
- Transport properties
- Other parameters

Stochastic Variabilities

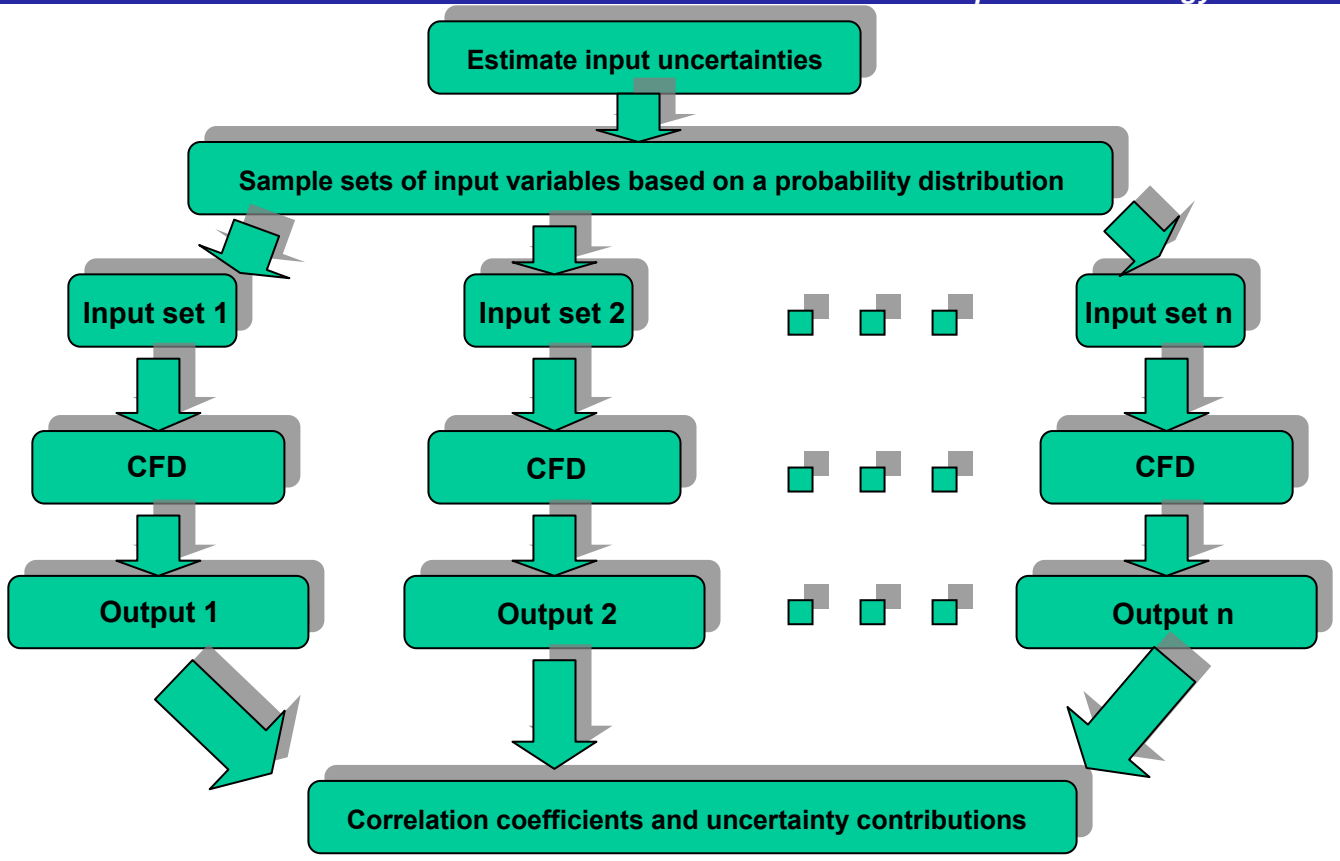
- Natural fluctuations in atmospheric conditions
- Trajectory adjustments
- Other unanticipated changes in the physical environment

Structural Uncertainties:

- Basic modeling assumptions
- Numerical representation
- Other simplifications

⇨ Parametric and stochastic uncertainties can be investigated probabalistically, but structural uncertainties can only be exposed through testing

Monte-Carlo Approach
to Uncertainty/Sensitivity Analysis



Types of Uncertainty

Parametric Uncertainties:

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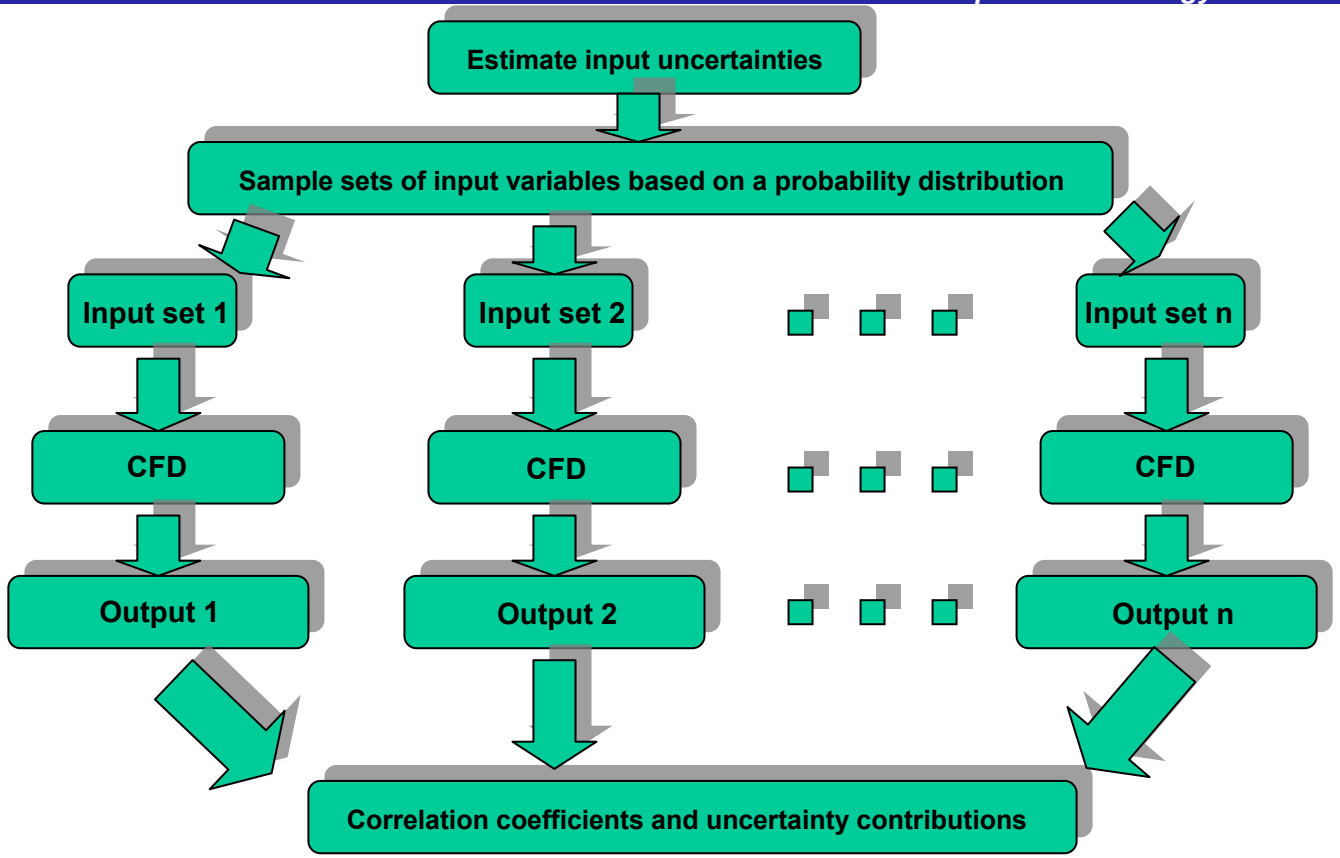
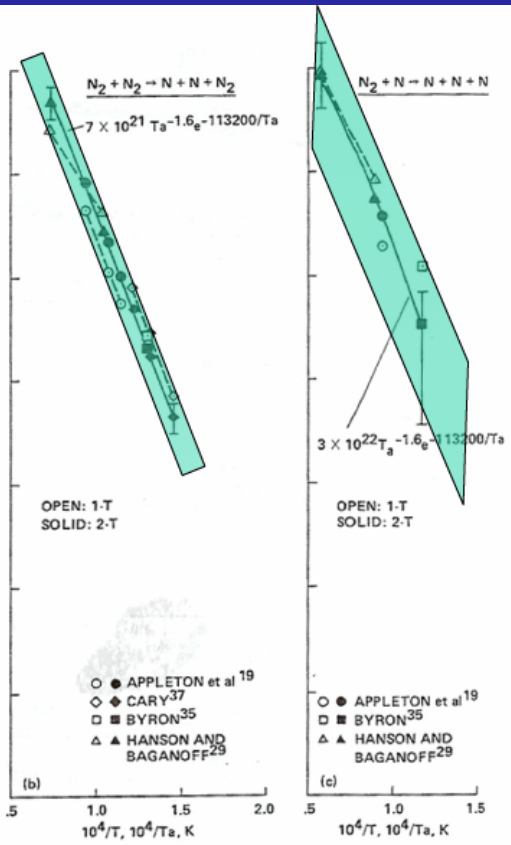


Assigning Input Uncertainties

Example: N_2 Dissociation Rate



Methods of Assigning Uncertainty

1) Combine sources of data & compute standard error
2) Evaluate experimental set-up, data reduction, or theoretical formulation
3) Recommendations in review articles
4) Quoted uncertainty in the data source
5) Expert judgment

For N_2 dissociation:

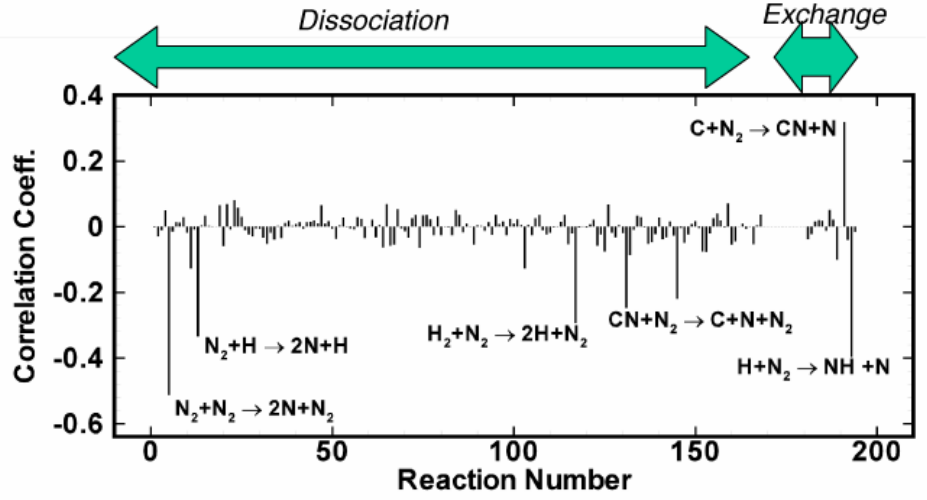
- **A few independent determinations exist using shock tube data from the 60s and 70s**
- **Data interpreted by Park using two temperature model**
- **Bands show resulting uncertainty in $N_2 + N_2$ and $N_2 + N$ dissociation rates**

Recent Example

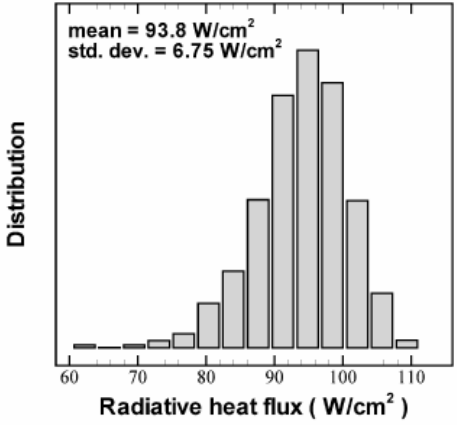
Titan Aerocapture Radiative Heating

- CN radiation dominates predicted aeroheating
- Determine sensitivity of radiative heating to reaction rates and other modeling parameters (total of 417 independent parameters)
- ~6000 CFD solutions run to determine heating distribution

Radiative heating sensitivities to reaction rates



Heating distribution



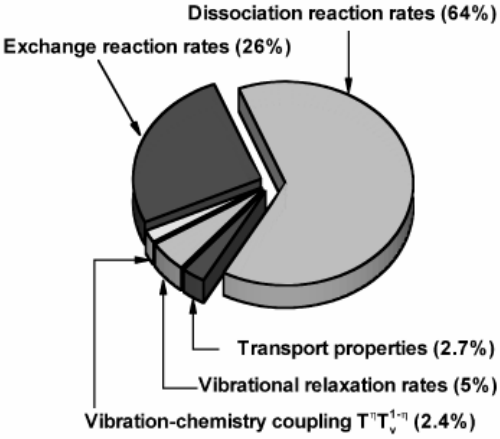
Most probable: 93.8 W/cm²
95% confidence: 81-104 W/cm²

Ref: AIAA 2004-2455

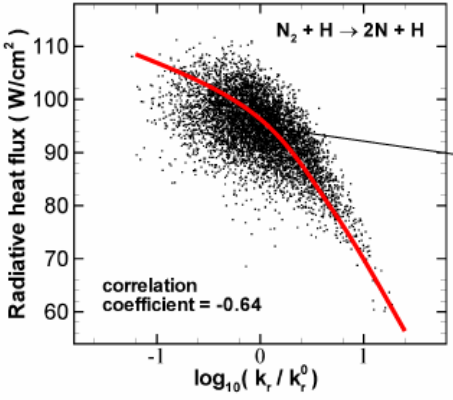
Recent Example

Titan Aerocapture Radiative Heating

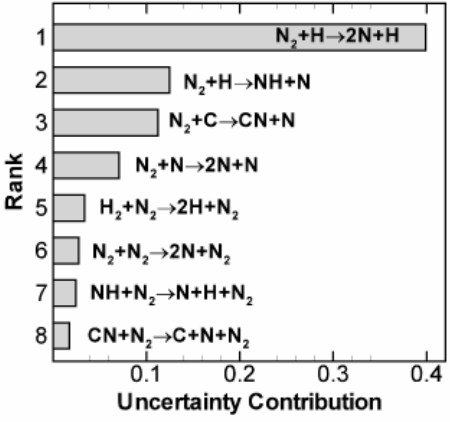
- Results indicate that majority of uncertainty in radiative heating is due to reaction rates
- One binary interaction (N_2 + H) is responsible for 55% of total parametric uncertainty
- Stochastic uncertainties were not explored (but they could be)



Sample Correlation Plot



Slope change in trend line indicates nonlinearity



Ref: AIAA 2004-2455

For Further Reading:
Uncertainty and Sensitivity

- Blottner, F., "Accurate Navier-Stokes Results for the Hypersonic Flow over a Spherical Nosetip," *Journal of Spacecraft and Rockets*, Vol. 27, No. 2, March 1990, pp. 113-122.
- Roache, P., "Quantification of Uncertainty in Computational Fluid Mechanics," *Annual Review of Fluid Mechanics*, Vol. 29, 1997, pp. 123-160.
- Mehta, U., "Some Aspects of Uncertainty in Computational Fluid Dynamics Results," *Journal of Fluids Engineering*, Vol. 113, 1991, pp. 538-542.
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- Saltelli, A., Chan, K., and Scott, E., Sensitivity Analysis, Wiley, New York, 2001.
- Dec, J. and Mitcheltree, R., "Probabalistic Design of a Mars Sample Return Earth Entry Vehicle Thermal Protection System," AIAA Paper No. 2002-0910, Jan. 2002
- Bose, D., Wright, M., and Gökçen, T., "Uncertainty and Sensitivity Analysis of Thermochemical Modeling for Titan Atmospheric Entry," AIAA Paper No. 2004-2455, Jun. 2004.

Outline

- Basic Equations and Kinetics
- Transport Modeling
- Turbulent Heating and Transition
- Afterbody Modeling
- Radiation/Flowfield/Ablation Coupling
- Uncertainties and Sensitivities
- **Validation and Verification**

What Does it Mean?

- **Verification: Are we solving the equations right?**
  - **Is the code employed accurate and correct**
  - **Is the solution obtained accurate and correct**

- **Validation: Are we solving the right equations?**
  - **Comparison of computational solution with experimental data**

Ref: ***AIAA Journal,*** **Vol 41, No. 1**

Verification:
Solution Accuracy

- **Compute cases for which analytical solutions exist**
  - Flat plate boundary layers, etc.
  - Typically analytical solutions exists only for trivial cases
- **Method of manufactured solutions**
  - Generate artificial solutions designed to test physics and numerics in codes
    - time consuming process, but valuable for certain applications
- **Standardized benchmark cases**
- **Code-to-code comparison**
  - Bootstrap from an already verified code by ensuring that both codes get the same result for a suite of test cases

Verification:
Minimizing Discretization Error

- **Grid resolution studies**
  - Ensure grid independence of solution
  - Do not stop resolution study when computation matches data!
- **Richardson extrapolation**
  - Solutions on several grids, coupled with an explicit knowledge of the exact order of accuracy of the method, can be used to estimate “exact” solution
    - time consuming process, but valuable for certain applications
    - for reacting hypersonic flows the exact order accuracy of method is not the formal order of accuracy
    - determination of exact order of accuracy can be very time consuming in itself, and will in general be problem-dependent
- **Grid convergence index (GCI)**
  - Developed for low speed flows, recently begun to be adapted for hypersonics

Validation:
Suitability of Physical Models to Problem

- **Frequently requires engineering judgment combined with sensitivity analysis**
  - Many models exist in literature for most physical phenomena of interest
  - Parametric analysis of suitable models can show whether choice is significant
    - Effort can then be focused on those areas where choice of model has a large impact on parameter of interest
- **Structural uncertainties cannot be detected parametrically**
  - All of the existing models may be incorrect for a given problem
  - Comparison to experiment is the only way to uncover such structural failings

Validation:
Comparisons to Ground/Flight Data

- **What can we do?**
  - **comparisons are generally good (within 15%) for acreage laminar forebody heating**
  - **reasonable agreement is generally obtained for acreage turbulent forebody heating (within 25%)**
  - **recent work on afterbody heating has demonstrated good agreement for laminar, non-ablating surfaces (within 20%)**

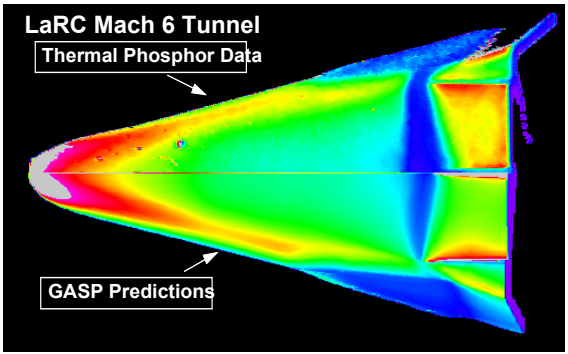
- **What can't we do?**
  - **little data exist to permit validation of CFD ability to predict the following:**
    - high energy entries (e.g. Pioneer Venus, Galileo)
    - local effects (gaps, protuberances, fins)
    - hypersonic turbulent separated flows

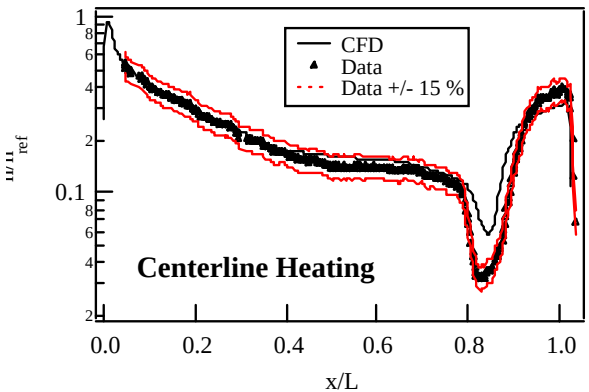
Ground Testing Facilities

- **No ground-based facility can simultaneously reproduce all necessary flight parameters**
- **General categories:**
  - **Wind tunnels (e.g. LaRC Mach 6, Mach 10, Mach 20 He)**
    - advantages: long test time, controlled environment
    - disadvantages: low enthalpy, cold models, fixed test gas
  - **Shock tunnels/expansion tubes (e.g. T3, T5, LENS, HEG)**
    - advantages: high enthalpy, variable gas mixtures
    - disadvantages: short test time, cold models
  - **Arc jets (e.g. Ames IHF/AHF/PTF, JSC, Sirocco)**
    - advantages: high enthalpy, long test time
    - disadvantages: cost, free stream characterization
  - **Free flight (e.g. Ames ballistics range, Eglin AFB range)**
    - advantages: quiescent freestream, no sting
    - disadvantages: model size, obtaining spatially resolved data

Validation:
Wind Tunnel Data

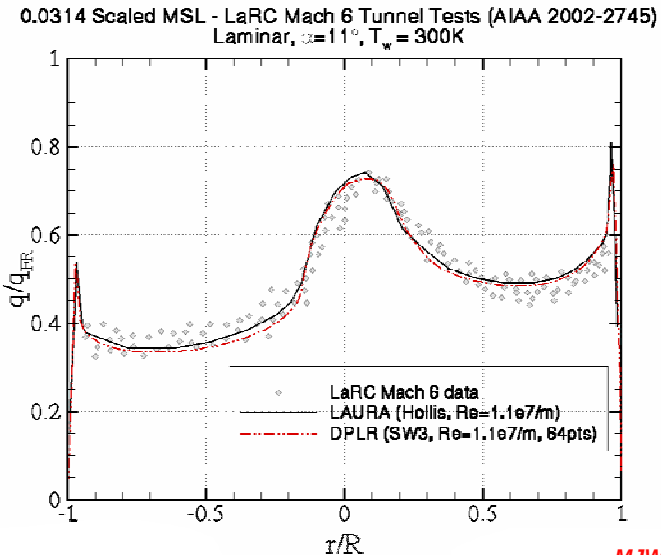
X38 Comparison to Tunnel Testing





Refs: AIAA Papers 97-2478, 97-2475

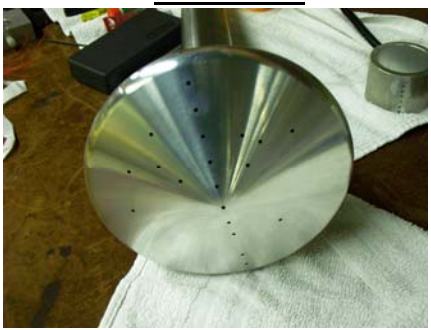
- Comparison to available data is an ongoing code validation activity
- Agreement between wind tunnel data and CFD is generally excellent (within 15%) for laminar acreage heating



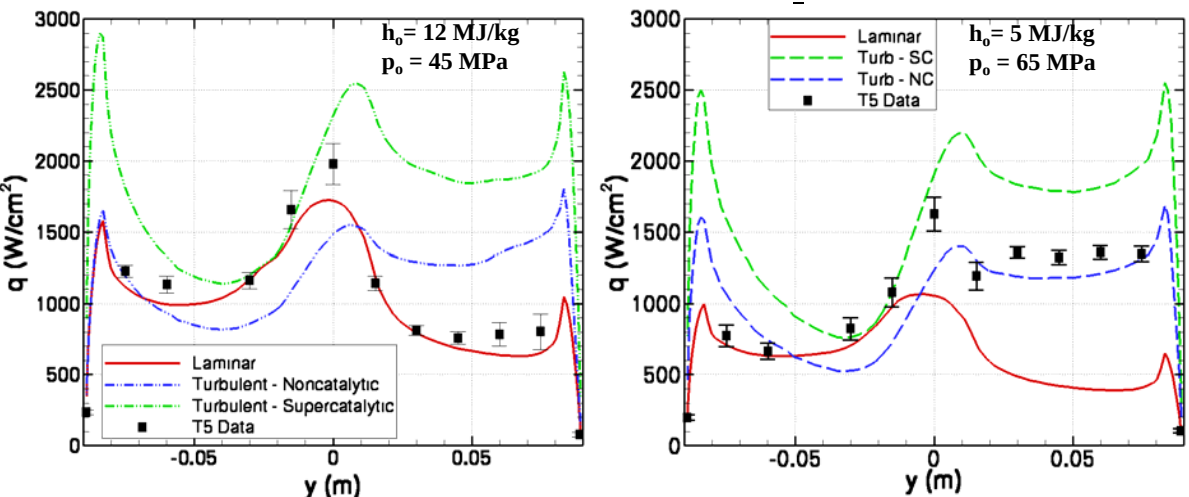
Validation:
Shock Tube Data

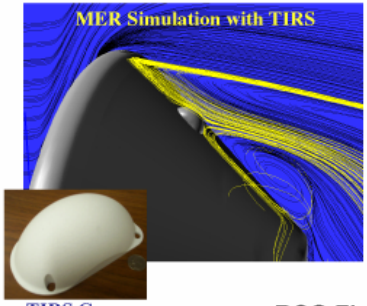
- Agreement between shock tube data and CFD is generally excellent within 15% for laminar acreage heating
- Agreement with turbulent acreage heating is generally within 20-25%

MSL Model



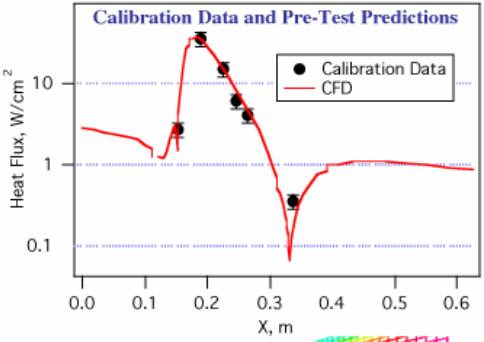
MSL Testing in CalTech T5 tunnel (CO_2 test gas)

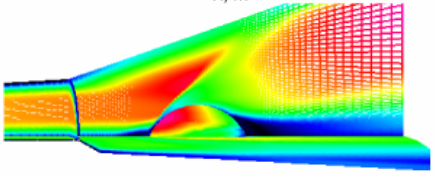




TIRS Cover

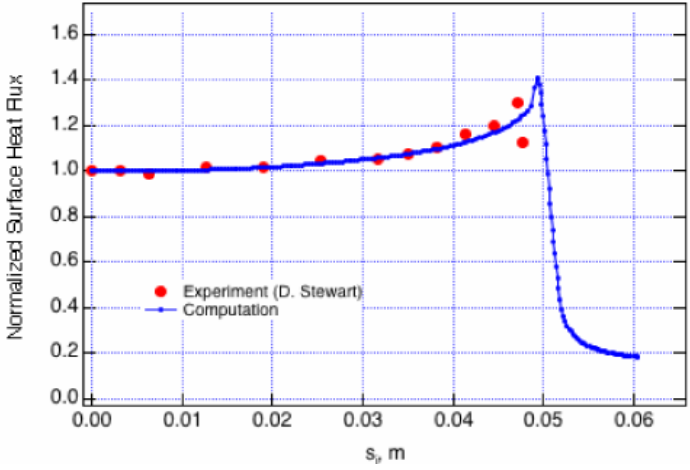
- Agreement to within 20% is possible





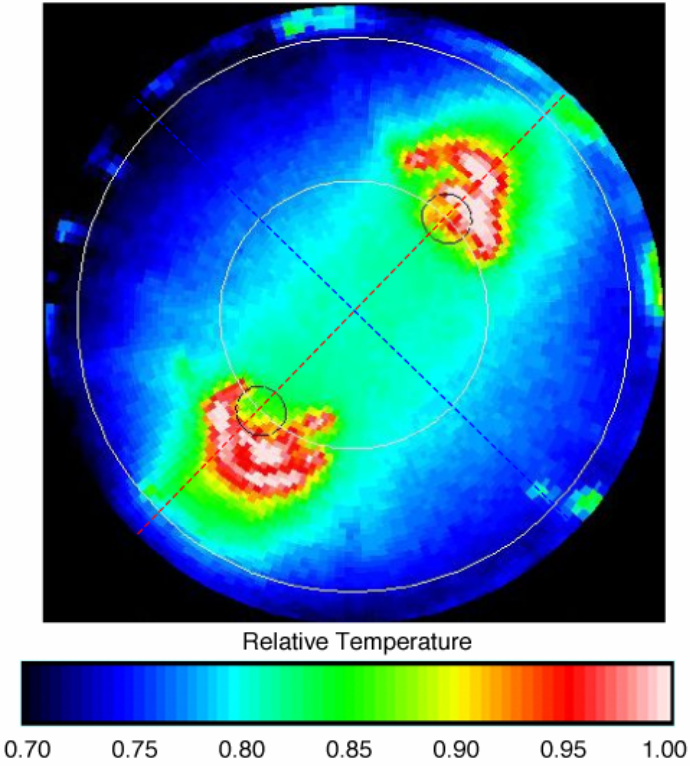
Panel Test Facility (PTF) simulations
h_o=9.3 MJ/kg, p_o=70 kPa

RCG Flat-faced Cylinder (D = 10.16 cm)
AHF 24-Inch Nozzle, p_o = 5.6 atm, h_o = 21 MJ/kg

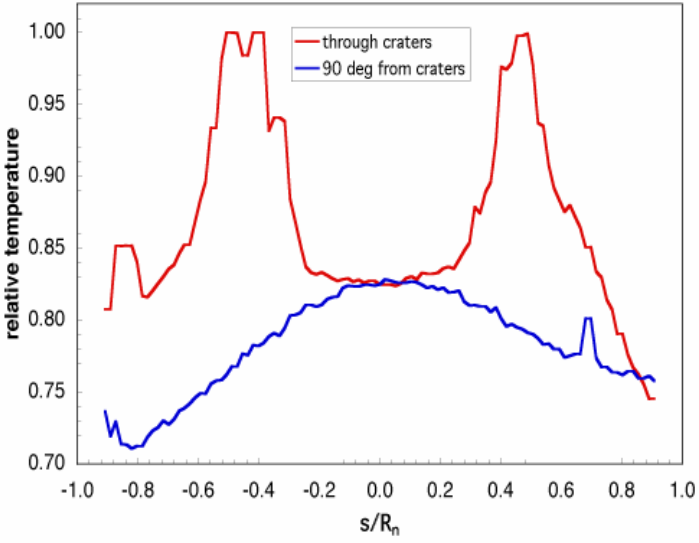


Validation:
Free Flight Data

Cavity Induced Transition



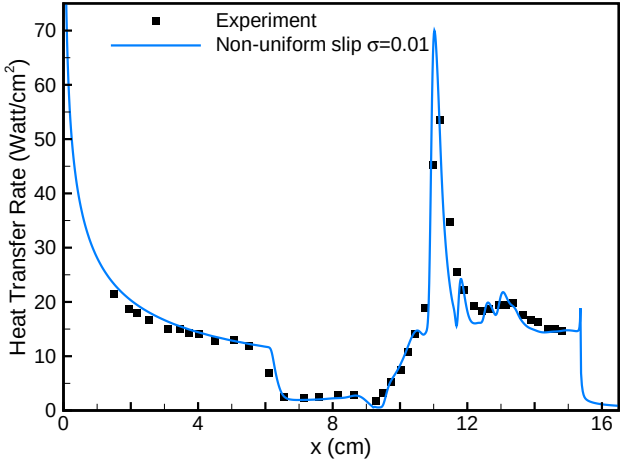
Graphite Nose, R_n = 18.5 mm
Two Cavities at ϕ = 20°, 180° Apart
Cavity Radius = 1.19mm = 0.064R_n



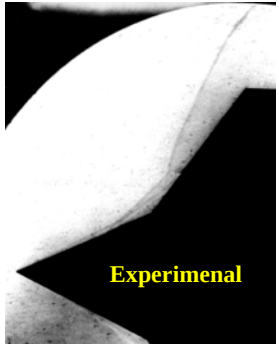
- **Thermal imagery enables quantitative heat transfer measurements**
- **Capability still under development (paper to be given at workshop)**

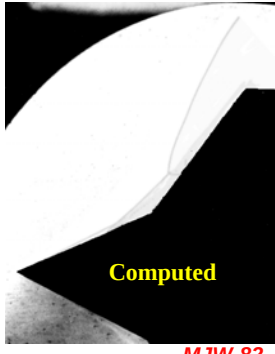
Validation:
AGARD WG10

- **Several test cases chosen for aerothermal CFD validation**
- **Experiments run in several facilities, "blind" computations solicited**
- **Results were generally encouraging, although some surprising differences were observed**
- **Example here is a shock interaction over a double cone geometry, which was previously shown to be extremely sensitive to details of the finite-rate relaxation processes occuring in the separation region**
- **Tests run at LENS facility, computations performed by Nompelis et al. (University of Minnesota)**



Schlieren Images





Refs: AIAA Paper 2002-0581

Heritage Flight Data

Dedicated Flight Tests

- NASA
  - Fire I&II, Apollo, Reentry F, PAET
- Other American
  - Military slender cone testing
  - Military funded basic research (BSUV, DEBI)
- European
  - MIRKA, ARD
- Japanese
  - OREX

Science Missions with Flight Data

- NASA (Viking, Pathfinder, Galileo, Shuttle)

For Further Reading:
Validation and Verification

- Gnoffo, P., "A Code Calibration Program in Support of the Aeroassist Flight Experiment," AIAA Paper 89-1673.
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- Roy, C., Oberkampf, W., and McWherter-Payne, M., " Verification and Validation for Laminar Hypersonic Flowfields, Part 2: Validation," AIAA Journal Vol. 41, No. 10, 2003, pp. 1944-1954.

For Further Reading:
Flight Data

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