Session: Major Efforts in Nonequilibrium Flows (Invited)

9:00 AM-9:30 AM
Oral Presentation. Modeling, Measurements, and Fundamental Database Development for Nonequilibrium Hypersonic Aerothermodynamics  
D. Bose

9:30 AM-10:00 AM
G. V. Candler

10:00 AM-10:30 AM
AIAA-2012-0725. Review of the VKI research on nonequilibrium phenomena in hypersonics  
T. E. Magin; O. Chazot

10:30 AM-11:00 AM
Oral Presentation. High-Speed Flow Studies at ITAM  
M. S. Ivanov; A. Maslov; Y. Bondar

11:00 AM-11:30 AM
Oral Presentation. Review of Experimental Studies Being Conducted in LENS Shock and Expansion Tunnels to Evaluate the Characteristics of Real Gas and Plasma Flows  
M. S. Holden; M. G. MacLean; R. A. Parker; T. P. Wadhams

11:30 AM-12:00 PM
AIAA-2012-0726. Study of hypervelocity non equilibrium flows in impulse facilities  
R. G. Morgan
Modeling, Measurements, and Fundamental Database Development for Nonequilibrium Hypersonic Aerothermodynamics

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Acknowledgements

- Aaron Brandis, Brett Cruden, Dinesh Prabhu, Rich Jaffe (NASA Ames)
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- Chris Johnston, Artem Dyakonov (NASA Langley)
- Winifred Huo (Huo Consulting)
- Prof. Doug Fletcher (University of Vermont)
- Matt MacLean (CUBRC)
Nonequilibrium Phenomena in Hypersonic Flow

- Nonequilibrium occurs when time scales of thermochemical processes are longer than fluid transport time scale
- Nonequilibrium conditions generally occur in low pressure environment and/or in flows with high gradients
- Nonequilibrium phenomena occurs
  - in shock wave
  - in boundary layer
  - on surfaces (catalycity, ablation)
  - in expanding flow (nozzles, plumes, wakes, etc.)
Impact of Nonequilibrium Phenomena

Radiative Heating: Nonequilibrium radiation can be several fold larger than equilibrium radiation

Convective Heating: Wall catalycity can raise aeroheating by several factors

Ablation: Nonequilibrium oxidation can significantly reduce recession

Aerodynamics: Nonequilibrium can alter trim angles by over 1-deg
Nonequilibrium phenomena exists at all flight regimes, however, its impact is dependent on flow enthalpy, vehicle size, pressure, etc.

In the upper right of the figures, nonequilibrium phenomena is driven by nonequilibrium ionization and non-Boltzmann kinetics.

Nonequilibrium can be important in the lower left part of the figure as well where it affects shock shapes and vehicle aerodynamics.
NASA Research Activities in Nonequilibrium

Fundamental Database
- Atomic Spectra
- Diatomic Spectra
- Triatomic Spectra
- Energy Transfer
- Reaction Cross Sections
- Electron Impact Cross Sections
- Radiative Processes

Measurements
- Shock Tube Measurements
- High Enthalpy Aerothermal Testing
- Gas-Surface Interactions
- MSL Entry Flight Instrumentation
- Arcjet Testing for Ablation
- Facility Characterization and Diagnostics

Modeling
- HyperRad Code
- Mars Chemistry
- Non-Boltzmann Excitation
- VUV Radiation
- Generalized Gas-Surface Interaction
- Nonequilibrium Ablation
- DSMC
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Ab-initio Computations of Triatomic Potentials

- **CO₂ Excitation & Dissociation:**
  - A critical process with impact on re-entry aerodynamics, IR radiation in the wake, freestream kinetics in high enthalpy tunnels
  - It is likely that CO₂ singlet → triplet transition is the bottleneck in CO₂ dissociation; its rate is being determined to describe CO₂ dissociation and recombination process

- **C₃ and C₂H Potentials:**
  - Key ablation products in boundary layer that significantly absorb incident shock layer radiation
  - C₃ Potential energy surfaces for two key transitions that absorb radiation are being characterized
    - Swings system (X¹Σ⁺ → A¹Πu): near UV 300-430 nm
    - (¹Σ⁺ → ¹Σ⁺⁺): VUV transition 140-190 nm

Content provided by Rich Jaffe (NASA Ames)
**N₂ Collisional Energy Transfer and Dissociation**

- **State-Specific Cross Sections**
  - Ab-inito potential energy surfaces generated for N₂+N and N₂+N₂ systems
  - Energy transfer and dissociation cross sections determined for binned ro-vibrational energies

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**Evaluation of Park’s TTv Vibration-Dissociation Model**

**Vibrational State-Specific Reaction Rate Quasi Classical Trajectories**

*Content provided by Rich Jaffe (NASA Ames)*
• **Nonequilibrium Electronic Excitation and Ionization:**
  
  - In low pressure flight regimes (occurs in Mars, Titan, and Earth entry), the electronic states of radiating species do not reach a Boltzmann equilibrium, and generally reduce radiation by a factor 2 or more.
  
  - A nonequilibrium model requires a collisional-radiative or a QSS (quasi steady state) model

• **Ab-Initio Cross Sections:**
  
  - Electron Impact Reactions:
    
    \[ e + M(X) \leftrightarrow e + M(A) \]
    
    \[ e + M \leftrightarrow M^+ + 2e \]

  - Photoionization and radiative recombination
    
    \[ e + M^+ \leftrightarrow M + h\nu \]

  \[ M : N, N_2, O \]
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Shock Tube Measurements

Developed in the mid 1960s; operational in early 1970s

- 10.16 cm dia. aluminum driven tube
- Unique capabilities
  - Shock speed range (up to 46 km/s)
  - Driven gas composition
  - Optical instrumentation with calibrated intensity measurements from VUV to mid-wave IR
Flight Relevance

- Emission measurements made at several planetary entry conditions
- ~800 images of detailed and quantified emission intensities obtained
- Unprecedented levels of model validation underway for both equilibrium and nonequilibrium radiation for Earth and Mars entry
  - Mars entry radiation is dominated by nonequilibrium phenomena

Figure provided by Brett Cruden (ERC-NASA Ames)
Nonequilibrium Relaxation

- Emission measurements made at Earth and Mars entry conditions
- ~800 images of detailed and quantified emission intensities obtained
- Unprecedented levels of model validation possible for both equilibrium and nonequilibrium radiation for Earth and Mars entry

Electron Density Profile Behind a 10 km/s Shock Inferred from Atomic Line Broadening

Figures provided by Brett Cruden (ERC-NASA Ames)

Nonequilibrium Vibrational and Rotational Temperature Profiles Inferred from CN violet Spectrum

Speed: 8.631 km/s
Pressure: 0.1 Torr
CO Fourth Positive Vacuum UV Radiation

- VUV radiation dominates radiative heating at high speed entries
- CO4+ radiation in the VUV spectrum measured for model validation
- Nonequilibrium excited state population at low pressure 0.1 Torr may be responsible for over prediction

Figures provided by Aaron Brandis (UC-Santa Cruz-NASA Ames)
High Enthalpy Aerothermal Measurements

- High enthalpy test campaign underway in CUBRC LENS XX expansion facility with freestream free of nonequilibrium
- High enthalpy aerothermal thermal tests in CO2 environment has enabled validation of
  - CO2 chemistry mechanism and energy transfer
  - Catalycity models

Figures provided by Matt MacLean (CUBRC) and Dinesh Prabhu (ERC-NASA Ames)
Gas-Surface Interaction Measurements

- Fundamental measurements in reacting boundary layers at flight relevant condition are rare
- University of Vermont (Prof. Doug Fletcher) 30 kW ICP Torch produces subsonic plasma representative of stagnation conditions in flight
- Two-photon LIF measurements of temperature and species density are made in the boundary layer
- Flight materials in CO₂ environment are being evaluated for high mass Mars entry system

Content provided by Prof. D. Fletcher (University of Vermont)
Mars Entry Aero/Aerothermal/TPS Response Measurements: MEDLI Project

- Mars Science Laboratory (MSL) heatshield instrumented with thermocouples and pressure sensors (Aug 2012 entry)
- Unprecedented opportunity to obtain flight data at Mars in nonequilibrium flow to validate
  - aerothermal models
  - aerodynamic models
  - ablation models
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HyperRad Radiation Code

- **HyperRad** is a new radiation code reliant on newly developed **ab-initio** database
  - Improved atomic lines; almost 5X as many lines as available in 2009 NEQAIR
    - Careful merger of NIST, Vanderbilt, and Top-Base line datasets
  - Improved Stark width and shift database
  - Line list driven molecular databases
  - Improved bound-free radiation routines based on ab initio cross sections
  - Three-dimensional radiation transport
  - Coupled thermal, chemical, and radiation nonequilibrium for excited state populations
  - Designed for high end computing and parallelization
  - First version released in 2011
  - **HyperRad** Development Team: Wray, Liu, Schwenke, Chaban, Huo, Carbon, Jaffe (NASA Ames)

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**Improved Line Database in HyperRad**

**Temperature Dependence of Stark Width**

Comparison of various CO4+ databases at 0.25 Torr
Currently used Mars entry chemistry mechanism was proposed by Park and co-workers nearly 20 years ago, based on very little measured data.

With detailed shock tube measurements and testing in high enthalpy facilities, it is now possible to significantly improve the chemistry model.

Content provided by Chris Johnston (NASA Langley)
Non-Boltzmann Excitation Modeling

Number Density of Excited CO A\(^1\Pi\)

Wall Directed Radiative Flux

Profiles along stagnation streamline showing influence of non-local absorption on excited state chemistry and radiation

Conditions: 7 km/s, 10\(^{-4}\) kg/m\(^3\), 5m diameter, 60-deg sphere cone

Excited State Chemistry Mechanism

1. \(\text{CO}(X^1\Sigma^+\text{)} + M \rightarrow \text{CO}(A^1\Pi) + M\)
2. \(\text{CO}(a^3\Pi_r\text{)} + M \rightarrow \text{CO}(A^1\Pi) + M\)
3. \(\text{CO}(X^1\Sigma^+\text{)} + e^- \rightarrow \text{CO}(A^1\Pi) + e^-\)
4. \(\text{CO}(X^1\Sigma^+\text{)} + e^- \rightarrow \text{CO}(a^3\Pi_r\text{)} + e^-\)
5. \(\text{CO}(a^3\Pi_r\text{)} + e^- \rightarrow \text{CO}(A^1\Pi) + e^-\)

- Non-Boltzmann modeling, integrated with CFD (HARA and LAURA), is being applied to model radiative heating environment on a high mass Mars entry system
- Validation data at low pressures to support modeling is expected from Ames 24-in shock tube

Content provided by Chris Johnston (NASA Langley)
Concluding Remarks

• Modeling of nonequilibrium phenomena is complex and must be supported by experimental measurements and fundamental database development
• Model development based on fundamental physics as well as phenomenological approaches are needed
• While NASA is supporting a wide range of research activities in nonequilibrium phenomena, several key areas lack a critical-mass (e.g. diagnostics development, DSMC, ...)
• NASA research in nonequilibrium phenomena for outer planet entries has languished
• We invite partnerships as much of our data and results can be shared openly

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