DSMC Shock Simulation of Saturn Entry Probe Conditions

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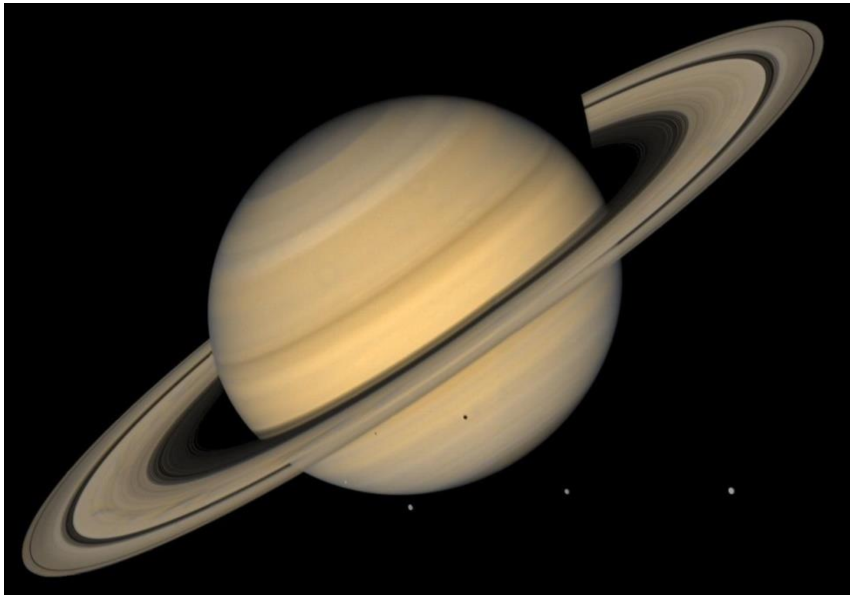
Work supported by NASA Space Technology Research Fellowship program. Computing resources provided by the Texas Advanced Computing Center.

Saturn Entry Probe

- The 2013 Decadal Survey identified a probe mission to Saturn as a high priority.
- Saturn entry conditions:
  - High speed trajectories of ~25-29 km/s.
  - H_2-He atmosphere mixture.
- Convective heating accounts for most of the total heat flux during entry.
- Significant uncertainty in the prediction of radiative heating.[1]

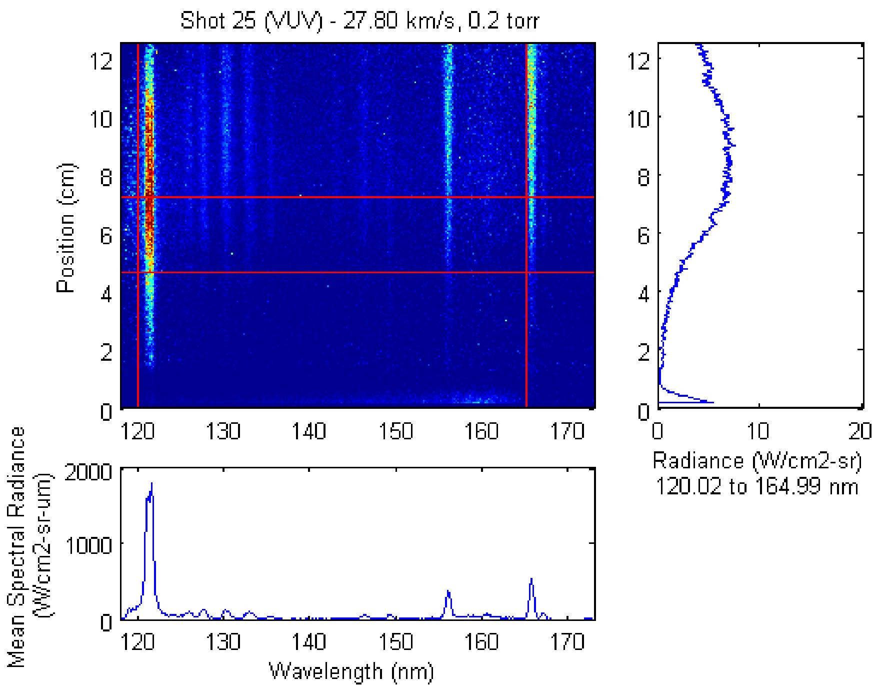


[1]Palmer, Prabhu, and Cruden, "Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method"
http://nssdc.gsfc.nasa.gov/planetary/image/saturn.jpg

Saturn Entry Experiments

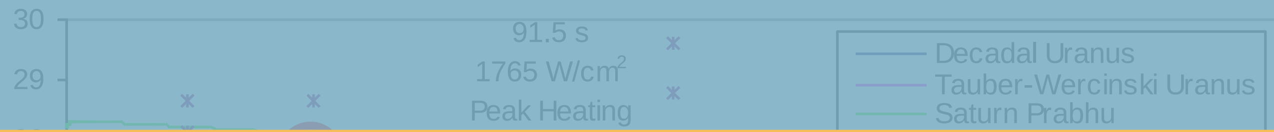
- Recent shock tube experiments of a H_2-He mixture have been performed in the NASA Ames Electric Arc Shock Tube (EAST)[1].
  - Spectrometers measured emission in the VUV, UV, visible, and near-IR ranges.
  - H and H_2 emission measured.
- Observations
  - Post-shock region did not equilibrium by 5 cm.
  - An induction period occurred several cm behind shock.
  - Radiance in the VUV range was observed in the pre-shock region indicating diffusion of hydrogen upstream of the shock.

27.8 km/s, 0.2 Torr, VUV range



[1]Cruden and Bogdanoff, "Shock Radiation Tests for Saturn and Uranus Entry Probes"

Saturn Entry Experiments



Motivation:

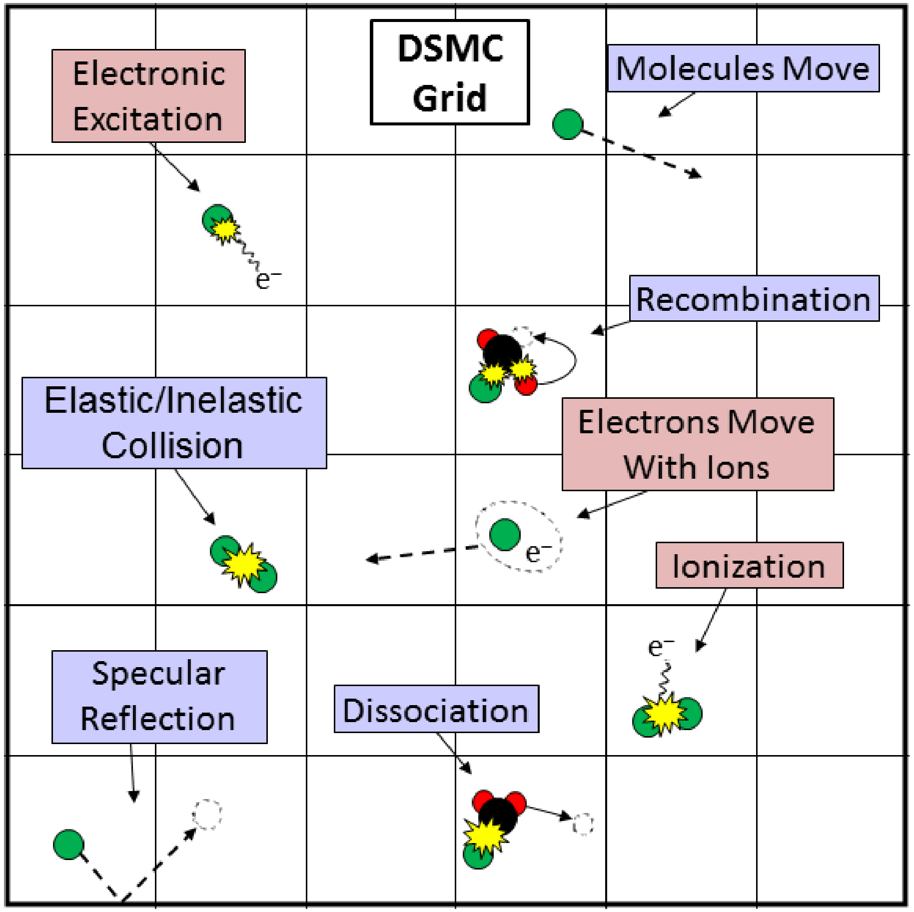
- Investigate the influence of non-equilibrium phenomena on Saturn entry conditions.
- Identify physical mechanisms that explain the EAST experimental results.
  - Direct Simulation Monte Carlo (DSMC) method is required to model non-continuum features.
- Complete a first attempt of modeling a high temperature H_2-He mixture with DSMC.
  - Develop high temperature parameters and identify areas requiring improvement.

- DSMC simulations of Shot 25 and Shot 17 are performed here.

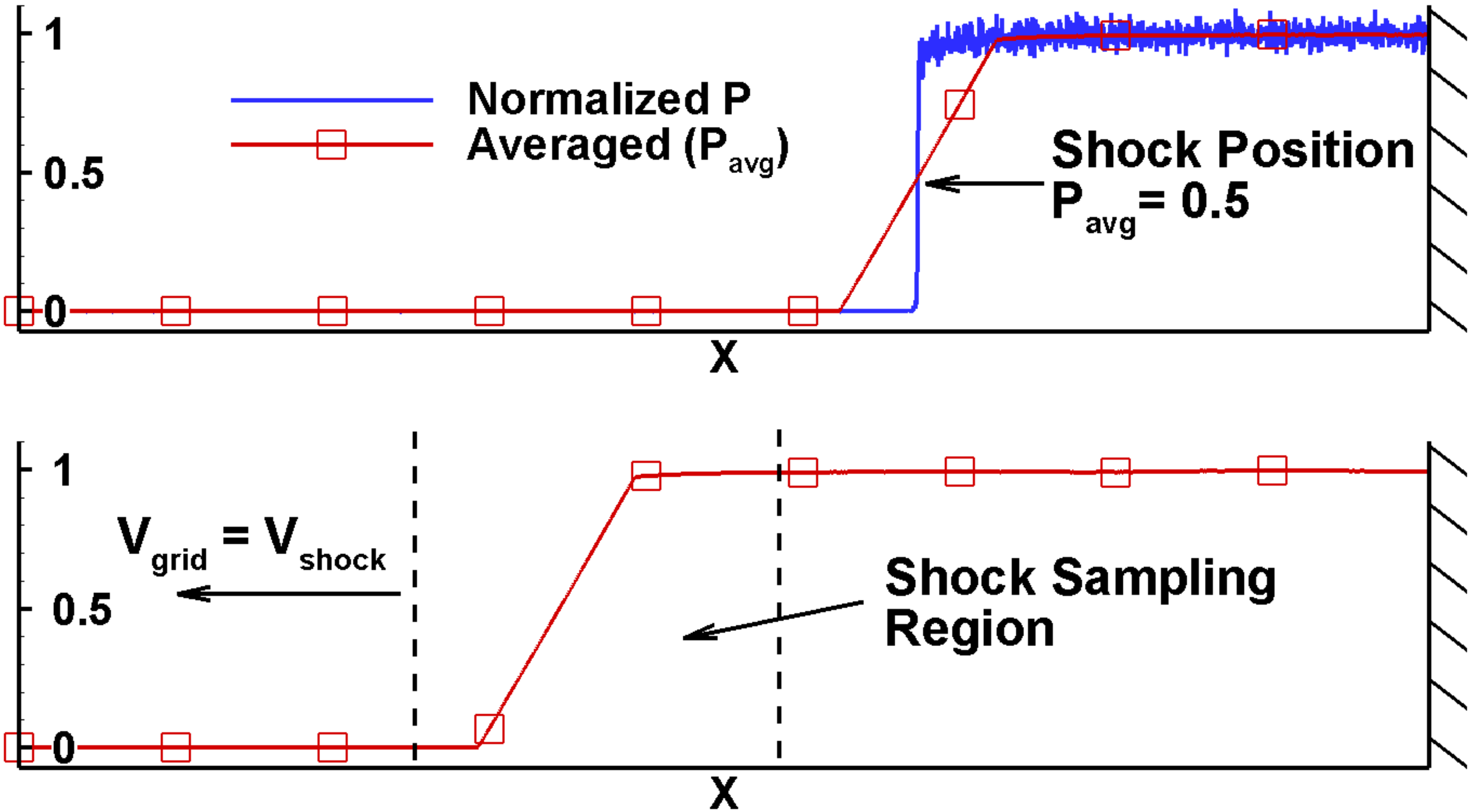
[1]Cruden and Bogdanoff, "Shock Radiation Tests for Saturn and Uranus Entry Probes"

Direct Simulation Monte Carlo (DSMC)

- Stochastic model of individual particles and their physics.
  - Each DSMC 'particle' represents many real particles.
  - Can model large non-equilibrium regions.
- Probabilistic approach
  - Simplified models use cross sections and probabilities determined from experiments.
- Applicable for rarefied flows
  - $Kn = {}^{\lambda}/_{D} > \ 0.01$
  - Continuum breaks down.
    - Must use Boltzmann equation.



1-D Unsteady Shock Simulation:

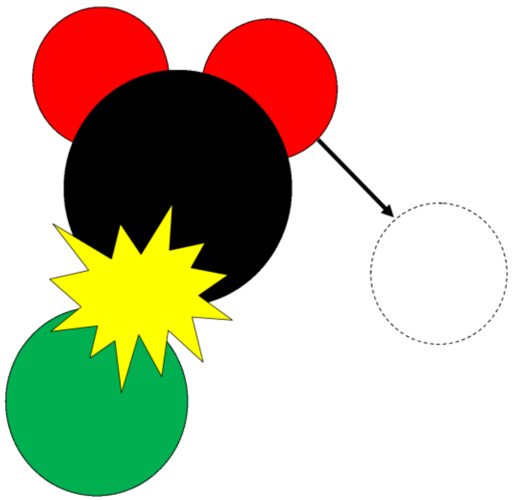


Electronic Excitation Model:

- Model scheme follows previous work by Liechty.[1]
  - Post-collision energy transfer is performed with an acceptance-rejection procedure following Larsen-Borgnakke.
  - Electronic energy and degeneracy parameters for each electronic level are required.
- *Electronic* temperature is currently modeled as the *electron* temperature.
  - Free electron kinetic energy is the only component in the electronic temperature.
  - Equilibrates rapidly with the translational temperature.
  - Misrepresents the non-equilibrium in the heavy particle electronically excited states.

[1]Liechty, D. S., and Lewis, M. J., "Extension of the Quantum-kinetic Model to Lunar and Mars Return Physics"

Collision Models:



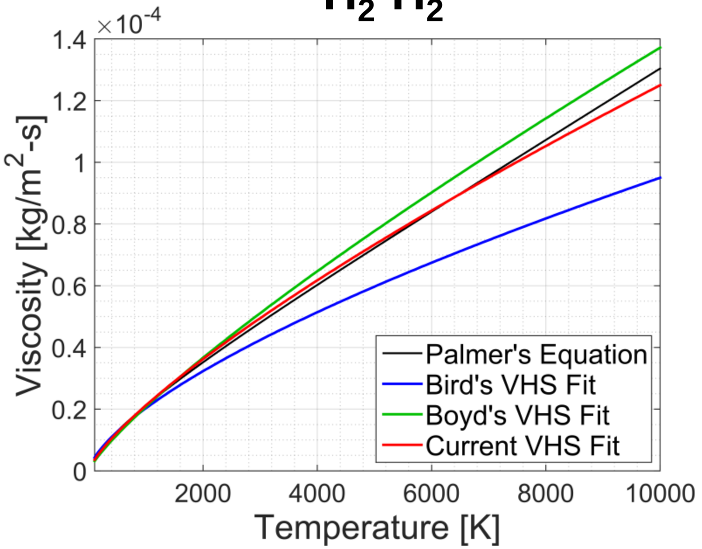
- Elastic collisions: Variable Hard Sphere (VHS)
- Inelastic collisions: Larsen-Borgnakke
  - Rotational relaxation: Parker's model
  - Vibrational relaxation: Millikan-White
- Chemical reactions: Total Collision Energy (TCE)
- Quasi-neutrality: Free electrons travel with ions

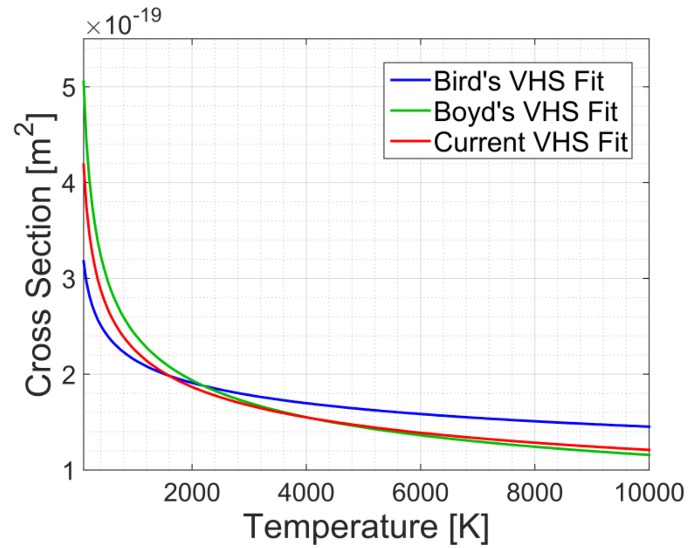
- From these models, over 50 input parameters are required for a 7-species H_2-He mixture (H_2, H, He, H_2^+, H^+, He^+, e^-).
  - Many of the DSMC parameters for H_2-He mixtures are outdated or unavailable in literature.
  - New or improved parameters were obtained when possible.

VHS Parameters:

- Previous general VHS parameters were published by Bird[1] and Boyd[2].
  - Collision partner independent.
  - Fit to low temperature data.
- Collision integrals provided by Palmer[3] were used to obtain high temperature VHS parameters.
- Species specific VHS parameters were curve fit for neutral-neutral and charge-neutral collisions.
- Charge-charge collision parameters were assumed to be identical to the charge-neutral parameters.
  - Necessary since the range of the VHS values is limited.
  - Introduces a small amount of error.

H_2-H_2

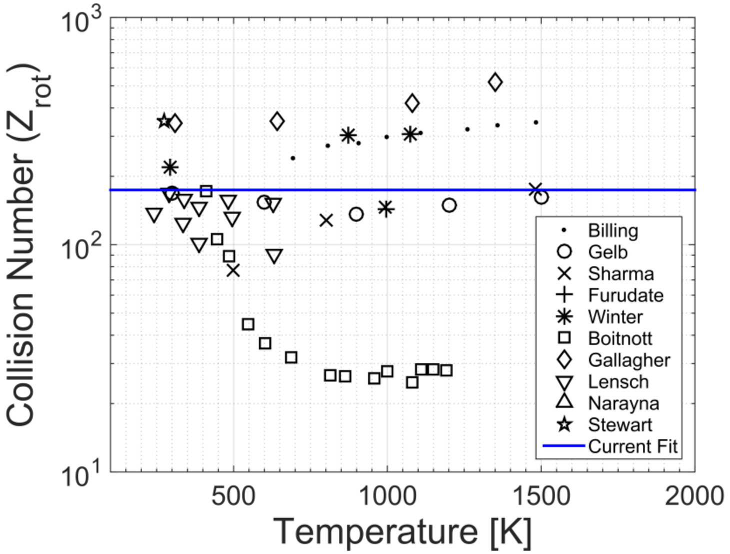




[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*
[2] I.D. Boyd, "Monte Carlo Simulation of Nonequilibrium Flow in a Low-power Hydrogen Arcjet"
[3] Palmer, Prabhu, and Cruden, "Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method"

H_2 Relaxation Parameters:

- Vibrational collision number is calculated from Millikan-White using Palmer's[1] parameters.
- A temperature dependent rotational collision number relationship is preferred (Parker).
  - H_2 is complex in rotation.
  - Compiled experimental data shows conflicting trends.
- Rotational collision number was "fit" to the data using a temperature independent value.
  - For a moderate temperature range between 200-1500 K, the fit was determined to be Z_{rot} = 174.



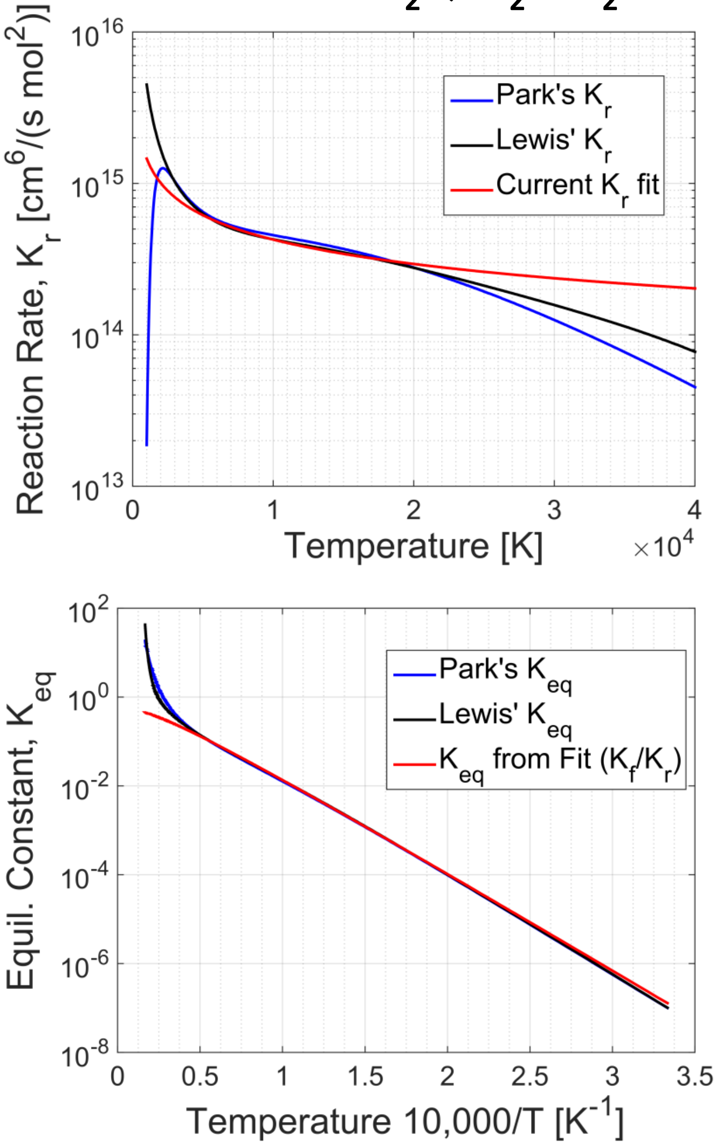
[1]Palmer, Prabhu, and Cruden, "Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method"

Chemical Reactions

Recombination Reaction Rates:

- Forward Arrhenius reaction rates (K_f) were obtained from Leibowitz[1].
- Reverse reaction rates (K_r) were calculated from the equilibrium constant (K_{eq}) and fit to an Arrhenius form.
  - Arrhenius fit is necessary for the TCE model.
- Neutral recombination reactions were fit to a temperature region between 5,000-20,000 K.
  - Over-predicts recombination at very high temperatures.
  - Under-predicts recombination at low temperatures.

$H + H + H_2 \rightarrow H_2 + H_2$



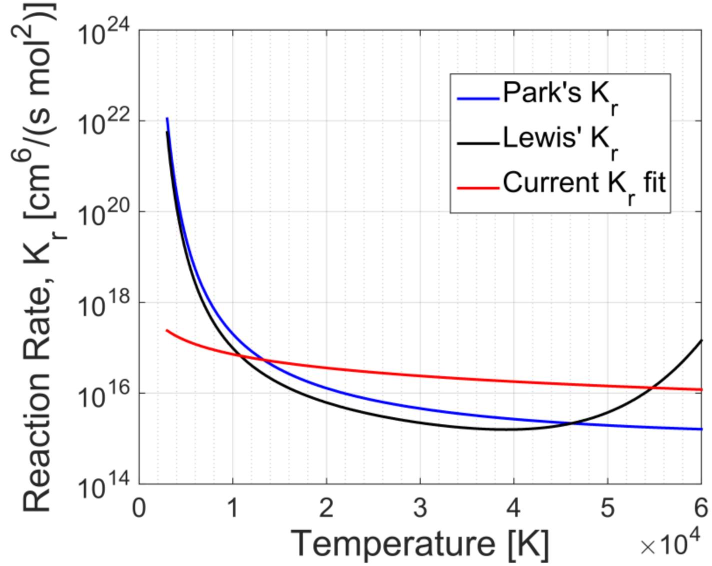
[1]L. P. Leibowitz and T. J.Kuo, "Ionizational Nonequilibrium Heating During Outer Planetary Entries"

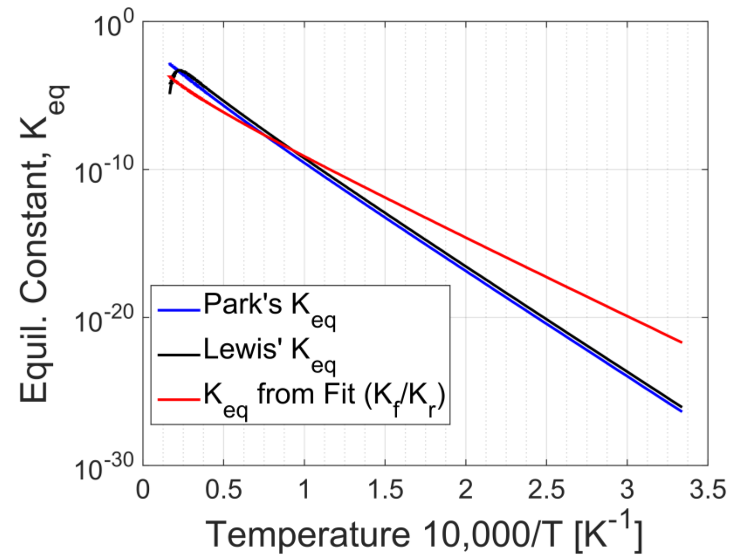
Chemical Reactions

Recombination Reaction Rates:

- Electron capture reaction rates are more difficult to curve fit.
  - Poor curve fits are due to constraints of the TCE model on the possible Arrhenius parameters.
- Large errors in the current electron capture rates are evident.
  - Over-predicts recombination at high temperatures.
  - Under-predicts recombination at low temperatures.
  - Leads to noticeable error in the equilibrium constant.

$H^+ + e^- + H \rightarrow H + H$





[1]L. P. Leibowitz and T. J.Kuo, "Ionizational Nonequilibrium Heating During Outer Planetary Entries"

0-D Relaxation Simulation

How can we compare the DSMC results directly to the experimental data?

- $T_{tr,o}$ = 20,000 K
- $T_{rot,o} = T_{vib,o} = T_{elec,o}$ = 300 K

- Experiments measure radiative emission.
  - Must post-process DSMC results with a radiative solver.
- Simulate Shots 25 and 17.
  - Compare simulated results to experiments for the VUV, UV, visible, and near-IR ranges.
  - Identify models and parameters for future improvement.

Radiation Model

NEQAIR:

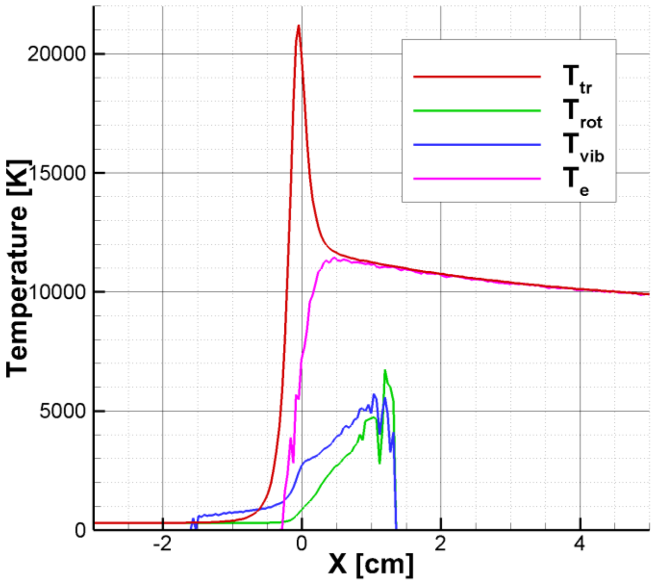
- Line-by-line, tangent slab computation along a line of sight.
- Multiple spectral and spatial broadening mechanisms are accounted for.
- Instruments convolutions are applied to mimic experimental smearing.
- Number densities and temperatures are passed to NEQAIR.
  - Four temperature calculation (T_{tr}, T_{rot}, T_{vib}, T_e).
  - Currently, only a Boltzmann calculation for H is available.

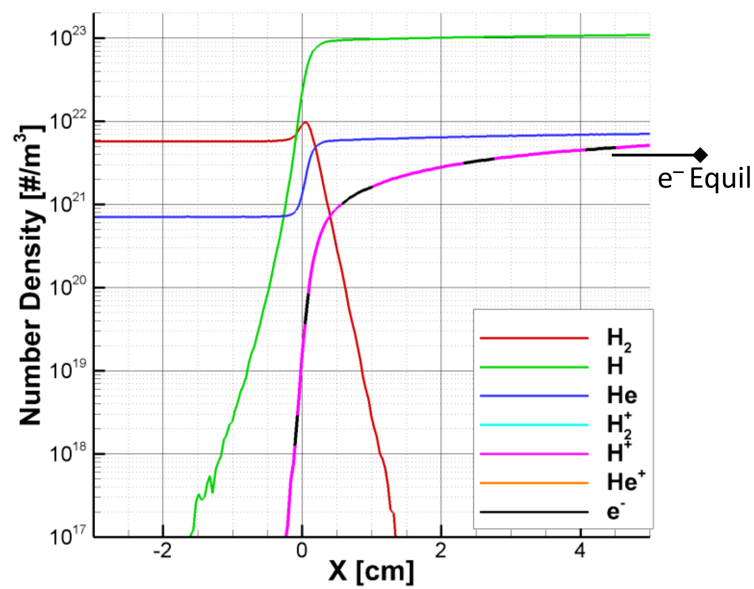
0.2 Torr Shock Simulation

EAST Shot 25:

- Shock velocity: 27.8 km/s
- Initial pressure: 0.2 Torr
- Initial temperature: 300 K
- Freestream 89% H_2: 11% He

- H_2 is dissociated by ~1.5 cm.
- H slightly diffuses upstream.
- Ionization begins immediately.
  - Degree of ionization is <10%.
  - Equilibrium has not been reached by 5 cm.
  - Higher electron number density than the experiment.
  - Expected equilibrium electron number density of 4.2×10^{21} m^{-3}.

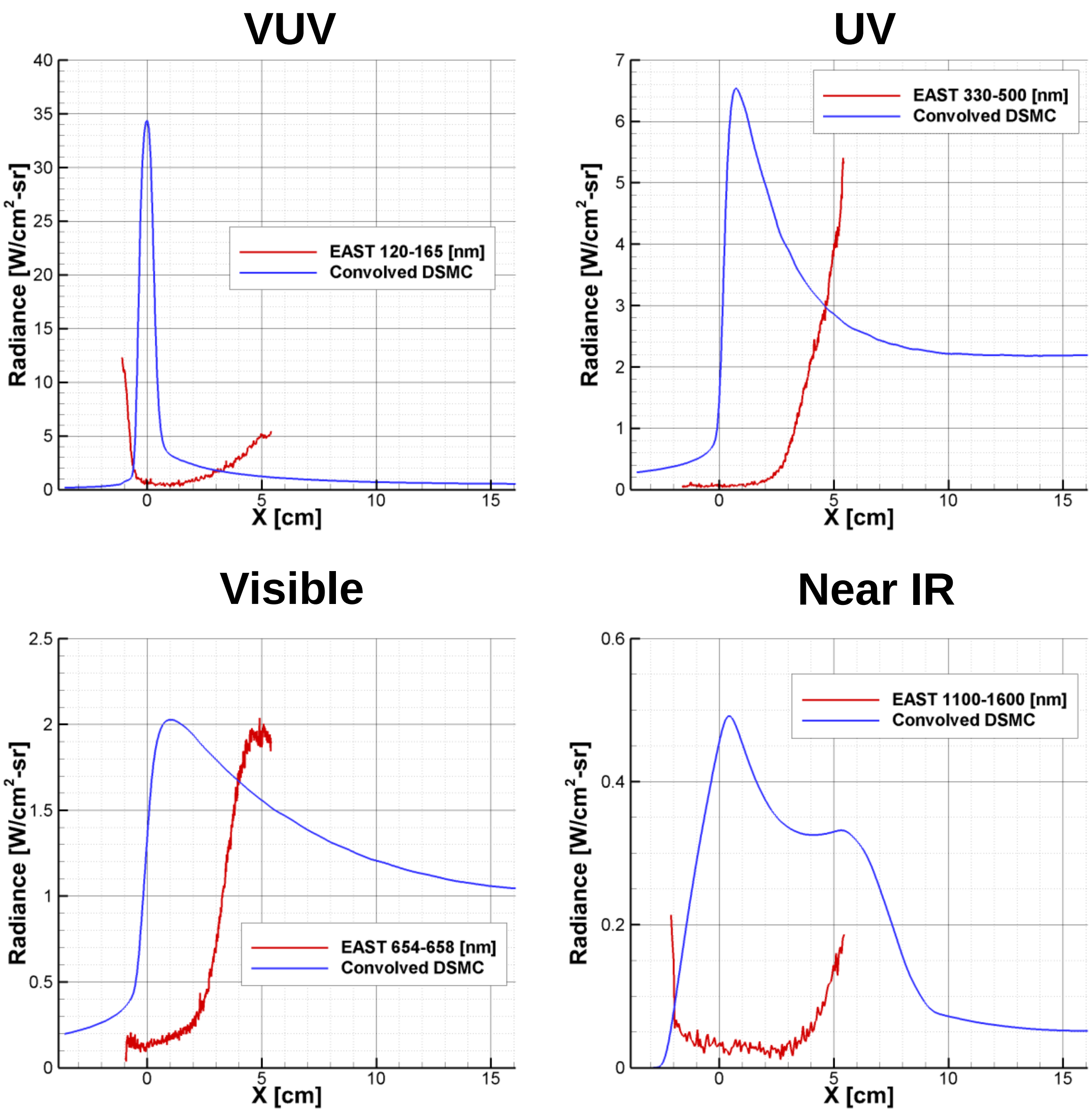




0.2 Torr Shock Simulation

NEQAIR Results:

- Radiance is generally over-predicted.
- Radiance measurements are roughly the correct shape.
- Molecular and Lyman-α emission occurs post-shock.
- Induction period is not seen in the simulation.

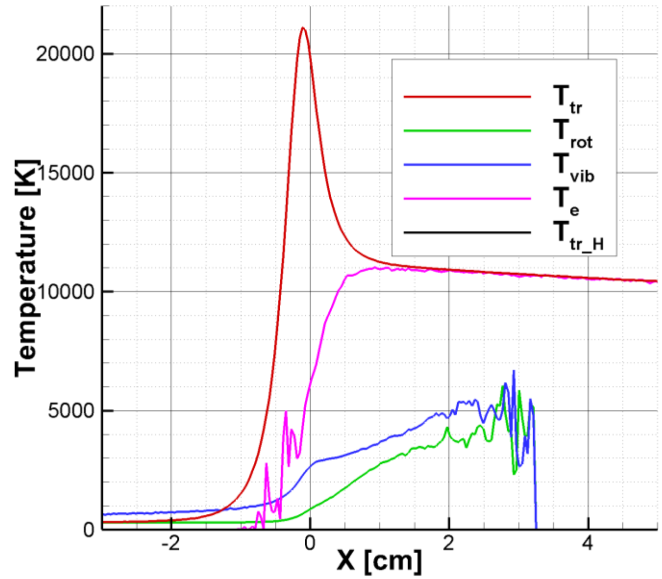


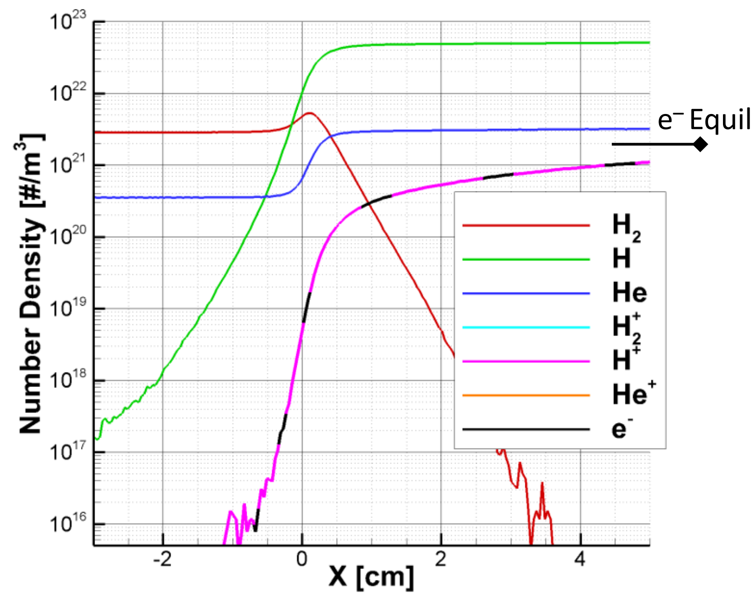
0.1 Torr Shock Simulation

EAST Shot 17:

- Shock velocity: 27.4 km/s
- Initial pressure: 0.1 Torr
- Initial temperature: 300 K
- Freestream 89% H_2: 11% He

- H_2 persists more than twice the post-shock distance than Shot 25.
- H diffuses much further upstream.
- Equilibrium has not been reached by 5 cm.
  - Expected equilibrium electron number density of 2.0×10^{21} m^{-3}.
  - Electron number density is trending towards this value, but still overshoots far downstream.



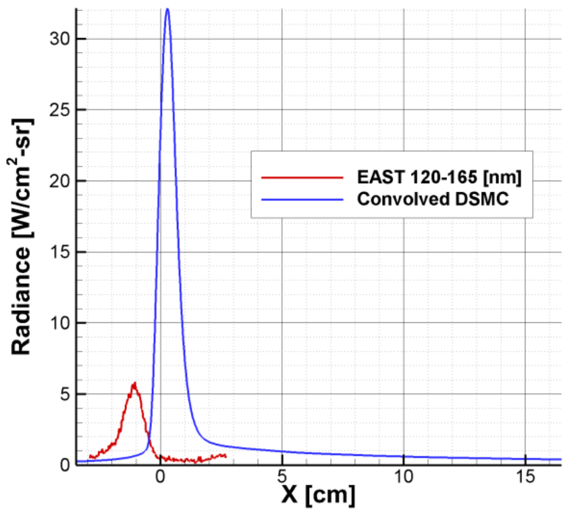


0.1 Torr Shock Simulation

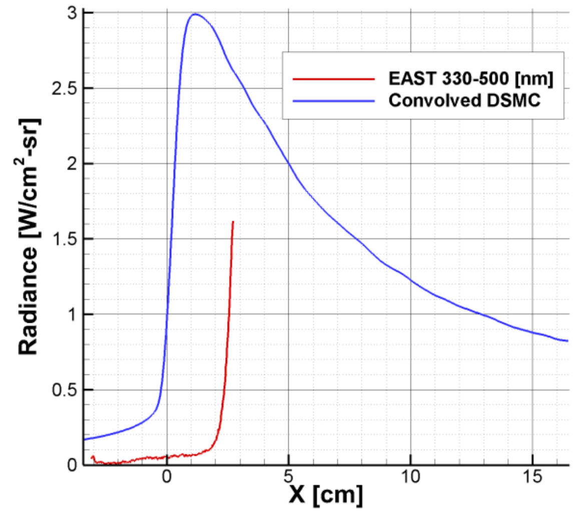
NEQAIR Results:

- Similar comparisons as Shot 25.
- Radiance seems to take the correct shape.
- VUV radiance spike is approximately the correct width.
- Induction period is not seen in the UV range.
- Visible range radiance increase at the shock front for both.

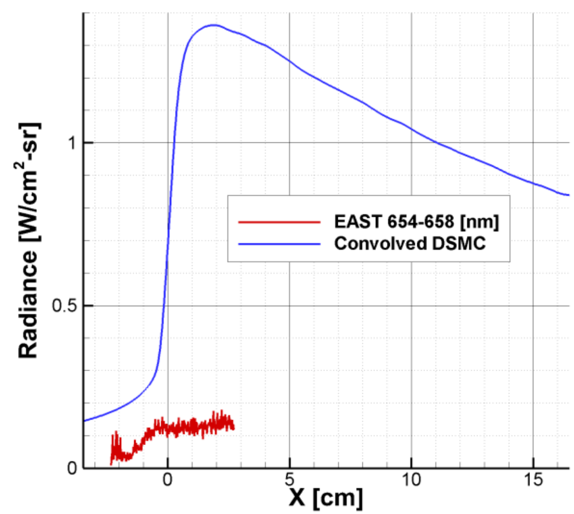
VUV



UV



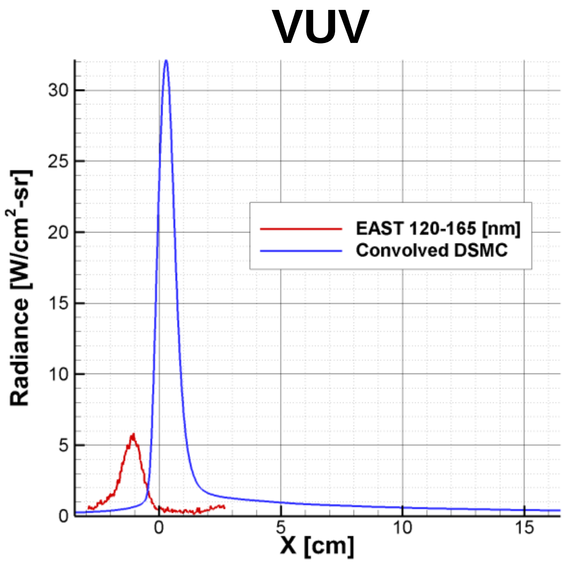
Visible

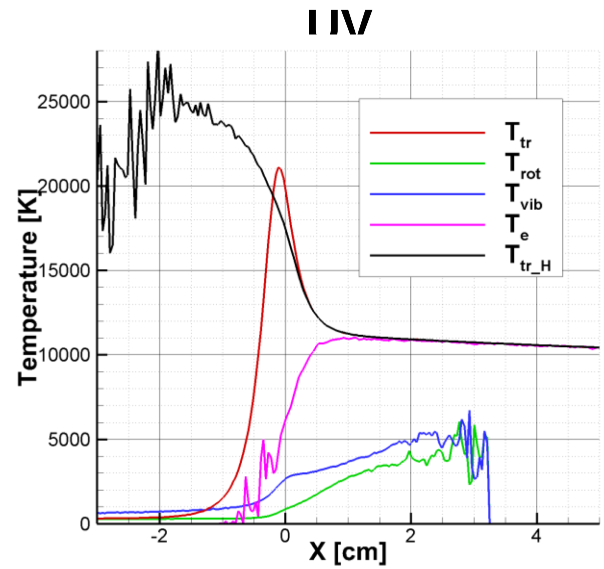


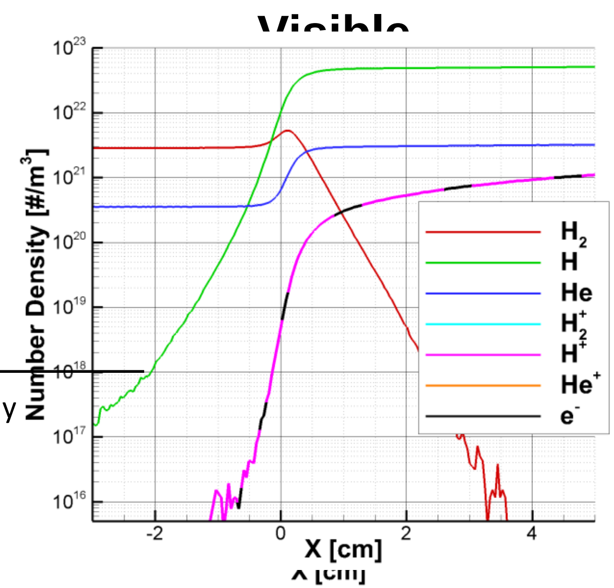
0.1 Torr Shock Simulation

NEQAIR Results:

- Pre-shock radiation misrepresentation could be due to
  - T_e is zero upstream of the shock.
  - Ambipolar diffusion is not included in the DSMC model.
- NEQAIR requires an electronic temperature due to various model shortcomings.
  - QSS rates for H are not yet included in NEQAIR.
  - T_e modeled as the free electron kinetic temperature.
- Hot Hydrogen diffuses upstream.
  - H Lyman-α emission (n=2 →1) should occur upstream.
  - With the correct T_e, these particles should be emitting.
- Cruden[1] determined that H is optically thick as low as $1.0{\times}10^{18}$ m^{-3}.
  - Simulated H passes this value at the same location that the experimental radiance increase.







Optically thick

[1]Cruden and Bogdanoff, "Shock Radiation Tests for Saturn and Uranus Entry Probes"

Conclusions

- An electronic excitation model was introduced to the DSMC code.
- High temperature DSMC parameters were obtained for a H_2-He mixture.
- A 0-D relaxation was performed and the correct equilibrium was obtained.
- First attempts at simulating a non-equilibrium H_2-He shock were completed and results were linked to the NEQAIR radiation solver.
  - Results were compared to the EAST experiments.
  - Non-equilibrium was confirmed with experiments to persist far downstream.
  - Atomic Hydrogen diffusion was observed upstream.
  - Simulated free electron number density was higher than the expected equilibrium values.
  - The ionization inductance period was not seen in the simulated radiance.
  - Simulated radiance was much higher than expected, but generally had the correct shape.

Future Work

High Priority:

- Formulate an improved representation of electronic temperature.
- Implement a more sophisticated chemical reaction model for recombination reactions in the DSMC code.
- Include quasi-steady state rates for H in NEQAIR.
- Perform a sensitivity analysis on the input parameters to identify the most important models and parameters that need improvements.

Low Priority:

- Model ambipolar diffusion in the DSMC code.
- Obtain high temperature data for H_2 rotational relaxation and develop a temperature dependent equation.

Questions?

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Questions?

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- Initial temperature: 300 K
- Freestream 89% H_2: 11% He

- H_2 is dissociated by ~1.5 cm.
- H slightly diffuses upstream.
- Ionization begins immediately.
  - Degree of ionization is <10%.
  - Temperature is static without electronic excitation.

- Comparing before (dashed) and after (solid) including an electronic excitation model.
  - Electron number density increase by two orders of magnitude.
  - Equilibrium has not been reached by 5 cm.
  - Higher electron number density than the experiment.
  - Expected equilibrium electron number density of 4.2×10^{21} m^{-3}.