DSMC Shock Simulation of Saturn Entry Probe Conditions

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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.
- H₂-He atmosphere mixture.

Convective heating accounts for most of the total heat flux during entry.

Significant uncertainty in the prediction of radiative heating.¹

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 achieve 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.

$^1$Cruden and Bogdanoff, “Shock Radiation Tests for Saturn and Uranus Entry Probes”
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.

1Cruden 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
  - $Kn = \frac{\lambda}{D} > 0.01$
  - Continuum breaks down.
    - Must use Boltzmann equation.
1-D Unsteady Shock Simulation:

- Normalized $P$ Averaged ($P_{\text{avg}}$)
- Shock Position $P_{\text{avg}} = 0.5$
- $V_{\text{grid}} = V_{\text{shock}}$
- Shock Sampling Region
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.

¹Liechty, 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.
Elastic Collisions

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.

\(^1\)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"
Inelastic Collisions

H₂ Relaxation Parameters:

• Vibrational collision number is calculated from Millikan-White using Palmer’s¹ parameters.

• A temperature dependent rotational collision number relationship is preferred (Parker).
  - H₂ 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 \( Z_{rot} = 174 \).

¹Palmer, Prabhu, and Cruden, “Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method”
Recombination Reaction Rates:

- Forward Arrhenius reaction rates ($K_f$) were obtained from Leibowitz\textsuperscript{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.
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.

$\text{H}^+ + e^- + \text{H} \rightarrow \text{H} + \text{H}$

1L. 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 ($T_{\text{tr}}$, $T_{\text{rot}}$, $T_{\text{vib}}$, $T_{\text{e}}$).
  - 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 \sim 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 $4.2 \times 10^{21}$ m$^{-3}$. 
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.
**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 \(2.0 \times 10^{21} \text{ m}^{-3}\).
  - Electron number density is trending towards this value, but still overshoots far downstream.
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.
NEQAIR Results:

- **NEQAIR radiation** representation temperature due to various model shortcomings.
  - Ambipolar diffusion is not included in the DSMC model.
  - QSS rates for H are not yet included in NEQAIR.
  - T_e modeled as the free electron kinetic temperature.
  - Cruden determined that H is optically thick as low as $1.0 \times 10^{18} \text{ m}^{-3}$.
  - Simulated H passes this value at the same location that the experimental radiance increase.

- Hot Hydrogen diffuses upstream.
  - H Lyman–$\alpha$ emission ($n=2 \rightarrow 1$) should occur upstream.
  - With the correct T_e, these particles should be emitting.

- **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.
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  - Results were compared to the EAST experiments.
  - Non-equilibrium was confirmed with experiments to persist far downstream.
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Questions?
EAST Shot 25:

- Shock velocity: 27.8 km/s
- Initial pressure: 0.2 Torr
- Initial temperature: 300 K
- Freestream 89% H\textsubscript{2}: 11% He

- H\textsubscript{2} is dissociated by ~1.5 cm and further by ~15 cm and after (solid) including an electronic excitation model.
- H slightly diffuses upstream.
- Ionization begins immediately.
  - Electron number density increase by two orders of magnitude.
  - Degree of ionization is <10%.
  - Temperature is static without electronic excitation.
  - Higher electron number density than the experiment.
  - Expected equilibrium electron number density of $4.2 \times 10^{21}$ m\textsuperscript{-3}.