DSMC Shock Simulation of Saturn Entry Probe Conditions

Kyle J. Higdon
The University of Texas at Austin

Brett A. Cruden, Aaron M. Brandis
AMA, Inc. at NASA Ames Research Center

Derek S. Liechty
NASA Langley Research Center

David B. Goldstein, Philip L. Varghese
The University of Texas at Austin

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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.
  - 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 H₂-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 H₂ emission measured.

- Observations
  - Post-shock region did not equilibrate 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.

¹Cruden 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.

\[\text{Cruden and Bogdanoff, "Shock Radiation Tests for Saturn and Uranus Entry Probes"}\]
• 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** ($P_{avg}$)

**Shock Position**
- $P_{avg} = 0.5$

**Shock Sampling Region**
- $V_{grid} = V_{shock}$
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 \( \text{H}_2\)-He mixture (\( \text{H}_2, \text{H}, \text{He}, \text{H}_2^+, \text{H}^+, \text{He}^+, \text{e}^- \)).
  - Many of the DSMC parameters for \( \text{H}_2\)-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’s\(^1\) 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 \(Z_{\text{rot}} = 174\).

\(^1\)Palmer, 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.

\textsuperscript{1}L. P. Leibowitz and T. J.Kuo, “Ionizational Nonequilibrium Heating During Outer Planetary Entries”
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.

\[ \text{H}^+ + e^- + \text{H} \rightarrow \text{H} + \text{H} \]

![Graph showing reaction rates and equilibrium constants vs. temperature](image)

\[^1\text{L. P. Leibowitz and T. J. Kuo, “Ionizational Nonequilibrium Heating During Outer Planetary Entries”}\]
How can we compare the DSMC results directly to the experimental data?

- $T_{tr,0} = 20,000$ K
- $T_{rot,0} = T_{vib,0} = T_{elec,0} = 300$ 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\textsubscript{2}: 11% He

- H\textsubscript{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 \(4.2 \times 10^{21} \text{ m}^{-3}\).
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% H₂: 11% He

- H₂ 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 $2.0 \times 10^{21}$ 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 radiancé increase.

1Cruden 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.
Conclusions:

• An electronic excitation model was introduced to the DSMC code.

• High temperature DSMC parameters were obtained for a H₂-He mixture.

• A 0-D relaxation was performed and the correct equilibrium was obtained.

• First attempts at simulating a non-equilibrium H₂-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.
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Questions?
**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.
  - Electron number density increase by 1.5 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 4.2×10\(^{21}\) m\(^{-3}\).