Gas-Surface Interaction Models in Hypersonic Flows

Master degree in Aerospace Engineering

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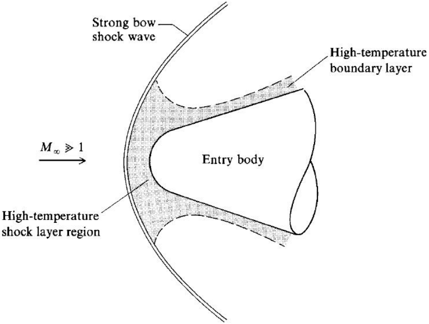
7th December 2015

Contents

Motivation

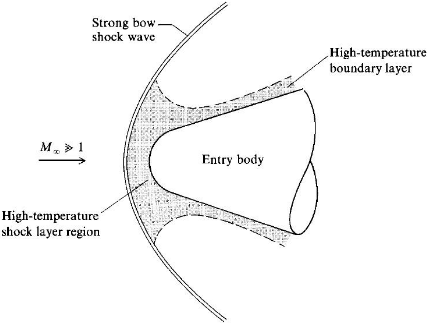
- Space vehicles enter planetary atmospheres at orbital speed $V_\infty \approx 7.9\ \frac{\text{km}}{\text{s}}$
- Shock wave upstream of vehicle
- Kinetic energy ($\approx \frac{1}{2}mV^2$) $\Rightarrow$ converted to internal energy.



Credit: Anderson

Objectives

- SPARK code
- Bla
- BlaBla
- BlaBlaBla

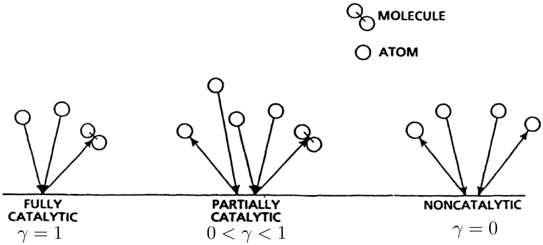


Credit: Anderson

1. Motivation
2. Theory and models
3. Implementation in SPARK
4. Results
5. Conclusions and future work

Catalytic Models

- Non catalytic
- Fully catalytic
- Partially catalytic
- Super catalytic
- Equilibrium wall
- Finite-rate catalycity

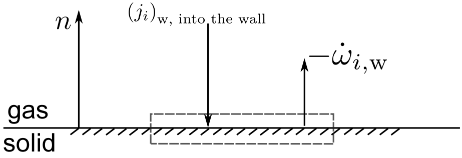


Credit: Scott

Where do these models fit in the overall SPARK code?

- As boundary conditions
- Wall mass and energy balances

Wall Species Mass Balance



- Fick's Law of diffusion: $(j_i)_{\text{w, into the wall}} = \left(\rho D_i \frac{\partial c_i}{\partial n}\right)_{\text{w}}$
- Production terms $\dot{\omega}_{i,\text{w}}$ are given by the catalytic model
- Final result

$$-\left(\rho D_i \frac{\partial c_i}{\partial n}\right)_{\text{w}} = (\dot{\omega}_{i,\text{w}})$$

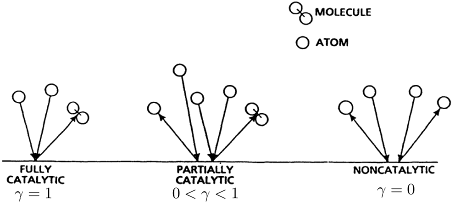
Modelling the Source Terms

- Macroscopic representation

$$\gamma_i \equiv \frac{|M_i|}{|M_i^{\downarrow}|}$$

- Kinetic Theory

$$M_i^{\downarrow} = c_{i,\mathrm{w}} \rho_{\mathrm{w}} \sqrt{\frac{R_i T_{\mathrm{w}}}{2\pi}}$$



- For Earth re-entry

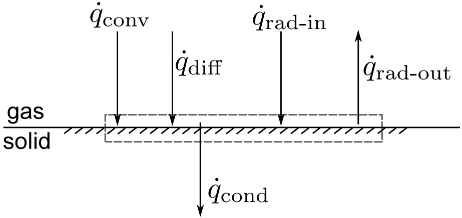
$$\mathrm{N} + \mathrm{N} \longrightarrow \mathrm{N}_2$$
$$\mathrm{O} + \mathrm{O} \longrightarrow \mathrm{O}_2$$

$$\dot{\omega}_{N,\mathrm{w}} = -\gamma_N c_{N,\mathrm{w}} \rho_{\mathrm{w}} \sqrt{\frac{R_N T_{\mathrm{w}}}{2\pi}}$$
$$\dot{\omega}_{N_2,\mathrm{w}} + \dot{\omega}_{N,\mathrm{w}} = 0$$

Improvements

1. γ = constant value
2. $\gamma = \gamma(T_{\mathrm{w}})$

Wall Energy Balance



- Surface at Radiative Equilibrium

$$\underbrace{\left(k\frac{\partial T}{\partial n}\right)_{\mathrm{w}}}_{\dot{q}_{\text{conv}}} + \underbrace{\left(\sum_{i=1}^{N_s} h_i \rho D_i \frac{\partial c_i}{\partial n}\right)_{\mathrm{w}}}_{\dot{q}_{\text{diff}}} = \underbrace{\epsilon\sigma T_{\mathrm{w}}^4}_{\dot{q}_{\text{rad-out}}}$$

1. Motivation

2. Theory and models

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Redesign SPARK's Boundary Condition Structure

Ghost Cell Concept

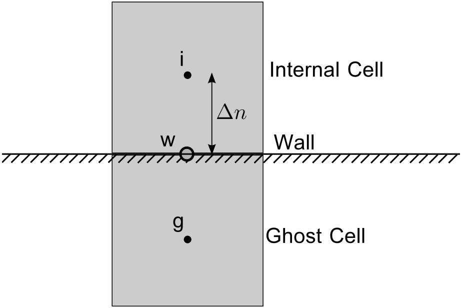
Implementation Mass Balance

$$-\left(\rho D_i \frac{\partial c_i}{\partial n}\right)_{\mathrm{w}} = \left(\dot{\omega}_{i,\mathrm{w}}\right)$$

Discretization:

$$\left(\frac{\partial c_i}{\partial n}\right)_{\mathrm{w}} = \frac{(c_i)_{\mathrm{i}} - (c_i)_{\mathrm{w}}}{\Delta n}$$

$$c^n_{i,\mathrm{w}} = c^n_{i,\mathrm{i}} + \dot{\omega}^n_{i,\mathrm{w}} \cdot \left(\frac{\Delta n}{\rho_{\mathrm{w}} D_{i,\mathrm{w}}}\right)^n$$



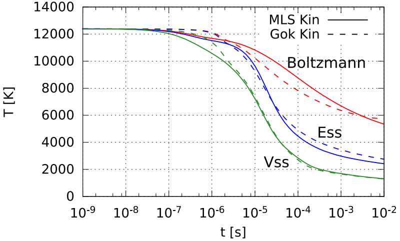
Summary of contributions

- The forward rate of reaction $N_2 + e^- \rightleftharpoons 2\,N + e^-$ was computed.
- The use of the Harmonic Oscillator model for the vibrational partition function was assessed in comparison with the analytical calculation.
- The spontaneous emission modeling has been improved.
- The vibrational redistribution method applied has an influence in the excited electronic states population of molecules.

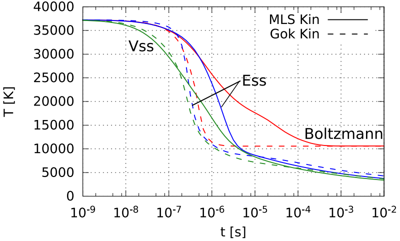
Results

1. Temperature results
2. Electronic excited levels results
3. Radiation results: 5.15 km/s
4. Radiation results: 9 km/s

Temperature results

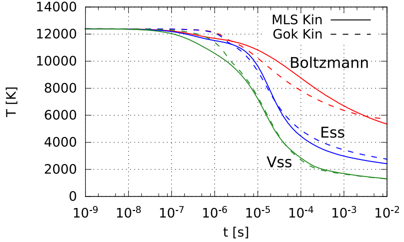


(a) 5.15 km/s

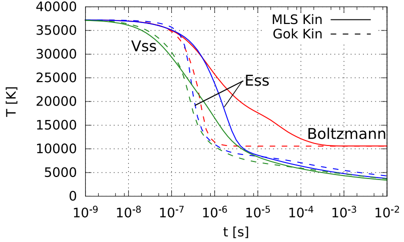


(b) 9 km/s

Temperature results



(a) 5.15 km/s



(b) 9 km/s

In regards to the kinetic model, Gökçen's or Lino da Silva's:

- Simulations agree for a shock speed of 5.15 km/s.
- There is a time discrepancy for the temperature decrease at 9 km/s between models.

In regards to the kinetics used, Boltzmann, ESS or VSS:

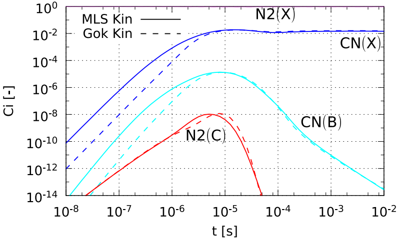
- VSS simulations exhibit the fastest decreasing temperature.
- Boltzmann are slowest to decrease their temperature.
- ESS simulations are a middle ground between VSS and Boltzmann.

Electronic excited levels results

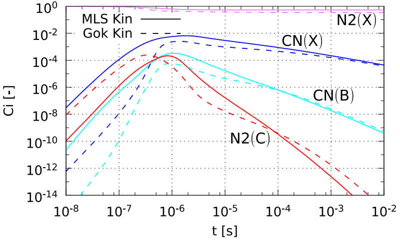
Time evolution of electronic excited levels shows:

- For 5.15 km/s there is agreement while there is a time shift for 9 km/s for Gökçen's and Lino da Silva's model.
- At 9 km/s the population of N_2(C) and CN(B) are on the same order of magnitude[1], at 5.15 km/s CN(B) dominates.

These trends are the same for ESS simulations.



(a) VSS at 5.15 km/s



(b) VSS at 9 km/s

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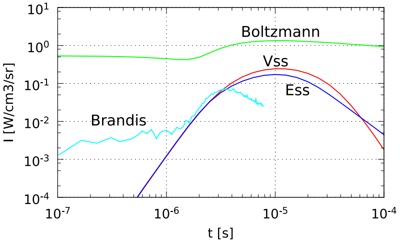
[1] Not seen experimentally.

Radiation results: 5.15 km/s

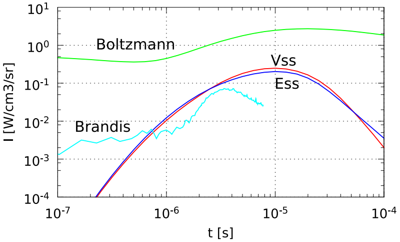
This simulated radiation intensity is the sum of radiation from CN Violet and N_2 second positive systems on a spectral window of $[310 - 450]$ nm. At 5.15 km/s, in regards to kinetics,

- Boltzmann overpredicts radiation intensity.
- The ESS and VSS curves are very similar.

Both Gökçen's and Lino da Silva's models are in reasonable agreement with the experiment[2]as with other previous results for this shock speed.



(a) Gökçen



(b) Lino da Silva

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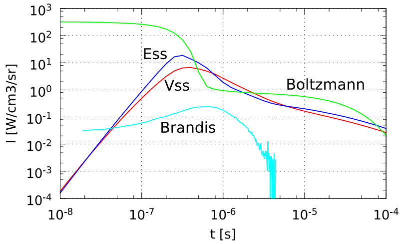
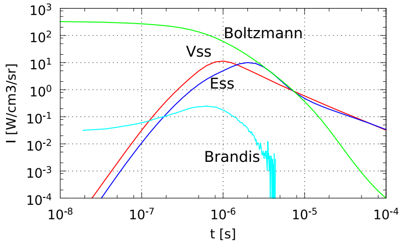
[2] Experimental data from A. Brandis PhD thesis (2009).

Radiation results: 9 km/s



(a) Gökçen



(b) Lino da Silva

For a shock speed of 9 km/s,

- No agreement can be found with the experimental results.
- ESS and VSS separate in magnitude using Gökçen's model.
- For Lino da Silva's model, ESS and VSS separate in time.

Lino da Silva's VSS curve seems to predict the peak time-wise but clearly does not agree with the experimental data.

Conclusions and future work

Regarding the comparison with the experimental results:

- At low shock speeds the results are in reasonable agreement with the experimental data.
- The results for a high shock wave speed are still not satisfactory.

Improved high temperature state-to-state data is required.

Conclusions and future work

Regarding the comparison with the experimental results:

- At low shock speeds the results are in reasonable agreement with the experimental data.
- The results for a high shock wave speed are still not satisfactory.

Improved high temperature state-to-state data is required.

To improve the results for higher shock speeds:

- Add dissociation of electronically excited molecules.
- Improve the vibrational redistribution model employed.
- Change the 0D system to a 1D system.

These changes might improve the agreement with the experimental results.

Number	Reaction
1	$N_2 + M_2 \rightleftarrows N + N + M_2$
2	$N_2 + M_3 \rightleftarrows N + N + M_3$
3	$CH_4 + M_1 \rightleftarrows CH_3 + H + M_1$
4	$CH_3 + M_1 \rightleftarrows CH_2 + H + M_1$
5	$CH_3 + M_1 \rightleftarrows CH + H_2 + M_1$
6	$CH_2 + M_1 \rightleftarrows CH + H + M_1$
7	$CH_2 + M_1 \rightleftarrows C + H_2 + M_1$
8	$CH + M_1 \rightleftarrows C + H + M_1$
9	$C_2 + M_1 \rightleftarrows C + C + M_1$
10	$H_2 + M_1 \rightleftarrows H + H + M_1$
11	$CN + M_1 \rightleftarrows C + N + M_1$
12	$NH + M_1 \rightleftarrows N + H + M_1$
13	$HCN + M_1 \rightleftarrows CN + H + M_1$
14	$CH_3 + N \rightleftarrows HCN + H + H$
15	$CH_3 + H \rightleftarrows CH_2 + H_2$
16	$CH_2 + N_2 \rightleftarrows HCN + NH$
17	$CH_2 + N \rightleftarrows HCN + H$
18	$CH_2 + H \rightleftarrows CH + H_2$
19	$CH + N_2 \rightleftarrows HCN + N$
20	$CH + C \rightleftarrows C_2 + H$
21	$C_2 + N_2 \rightleftarrows CN + CN$
22	$CN + H_2 \rightleftarrows HCN + H$

Number	Reaction
23	$CN + C \rightleftarrows C_2 + N$
24	$N + H_2 \rightleftarrows NH + H$
25	$C + N_2 \rightleftarrows CH + N$
26	$C + H_2 \rightleftarrows CH + H$
27	$H + N_2 \rightleftarrows NH + N$
28	$H + H \rightleftarrows {H_2}^+ + E^-$
29	$C + H \rightleftarrows CH^+ + E^-$
30	$C + N \rightleftarrows CN^+ + E^-$
31	$N + H \rightleftarrows NH^+ + E^-$
32	$N + N \rightleftarrows {N_2}^+ + E^-$
33	$N + E^- \rightleftarrows N^+ + E^- + E^-$
34	$C + E^- \rightleftarrows C^+ + E^- + E^-$
35	$H + E^- \rightleftarrows H^+ + E^- + E^-$
36	$Ar + E^- \rightleftarrows Ar^+ + E^- + E^-$
37	$H_2 + E^- \rightleftarrows {H_2}^+ + E^- + E^-$
38	$CH + E^- \rightleftarrows CH^+ + E^- + E^-$
39	$NH + E^- \rightleftarrows NH^+ + E^- + E^-$
40	$N_2 + E^- \rightleftarrows {N_2}^+ + E^- + E^-$
41	${N_2}^+ + E^- \rightleftarrows N^+ + N + E^-$
42	$C^+ + N_2 \rightleftarrows {N_2}^+ + C$
43	$C^+ + N_2 \rightleftarrows CN^+ + N$
44	$C^+ + N_2 \rightleftarrows N^+ + CN$
45	$N_2 + E^- \rightleftarrows N + N + E^-$

Number	Reaction
5	$\mathrm{CN(X) + M \rightleftarrows CN(A) + M}$
6	$\mathrm{CN(X) + M \rightleftarrows CN(B) + M}$
7	$\mathrm{N_2(X) + M \rightleftarrows N_2(A) + M}$
8	$\mathrm{N_2(A) + M \rightleftarrows N_2(B) + M}$
9	$\mathrm{N_2(C) + M \rightleftarrows N_2(B) + M}$
10	$\mathrm{CN(X) + E^- \rightleftarrows CN(A) + E^-}$
11	$\mathrm{CN(X) + E^- \rightleftarrows CN(B) + E^-}$
12	$\mathrm{N_2(X) + E^- \rightleftarrows N_2(A) + E^-}$
13	$\mathrm{N_2(X) + E^- \rightleftarrows N_2(B) + E^-}$
14	$\mathrm{N_2(X) + E^- \rightleftarrows N_2(C) + E^-}$
15	$\mathrm{N_2(A) + E^- \rightleftarrows N_2(B) + E^-}$
16	$\mathrm{N_2(A) + N_2(A) \rightleftarrows N_2(X) + N_2(B)}$
17	$\mathrm{N_2(A) + N_2(A) \rightleftarrows N_2(X) + N_2(C)}$
18	$\mathrm{N_2(A) + CN(X) \rightleftarrows N_2(X) + CN(B)}$
19	$\mathrm{CN(X) + N_2(X, 4\,) \rightleftarrows CN(A) + N_2(X, 0\,)}$
20	$\mathrm{CN(X) + N_2(X, 11\,) \rightleftarrows CN(B) + N_2(X, 0\,)}$