DSMC Simulations of Mars Science Laboratory Entry from Rarefied to Continuum Conditions

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# Mars Science Laboratory Mission

<table>
<thead>
<tr>
<th>Mission Type</th>
<th>Mars Rover</th>
</tr>
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<tbody>
<tr>
<td>Operator</td>
<td>NASA</td>
</tr>
<tr>
<td>Launch Date</td>
<td>11/26/11</td>
</tr>
<tr>
<td>Launch Mass</td>
<td>3839 kg</td>
</tr>
<tr>
<td>Rocket</td>
<td>Atlas V</td>
</tr>
<tr>
<td>Launch Date</td>
<td>08/06/12</td>
</tr>
<tr>
<td>Launch Site</td>
<td>Gale Crater</td>
</tr>
</tbody>
</table>

credit: NASA JPL
Overview – Coupling aerothermal environment and material response

MSL PICA heatshield

Aeroshell Geometry[1]

Image processing and material meshing POINTWISE

Material mesh

Spatial and temporal interpolations

Material response PATO [4]

Recession, temperature and internal velocity

Environment meshing POINTWISE


Aerothermal environment around aeroshell

Boundary layer edges BLAYER

Aerothermal environment at the surface

LEGEND

Overview – Coupling aerothermal environment and material response

From literature

Material meshing POINTWISE

Soft coupling OPENFOAM

BOUNDARY LAYER

AEROTHERMAL ENVIRONMENT

ENVIRONMENT MESH

MATERIAL RESPONSE
Aerothermal environment computed from DPLR

DPLR assumptions

- **Laminar** boundary layer
- **Non-blowing** & smooth wall
- Chemical and thermal non-equilibrium
- 2 temperatures model
- Radiative equilibrium wall with $\varepsilon = 0.85$
- Super-catalytic wall: recombination to freestream mole fraction
- Mars atmosphere: $y_{CO2} = 0.97$, $y_{N2} = 0.03$
- 8 species and 24 reactions (12 forward + 12 backward): Mitcheltree model [5]
- Park hypersonics correction to vibrational relaxation [6]
- Used from 48.4s to 100.5s of entry

BLAYER calculates the **boundary layer edges** using a curvature-based method

Surface pressure $p_w$, heat transfer coefficient $C_H$ and enthalpy $h_e$ at the **boundary layer edges** are used as inputs in the material response code: PATO

credit: C. Tang, NASA Ames
Aerothermal environment computed from SPARTA

SPARTA assumptions

- 3 temperatures model
- Radiative equilibrium wall with $\varepsilon = 0.85$
- Super-catalytic wall: recombination to freestream mole fraction
- Mars atmosphere: $y_{\text{CO}_2} = 0.97$, $y_{\text{N}_2} = 0.03$
- 8 species and 24 reactions(12 forward + 12 backward): Mitchelltree model [5]
- VSS model with high temperature transport calibration [6]
- Parker equation for rotational relaxation and Millikan-White equation + Park correction for vibrational relaxation [7]
- Discrete vibrational temperature
- Used from 0s to 48.4s of entry

Boundary layer edges calculated using an edge-based method

Surface pressure $p_w$, heat transfer coefficient $C_H$ and enthalpy $h_e$ at the boundary layer edges are used as inputs in the material response code: PATO
# High temperature transport model

<table>
<thead>
<tr>
<th></th>
<th>d (Å)</th>
<th>ω</th>
<th>α</th>
<th>$Z_{\text{rot}}^\infty$</th>
<th>$T^* (K)$</th>
<th>$C_1 (K)$</th>
<th>$C_2 (K^{0.33})$</th>
<th>$\sigma_v^{\text{Park}} (\text{Å}^2)$</th>
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<tbody>
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<td>O$_2$</td>
<td>3.896</td>
<td>0.7</td>
<td>1.463</td>
<td>14.4</td>
<td>90</td>
<td>100.7</td>
<td>138</td>
<td>0.3</td>
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<td>N$_2$</td>
<td>4.04</td>
<td>0.686</td>
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<td>O</td>
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<td>N</td>
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<tr>
<td>NO</td>
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<td>0.737</td>
<td>1.542</td>
<td>5</td>
<td>117</td>
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<tr>
<td>CO</td>
<td>4.684</td>
<td>0.787</td>
<td>1.494</td>
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<td>92</td>
<td>18.36</td>
<td>198</td>
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<td>CO$_2$</td>
<td>4.147</td>
<td>0.632</td>
<td>1.259</td>
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<td>C</td>
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<td>0.883</td>
<td>1.523</td>
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VSS: $T_{\text{ref}} = 273$ K

<table>
<thead>
<tr>
<th></th>
<th>Parker</th>
<th>Millikan White</th>
<th>Park [7]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_1 (K)$</td>
<td>$C_2 (K^{0.33})$</td>
<td>$\sigma_v^{\text{Park}} (\text{Å}^2)$</td>
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<tr>
<td>O$_2$</td>
<td>100.7</td>
<td>138</td>
<td>0.3</td>
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<tr>
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<td>221</td>
<td>0.3</td>
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<tr>
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<tr>
<td>C</td>
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</table>

### Chemistry model

#### Reaction parameters for the Micheltree and Gnoffo reaction model [5]

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>$A$ (cm$^3$/mol/s)</th>
<th>$B$</th>
<th>$C$ (K)</th>
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<tbody>
<tr>
<td>1</td>
<td>CO + M ↔ C + O + M (M = atom)</td>
<td>3.4×10$^{20}$</td>
<td>-1.00</td>
<td>129,000</td>
</tr>
<tr>
<td>2</td>
<td>CO + M ↔ C + O + M (M = mol.)</td>
<td>2.3×10$^{20}$</td>
<td>-1.00</td>
<td>129,000</td>
</tr>
<tr>
<td>3</td>
<td>CO$_2$ + M ↔ CO + O + M (M = atom)</td>
<td>1.4×10$^{22}$</td>
<td>-1.50</td>
<td>63,275</td>
</tr>
<tr>
<td>4</td>
<td>CO$_2$ + M ↔ CO + O + M (M = mol.)</td>
<td>6.9×10$^{21}$</td>
<td>-1.50</td>
<td>63,275</td>
</tr>
<tr>
<td>5</td>
<td>O$_2$ + M ↔ O + O + M (M = atom)</td>
<td>1.0×10$^{22}$</td>
<td>-1.50</td>
<td>59,750</td>
</tr>
<tr>
<td>6</td>
<td>O$_2$ + M ↔ O + O + M (M = mol.)</td>
<td>2.0×10$^{21}$</td>
<td>-1.50</td>
<td>59,750</td>
</tr>
<tr>
<td>7</td>
<td>N$_2$ + M ↔ N + N + M (M = atom)</td>
<td>3.0×10$^{22}$</td>
<td>-1.60</td>
<td>113,200</td>
</tr>
<tr>
<td>8</td>
<td>N$_2$ + M ↔ N + N + M (M = mol.)</td>
<td>7.0×10$^{21}$</td>
<td>-1.60</td>
<td>113,200</td>
</tr>
<tr>
<td>9</td>
<td>NO + M ↔ N + O + M (M = C, N, O, NO, CO$_2$)</td>
<td>1.1×10$^{17}$</td>
<td>0.00</td>
<td>75,500</td>
</tr>
<tr>
<td>10</td>
<td>NO + M ↔ N + O + M (M = N$_2$, O$_2$, CO)</td>
<td>5.0×10$^{15}$</td>
<td>0.00</td>
<td>75,500</td>
</tr>
<tr>
<td>11</td>
<td>NO + O ↔ O$_2$ + N</td>
<td>8.4×10$^{12}$</td>
<td>0.00</td>
<td>19,450</td>
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<tr>
<td>12</td>
<td>N$_2$ + O ↔ NO + N</td>
<td>6.4×10$^{17}$</td>
<td>-1.00</td>
<td>38,370</td>
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<tr>
<td>13</td>
<td>CO + O ↔ O$_2$ + C</td>
<td>3.9×10$^{13}$</td>
<td>-0.18</td>
<td>69,200</td>
</tr>
<tr>
<td>14</td>
<td>CO$_2$ + O ↔ O$_2$ + CO</td>
<td>2.1×10$^{13}$</td>
<td>0.00</td>
<td>27,800</td>
</tr>
<tr>
<td>15</td>
<td>CO + N ↔ NO + C</td>
<td>2.86×10$^{11}$</td>
<td>0.50</td>
<td>53,630</td>
</tr>
<tr>
<td>16</td>
<td>CO + CO ↔ CO$_2$ + C</td>
<td>2.33×10$^9$</td>
<td>0.50</td>
<td>65,710</td>
</tr>
<tr>
<td>17</td>
<td>NO + CO ↔ CO$_2$ + N</td>
<td>4.59×10$^8$</td>
<td>0.50</td>
<td>12,070</td>
</tr>
</tbody>
</table>

- Backward rates computed using forward rates and equilibrium constants.
- Equilibrium constants computed using van’t Hoff equation (Gibbs free energy).
- Backward rates fit to modified Arrhenius form between 5,000 and 20,000 K.
Radiative equilibrium boundary condition

\[ q_w = \varepsilon \sigma T_w^4 \]
Translational temperature at different altitudes
Number density at different altitudes
Surface temperature and pressure from DSMC at 40s.
The 48.4s of entry point: DSMC vs CFD
Continuum breakdown parameters: CFD

\[ Kn_{GLL} = \frac{\lambda}{Q} \left| \frac{dQ}{dl} \right| \] [8]
Continuum breakdown parameters: DSMC

\[ Kn_{GLL} = \frac{\lambda}{Q} \left| \frac{dQ}{dl} \right| \] [8]
The 48.4s of entry point: DSMC mole fractions
Temperature from PATO

![Graph showing temperature over time for different MISPs](image)

- **Temperature from PATO**
- **Surface**
- **DSMC**
- **DPLR**
- **MISP1**
- **MISP2**
- **MISP3**
- **MISP4**
- **MISP5**
- **MISP6**
- **MISP7**

**Diagram showing spatial distribution of MISPs**

- **MISP1**
- **MISP2**
- **MISP3**
- **MISP4**
- **MISP5**
- **MISP6**
- **MISP7**

**Legend**
- **MISP1**
- **MISP2,3**
- **MISP4**
- **MISP5**
- **MISP6**
- **MISP7**

**Temperature (K)**
- 0
- 20
- 40
- 60
- 80
- 100

**Time (s)**
- 0
- 20
- 40
- 60
- 80
- 100
• Addition of DSMC results significantly modify temperature prediction for first 60s of Entry Interface
Recession from PATO

Recension (mm) vs Time (s)

- DSMC
- DPLR

- MISP1
- MISP2,3
- MISP4
- MISP5
- MISP6
- MISP7

DSMC+DPLR (solid)
DPLR (dotted)
Conclusion

Hypersonic environment (DPLR)
- Laminar
- Super-catalytic wall
- Non-blowing
  (SPARTA)
- High T transport calibration
- Parker +Millikan White + Park for relaxation
- Discrete vibrational levels
  (common)
- Super-catalytic wall with radiative equilibrium
- Mitcheltree 8 species reaction model

DSMC simulations from 20 to 48.4s
- Shock narrows with decreasing altitude
- Compute surface pressure and heat flux

Shock standoff offset at 48.4s
- Continuum breakdown?
- Differences between models?
Conclusion

Hypersonic environment (DPLR)
- Laminar
- Super-catalytic wall
- Non-blowing
  (SPARTA)
- High T transport calibration
- Parker + Millikan White + Park for relaxation
- Discrete vibrational levels
  (common)
- Super-catalytic wall with radiative equilibrium
- Mitcheltree 8 species reaction model

Soft coupling

Porous material response (PATO)
- Pyrolysis
- CMA-type BL approx.
- No finite-rate
- Equilibrium

Outputs
- Temperature
- Recession
References

Questions?

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