High-Temperature Modeling of Transport Properties in Hypersonic Flows

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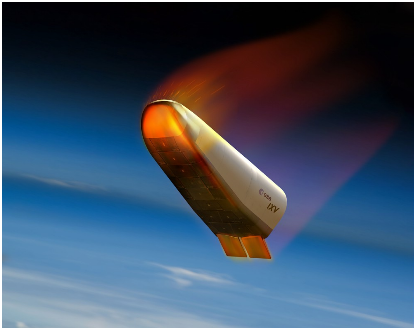
Hypersonic Reentry Flows



Artist rendering, credit: Dassault Aviation

esa's IXV

Intermediate eXperimental Vehicle
Reentering at 7700 m/s, Feb. 2015

Blunt bodies, Ma = 20 to 50:

- Detached bow shock
  - Extreme deceleration
- High temperature gas
  - Chemically reacting
  - Partially ionized (plasma)
- Electrically charged flow
  - Loss of telemetry (Blackout)
- Radiative and **convective heating**
  - Thermal protection system

Chemical Non-Equilibrium

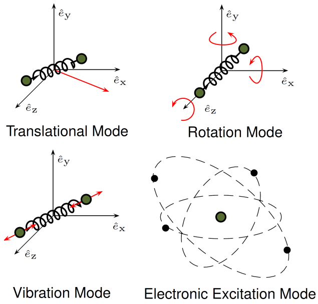
- Chemical Kinetic timescales $\approx$ Flow timescales,
  - composition of the flow-field is determined as part of the simulation procedure.

- Earth atmosphere is described as a mixture of 11 chemical species:

$$N_2,\ O_2,\ N,\ O,\ NO,\ NO^+,\ N^+,\ O^+,\ {N_2}^+,\ {O_2}^+,\ e^-$$

Thermal Non-Equilibrium

- Molecules and atoms can store energy in various modes (degrees of freedom).
- In low density conditions, energy exchanges between modes may be slow relative to flow velocity.
- The flow is characterized by multiple temperatures T_k.



Conservation Equations

- **Mass of species s:**

$$\frac{\partial}{\partial t}(\rho c_s) + \vec{\nabla}\cdot(\rho\vec{u}c_s) = \vec{\nabla}\cdot\vec{J}_s + \dot{\omega}_s$$

- **Momentum:**

$$\frac{\partial}{\partial t}(\rho\vec{u}) + \vec{\nabla}\cdot(\rho\vec{u}\otimes\vec{u}) = \vec{\nabla}\cdot[\tau] - \vec{\nabla}P$$

- **Total energy:**

$$\frac{\partial}{\partial t}(\rho E) + \vec{\nabla}\cdot(\rho\vec{u}E) = \vec{\nabla}\cdot\left(\sum_k \vec{q_{\mathrm{C}}}_k + \sum_s \vec{J}_s h_s + \vec{u}\cdot[\tau] - P\vec{u}\right)$$

- **Non-equilibrium energy k:**

$$\frac{\partial}{\partial t}(\rho\varepsilon_k) + \vec{\nabla}\cdot(\rho\vec{u}h_k) = \vec{\nabla}\cdot\left(\vec{q_{\mathrm{C}}}_k + \sum_s \vec{J}_s h_{s,k}\right) + \dot{\Omega}_k$$

SPARK Aerothermodynamics code:

- Multi-Species, Multi-Temperature
- Finite Volumes Method
- Multi-block structured mesh
- Thermo-chemical database
- Modular and object oriented, programed in Fortran 2008

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This work provides models to compute the dissipative terms

Dissipative fluxes

- The **mass diffusion flux** $\vec{J_s}$ is modeled by Fick's Law of diffusion, for each species s relative to the mixture:

$$\vec{J_s} = \rho D_s \vec{\nabla}(c_s)$$

- The **viscous stress tensor** $[\tau]$ assumes a Newtonian fluid and Stokes hypothesis:

$$[\tau] = \mu \left(\vec{\nabla}\vec{u} + (\vec{\nabla}\vec{u})^{\intercal} \right) - \frac{3}{2}\mu(\vec{\nabla} \cdot \vec{u}) \, [\, \mathrm{I} \,]$$

- The **conduction heat flux** $\vec{q_{\mathrm{C}}}_k$ is given by Fourier's Law, for each non-equilibrium temperature T_k:

$$\vec{q_{\mathrm{C}}}_k = \lambda_k \vec{\nabla} T_k$$

Transport Coefficients

Mass Diffusion	D_s
Viscosity	μ
Thermal Conductivity	λ_k

- Consequence of the interactions between particles at microscopic level.
- Functions of temperature and local chemical composition, requiring computation in real-time.
- Exact solutions computationally expensive $\rightarrow$ **Approximate methods**

Wilke/Blottner/Eucken Model

Blottner Model
Viscosity μ_s determined for each species s, using curve fits as function of T

$$\mu_s = 0.1 \exp\left((A_s \ln T + B_s)\ln T + C_s\right)$$

Eucken Relation
Thermal conductivity $\lambda_{k,s}$ given by μ_s and specific heat $C_{\mathrm{V}\,k,s}$, per species s and energy mode k

$$\lambda_{k,s} = \begin{cases} \dfrac{5}{2}\mu_s C_{\mathrm{V}\,\mathrm{tra},s} & \text{if } k{=}\mathrm{tra} \\ \mu_s C_{\mathrm{V}\,k,s} & \text{if } k{=}\mathrm{rot,vib,exc} \end{cases}$$

Wilke Mixing Rule
Global viscosity μ and thermal conductivities λ_k are averaged according to gas composition x_s

$$\mu = \sum_s \frac{x_s \mu_s}{\phi_s} \quad \text{and} \quad \lambda_k = \sum_s \frac{x_s \lambda_{k,s}}{\phi_s} \quad \text{with:}$$

$$\phi_s = \sum_r x_r \left[1 + \left(\frac{\mu_s}{\mu_r}\right)^{1/2}\left(\frac{M_r}{M_s}\right)^{1/4}\right]^2 \left[8\left(1 + \frac{M_s}{M_r}\right)\right]^{-1/2}$$

Constant Lewis Number
Diffusion coefficient D_s assumes a constant Lewis number (same for all species)

$$D_s = D = \frac{\mathrm{Le}\,\lambda}{\rho C_{\mathrm{P}}} \quad \text{with} \quad \mathrm{Le} = 1.2$$

Gupta-Yos/CCS Model

Collision Cross-Section
Cross-section areas $\pi\overline{\Omega}_{sr}^{(l,l)}$, are defined by curve fits as function of T for each pair of chemical species $(s, r$ combinations)

$$\pi\overline{\Omega}_{sr}^{(l,l)} = D_{\overline{\Omega}_{sr}^{(l,l)}} T^{\left[A_{\overline{\Omega}_{sr}^{(l,l)}}(\ln T)^2 + B_{\overline{\Omega}_{sr}^{(l,l)}} \ln T + C_{\overline{\Omega}_{sr}^{(l,l)}}\right]}$$

$$\Delta_{sr}^{(l)} = \frac{8}{3}\left[\frac{2M_sM_r}{\pi R_{\mathrm{u}} T_c (M_s + M_r)}\right]^{1/2} \pi\overline{\Omega}_{sr}^{(l,l)} \quad \text{with } l = \{1,2\}$$

Gupta-Yos Mixing Rule
Global viscosity μ and thermal conductivities λ_k are averaged according to gas composition x_s

$$\mu = \sum_s \frac{x_s m_s}{\sum_r x_r \Delta_{sr}^{(2)}}$$

$$\lambda_{\mathrm{tra}} = \frac{5}{2}\sum_s \frac{x_s m_s C_{\mathrm{V}\,\mathrm{tra},s}}{\sum_r \alpha_{sr} x_r \Delta_{sr}^{(2)}}$$

$$\lambda_{k\neq\mathrm{tra}} = \sum_s \frac{x_s m_s C_{\mathrm{V}\,k,s}}{\sum_r x_r \Delta_{sr}^{(1)}}$$

Effective diffusion
The diffusion coefficient of each chemical species relative to the mixture D_s is averaged from the binary diffusion coefficients D_{sr}

$$D_{sr} = \frac{k_{\mathrm{B}} T_c}{P\Delta_{sr}^{(1)}} \qquad \rightarrow \qquad D_s = \frac{1 - x_s}{\sum_{r\neq s} \frac{x_r}{D_{sr}}}$$

Diffusion Flux

- Generalized Fick Law: $\vec{J}_s^* = \rho D_s \vec{\nabla}(c_s)$

Mass Conservation

Due to approximations, the total diffusion flux violates the mass conservation condition

$$\sum \vec{J}_s = \vec{\varepsilon} \neq 0$$

Ambipolar Effect

Due to charge interaction, ions and electrons have similar diffusion velocities. Can be introduced by ensuring neutral flux:

$$\sum q_s \vec{J}_s = 0$$

and correcting the ion diffusion coefficient:

$$D_{\text{ion}}^a = \left(1 + \frac{T_{\text{e}}}{T_{\text{ion}}}\right) D_{\text{ion}}$$

Flux Correction

An improved normalization method was implemented that ensures both conditions:

$$\vec{\varepsilon} = \frac{\sum\limits_{s \neq \text{e}} \vec{J}_s^* + \sum\limits_{s=\text{ion}} \frac{M_{\text{e}}}{M_s} \vec{J}_s^*}{1 + \sum\limits_{s=\text{ion}} \frac{M_{\text{e}}}{M_s} \frac{c_s}{1 - c_{\text{e}}}}$$

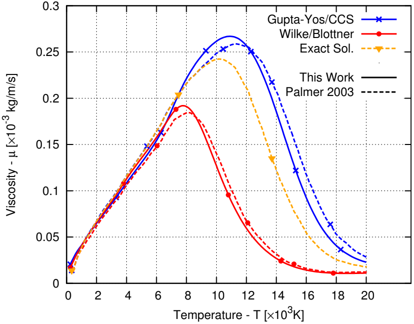
$$\vec{J}_{s \neq \text{e}} = \vec{J}_s^* - \frac{c_s}{1 - c_{\text{e}}} \vec{\varepsilon}$$

$$\vec{J}_{\text{e}} = M_{\text{e}} \sum_{s=\text{ion}} \frac{1}{M_s} \vec{J}_s$$

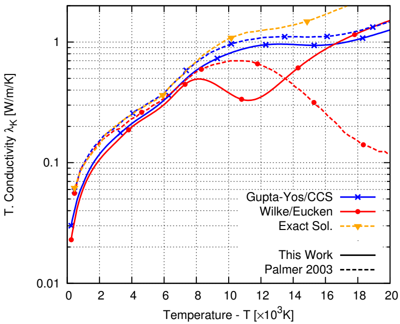
Verification & Validation

Results for the equilibrium composition of Air (11 species) at $P = 1\,\text{atm}$

Viscosity μ



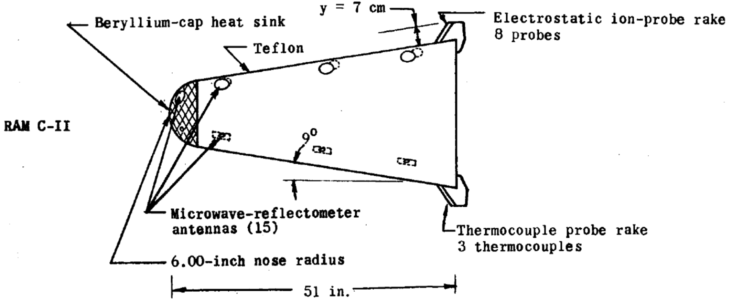
Total Thermal Conductivity λ



- Good correlation with previous work. Discrepancies due to different input data.
- Both models are valid only at low temperatures (weakly ionized gas).
- Gupta-Yos/CCS model is accurate for a larger temperature range.
- Wilke/Blottner/Eucken model is 50% faster to compute.

Application: RAM-C II Experiment

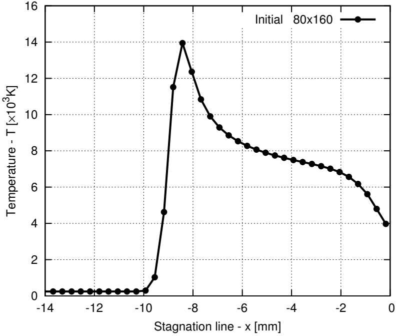
Experiments in the late 1960's for studying communications blackout, measured the electron density in the plasma around a blunt capsule, as it reenters earth atmosphere.

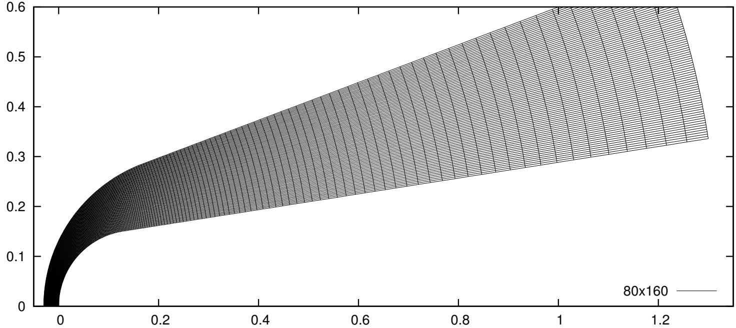


- The conditions at 61 km altitude, $\mathrm{Ma} = 24$, have been simulated.

Computational Mesh
Axisymmetric Flow → 2D Mesh

1. Initial Uniform Mesh 80×160 cells





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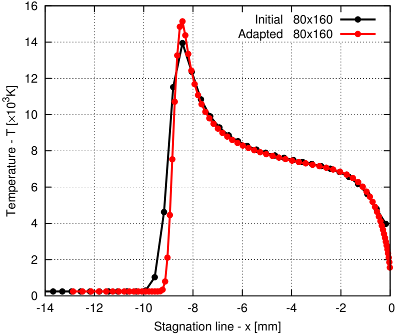
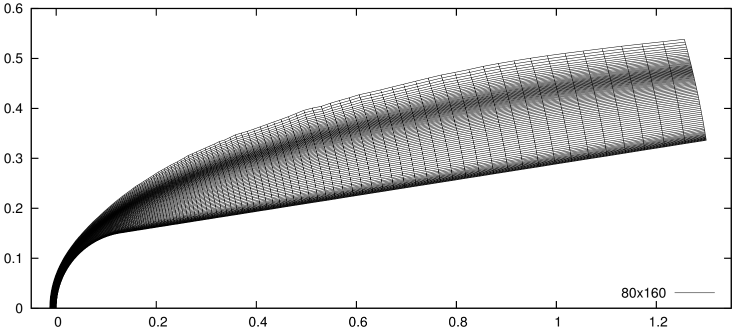
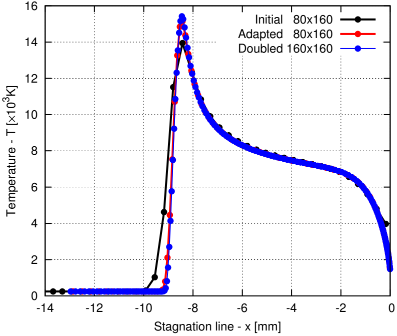


1. Initial Uniform Mesh 80×160 cells
2. Clustering at Shock and Wall

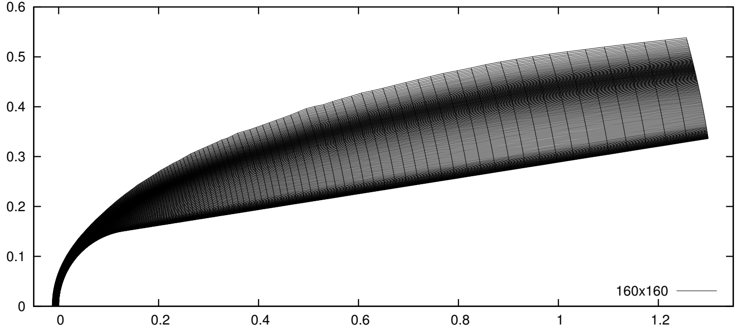


Computational Mesh

Axisymmetric Flow $\rightarrow$ 2D Mesh



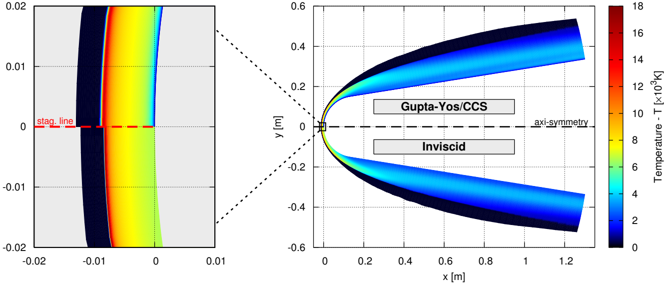
1. Initial Uniform Mesh 80×160 cells
2. Clustering at Shock and Wall
3. Doubling for convergence check

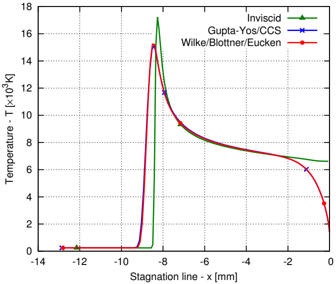


Temperature

Thermal equilibrium

RAM-C II $h = 61$ km Ma $= 24$
$T_\infty = 244$ K $P_\infty = 19.3$ Pa $V_\infty = 7650$ m/s
$T_{\mathrm{wall}} = 1200$ K (BC: Isothermal, Non-Catalytic)



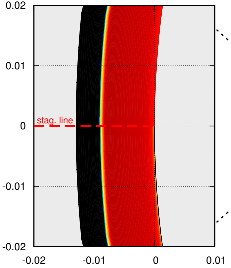


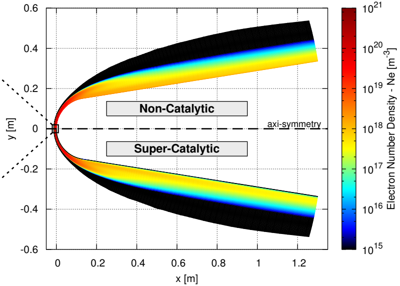
- When transport processes (dissipation) are considered:
  - Peak temperature 13% lower.
  - Significant improvement in behavior at the wall.
  - Better solver stability.
- Difference between the two transport models is negligible.

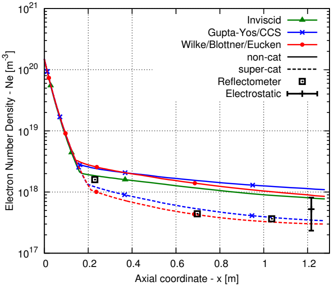
Electron Density (experiment results)

Thermal equilibrium, catalytic effect

RAM-C II	h = 61 km	Ma = 24
T_∞ = 244 K	P_∞ = 19.3 Pa	V_∞ = 7650 m/s
T_{wall} = 1200 K	(BC: Isothermal)	





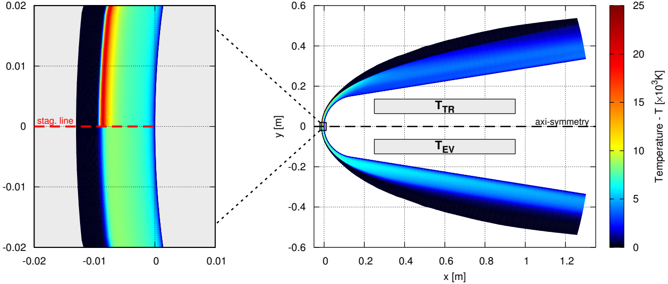


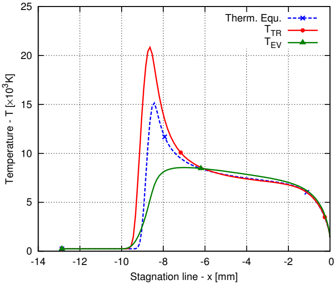
- Wall catalicity condition has a significant effect.
- Excellent agreement of the results with experimental data, when total ion recombination at the wall is considered.
- The influence of the transport model is negligible.

Thermal Non-Equilibrium

Two temperature model: T_{TR}, T_{EV}

RAM-C II h = 61 km Ma = 24
T_∞ = 244 K P_∞ = 19.3 Pa V_∞ = 7650 m/s
T_{wall} = 1200 K (BC: Isothermal, Non-Catalytic)

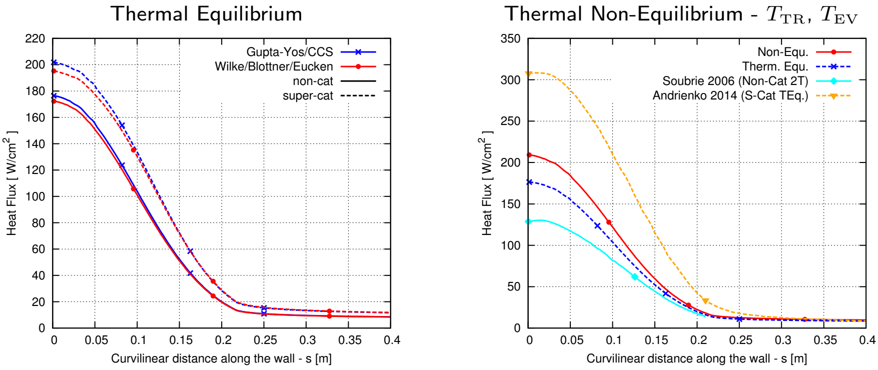




- The non-equilibrium effect is very strong with 40% difference of T_{TR} relative to equilibrium, and 60% between T_{TR} and T_{EV}.
- Causes increase in shock thickness and standoff distance.
- Correlation with experimental results for electron density not significantly affected.

Wall Heat Flux

RAM-C II	h = 61 km	Ma = 24
T_∞ = 244 K	P_∞ = 19.3 Pa	V_∞ = 7650 m/s
T_{wall} = 1200 K	(BC: Isothermal)	



- Negligible effect of the transport model (2%).
- Significant influence of wall catalicity (14%).
- Significant effect of thermal non-equilibrium (19%).
- Within the range of predictions found on previous works.

Conclusions

- Two transport models were successfully implemented with flexibility for any multi-temperature model. Improvements introduced in charged particle diffusion.

- Implementation validated against previous works and experimental data in an application case. Both models are well suited for the case tested, although the Gupta-Yos/CCS model is known to be more accurate for higher entry velocities.

- New capabilities added to the SPARK code, such as the computation of the heat flux at the wall.

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Future Works:

- Additional V&V should be performed for other multi-temperature and chemical models, and also on different flow conditions.
- Update the collision cross section and viscosity database for Air, and complement data with additional chemical species – different planetary atmospheres.
- Extend the transport modeling for use with state-to-state chemistry.

Thank you!

Questions?

Suggestions?