Abstract Preparation Instructions

Authors are requested to prepare their abstract directly in the Indico abstract submission form. The abstract editor supports **Markdown** formatting and a limited subset of **LaTeX mathematical expressions**.

Please submit your abstract under contributions

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The Don'ts

- **Do not use \ce{N2}** or other mhchem commands, as packages such as mhchem are not supported by the Indico abstract editor. Instead, use inline LaTeX notation such as N_2 when chemical formulas are embedded in a sentence.
- Do not use HTML tags <sup> or <sub>. Instead, use LaTeX notation, e.g. ^{2} for superscripts and $_2$ for subscripts.
- Do not capitalize the entire title. Use sentence case and capitalize only the first letter of the title (except for proper nouns and standard acronyms).
- Do not include the authors at the top of the contribution. There is a dedicated section at the bottom of the submission form for entering author information. Your contribution should begin directly with the abstract text.

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Text Formatting

The following Markdown syntax may be used:

```
# Section Heading

## Subsection Heading

**Bold text**

*Italic text*

- Bullet item 1
- Bullet item 2

1. Numbered item 1
2. Numbered item 2
```

Mathematical Formulae

Simple LaTeX expressions can be **included inline using single dollar signs**. (Do not use \ce{}):

The heat flux is given by $q = k \nabla T$.

Chemical Species and Formulae

Chemical species, reactions, and material compositions should be written using standard LaTeX mathematical notation.

```
$N_2$, $O_2$, $NO$, $CO_2$, $H_2O$

$N + O \rightarrow NO$

$C_f/C-SiC$
```

```
$N_2^+$
$O^-$
$SiO_2$
$Al_2O_3$
``
```

-

Tables

Tables can be created directly in Markdown using the pipe (|) character.

Example:

```
*Table 1. Test conditions for the investigated cases.*

| Case | Velocity (km/s) | Enthalpy (MJ/kg) |
|------|----------------:|-----------------:|
| 1    | 10.0            | 30.5             |
| 2    | 12.5            | 42.7             |
| 3    | 15.0            | 58.1             |
```

Renders as:

Table 1. Test conditions for the investigated cases.

Case	Velocity (km/s)	Enthalpy (MJ/kg)
1	10.0	30.5
2	12.5	42.7
3	15.0	58.1

Please note:

- Keep tables simple.
- Avoid merged cells, multi-row headers, and complex formatting.
- Use SI units in column headers whenever possible.

- Provide a table caption immediately above or below the table.

References

References should be included at the end of the abstract in a dedicated **References** section.

The Indico abstract editor does **not** support BibTeX or LaTeX citation commands such as \cite{}. Therefore, references must be entered manually and cited in the text using numbered brackets.

Example citation within the text:

The catalytic recombination behaviour of ceramic TPS materials has been studied extensively [1].

Example citation within the text:

```
## References

[1] Smith, J., and Jones, P., "Catalytic Surface Effects on High-Temperature Ceramics," Journal of Thermophysics and Heat Transfer, Vol. 35, No. 2, 2021, pp. 123–135.

[2] Brown, A. et al., "Experimental Investigation of Reusable Thermal Protection Systems," Proceedings of the 10th International Workshop on Radiation of High Temperature Gases in Atmospheric Entry, 2024.

```

Please ensure that all references are complete and contain sufficient bibliographic information (authors, title, publication, year, volume, pages, DOI where available) to allow readers to locate the source. Citations should be numbered in the order in which they first appear in the text.

Figures

Figures should be uploaded directly through the Indico abstract editor. To ensure unique file names and avoid conflicts, please name figure files according to the convention:

```
figure_<ID>_<number>.png
```

where:

- <ID> is the abstract/contribution ID assigned by Indico.
- <number> is the figure number within the abstract.

```
figure_6997_01.png
figure_6997_02.png
figure_6997_03.png
```

After uploading a figure, hover the mouse cursor over the uploaded image or image link and copy the displayed URL. Insert the figure in the Markdown editor using this URL. Each figure should be accompanied by a caption placed directly below the image.

Example:

```
![Figure 1](https://indico.esa.int/event/.../figure_6997_01.png)

*Figure 1. T6 Stalker Tunnel schematic.*
`
```

Figures should be referenced in the text as **Fig. 1**, **Fig. 2**, etc. Images should be provided in PNG, JPG, or JPEG format and with sufficient resolution to ensure readability.

To include Movies mp4:

<img src="PASTE_YOUR_IMAGE_URL_HERE" alt="Click to Watch Video" width="500">

Equations

Mathematical expressions may be included using LaTeX notation. Inline equations should be enclosed in single dollar signs ($...$), while displayed equations should be written using the equation environment. Display equation can only be used with \begin{equation} ....

Inline equation:

```
The vibrational temperature is denoted by $T_v$.
```

Displayed equation:

```
The global direct reaction rate is given by

\begin{equation}
K^d(T,T_v)=\sum_v k_v^d(T)f_v(T_v)
\end{equation}
```

If you like to number your equation use \tag{}

```
\begin{equation}
K^r(T)=\frac{K^d(T,T)}{K_{eq}(T)}
\tag{2}
\end{equation}
```

Please note:

- Use standard LaTeX notation for equations.
- Number equations manually using \tag{1}, \tag{2}, etc.
- Use ${N_2}$, ${O_2}$, ${H_2}$, etc. for chemical species.
- Do **not** use commands from unsupported packages such as \ce{}.
- Avoid advanced LaTeX environments that require additional packages.
- do not use $$..$$ for display equations

Examples:

1. INTRODUCTION

One of the side effects of using drag to slow-down spacecraft during their entry into an atmosphere is the resulting substantial heating to the vehicle. The resulting heat flux, which can lead to failure of the structure, is strongly influenced by a change in gas composition due to the sudden and steep temperature gradient through the shock near the surface [Jr.19]. These strong thermochemical reactions take place within the shock layer, in which the imbalance in gas species initially results in a state of nonequilibrium where the internal degrees of freedom of the gas are excited, heavily influencing radiation. For missions such as Mars return, during which entry velocities can be as high as 15 km/s, radiative heating becomes the primary source of heat load on the vehicle's surface [BJ14]. As this process involves complex models and is computationally expensive, laboratory ground testing can reduce uncertainty by providing validation data. Shock tube experiments are a tool to recreate these thermochemical phenomena in a ground-based facility.

Emission spectroscopy can be used to investigate a slug of gas thermochemically similar to the gas encountered by the vehicle during re-entry in order to measure radiative emission and spatially resolve temperature and gas species densities. Knowledge of these quantities offers a better understanding of the flowfield around the vehicle, and a better prediction of the contribution from radiative heat transfer, currently predicted with an uncertainty of the order of 80% [JMG+13]. This uncertainty leads to excessive safety margins in the design of thermal protection systems, which amount to a substantial portion of the vehicles' mass. It is therefore crucial to be able to quantify it.

spectral data particularly useful to characterise the flow. As density is especially low during high-altitude flight, or in atmospheres as thin as Mars', equilibrium states take more time to be reached. The non-equilibrium component of the shock layer, where dissociation, ionisation and excitation are not in equilibrium with their backwards

reactions, can account for a large proportion of the emitted radiation [BJC16]. Although critical, the quantity of existing spectra dataset in the VUV region is limited due to its challenging acquisition.

2. Experimental arrangement

2.1. Facility

The T6 Stalker Tunnel shock tube was previously used to perform emission spectroscopy in the wavelength regime of 300-850 nm to measure radiation in the shock layer [CDM19a, GCM21, GCJ+]. A VUV emission spectroscopic system is currently under development to use on T6 in its shock tube mode, with the goal to perform spectroscopy for shots in the velocity range of 10-15 km/s. The T6 Stalker Tunnel is a high enthalpy ground testing facility, able to perform as a reflected shock tunnel, an expansion tube, or a shock tube of different diameters. Its latter mode is of interest in this paper, but details of the facility's development were reported in various publications [CDS+21, SCG+]. A schematic of the tunnel in its different configurations is shown in Fig.1.

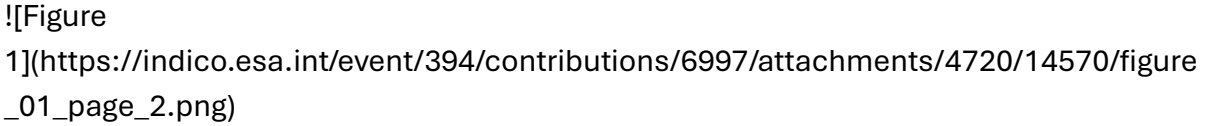

Figure 1. T6 Stalker Tunnel schematic [CDM+19b].

The driver section contains a piston separating high pressure reservoir gas and lower-pressure, low molecular weight compression tube gas. The piston is accelerated by the reservoir gas and quickly compresses the driver gas to high pressure and temperature against a metal diaphragm separating the driver and the shock tube. When the

diaphragm ruptures, the driver gas is free to expand into the low-pressure test gas, driving a shock wave, while still compressed by the piston to maintain pressure in the driver section and avoid expansion waves to travel downstream and interact with the shock. The slug of gas following the shock undergoes the same non-equilibrium thermochemical processes as the stagnation streamline in front of a (re-)entering vehicle, allowing investigation of

emitted radiation of interest.

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Introduction

In the last years, state-to-state (StS) chemical kinetics have been used to model high-enthalpy flows in 2D configurations in dissociating air [Bonelli et al., 2024; Guo et al., 2024; Wang et al., 2023]. The recent interest in the exploration of ice giant planets [Blanc et al., 2021] needs the construction of kinetic schemes for Hydrogen/Helium mixture plus some impurities (CH_4), which give a relevant contribution to the radiation emission in the shock layer.

A pure H_2/He StS kinetic scheme, originally developed to describe volume sources of negative ion production [Celiberto et al., 2023; Colonna et al., 2017], has been used to model EAST shock tube experiment in conditions of Saturn entry [Cruden et al., 2017], reproducing the ionisation profile [Colonna et al., 2020]. It has been shown that ionisation is more efficiently initiated by the reaction $2\text{H}_2 \rightleftharpoons \text{H}_3^+ + \text{H}^-$ than by ionising recombination ($2\text{H} \rightleftharpoons \text{H}_2^+ + e^-$), the latter limited by the dissociation kinetics.

A StS model accounting for ionisation should also describe the free electron kinetics, through the solution of the Boltzmann equation [Colonna et al., 2022], and, together with the vibrational levels, the evolution of electronically excited states of atoms and molecules [Colonna et al., 2001].

A multi-temperature (mT) model rigorously derived from the StS is here presented. The state-specific cross section database has been updated so as to include the most accurate data available for the electron-impact induced inelastic and dissociative processes of H_2 [Scarlett et al., 2021] and the mT model still follows the kinetics of selected electronically excited states of molecular hydrogen. The equation for vibrational energy relaxation includes also the contribution of chemical processes.

Implementation of Rapidly-Scanned, Infrared Laser Absorption Diagnostics in NASA utilizes a laser at 226 nm with a bandwidth of $\approx 15\text{ cm}^{-1}$ to excite multiple levels near the (0,0) bandhead of the NO $\text{A}^2\Sigma^- - \text{X}^2\Pi$ system. The NO MTV beam is critical for these high-enthalpy measurements.

From State-to-State to multi-Temperature

A mT model assumes that the internal distributions follow the Boltzmann function with independent internal temperatures T_v. Given a process like $\text{H}_2(v) + X \rightleftharpoons \cdots$ with k_v^d and k_v^r direct and reverse rate respectively, the kinetic equation contains the term proportional to $k_v^d(T)f_v(T_v)$ and to $k_v^r(T)$, where f_v is the vibrational distribution. The global rates are given by:

\begin{equation}

K^d(T,T_v) = \sum_v k_v^d(T)f_v(T_v) \tag{1}

\end{equation}

\begin{equation} K^r(T) = \sum_v k_v^r(T) \tag{2} \end{equation}

and the contribution to the internal energy by:

\begin{equation}

\mathcal{L}(T,T_v) = \sum_v \varepsilon_v k_v^d(T)f_v(T_v) \tag{3} \end{equation}

\begin{equation}

\mathcal{G}(T) = \sum_v \varepsilon_v k_v^r(T) \tag{4}

\end{equation}

where the symbols $\mathcal{L}$ and $\mathcal{G}$ indicate the rate of energy loss and gain respectively. It should be noted that only K^d and $\mathcal{L}$ depend on T_v, while K^r and $\mathcal{G}$ are only a function of T. The reverse rates are not independent and can be calculated from the direct ones using the detailed balance principle:

\begin{equation}

K^r(T) = K^d(T,T) / K_{eq}(T) \tag{5}

\end{equation}

A similar procedure is followed to calculate global rates for processes induced by electron collision, $e^- + \text{H}_2(v)$. The first step consists in calculating the StS rates as a function of the electron temperature T_e:

\begin{equation}

k^d_v(T_e) = \int_{\varepsilon^\star_v}^{\infty} f^M_e(\varepsilon,T_e) u(\varepsilon) \sigma_v(\varepsilon) \varepsilon \tag{6}

\end{equation}

where f^M_e is a Maxwell electron energy distribution function, ε the electron energy, u the electron velocity and σ_v the cross section of the process. The quantity $\varepsilon^\star_v$ is the threshold corresponding to the amount of energy lost by electrons in the process. Then the global rates as a function of T_e and T_v can be calculated using the previous global rate equations.

In the absence of an applied electromagnetic field, it is reasonable to assume that free electrons are in equilibrium with the gas temperature [Colonna et al., 2020]. For the sake of completeness, the contribution of these processes to the electron energy equation are given by:

\begin{equation} \mathcal{L}(T,T_v) = \sum_v \varepsilon_v^\star k_v^d(T)f_v(T_v) \tag{7} \end{equation}

\begin{equation} \mathcal{G}(T) = \sum_v \varepsilon_v^\star k_v^r(T) \tag{8}

\end{equation}

that should be added to the Landau-Teller terms due to elastic collisions with heavy particles.

To evaluate the emission accurately, the emission coefficient is calculated using the following relations:

\begin{equation} \varepsilon_{u l}=\frac{E_u-E_l}{4 \pi} \mathcal{A}_{u l} n_i(p, T) g_u \frac{e^{-E_u /\left(k_{\mathrm{B}} T\right)}}{Q_{\mathrm{int}, i}(T)}, \tag{9} \end{equation}

\begin{equation} \mathcal{R}(T_{SF_{\lambda_1-\lambda_2}})=\sum_p \left[\varepsilon^\text{synth}\left(\lambda_p,T\right)-\varepsilon^\text{meas}\left(\lambda_p\right)\right]^2 / \left[\varepsilon^\text{meas}\left(\lambda_p\right)\right]^2, \tag{10} \end{equation}

The numerical values of the K^d have been fitted as a function of T and T_v with a 2D best fitting procedure. Quantum effects and anharmonicity of the vibrational levels make the Arrhenius expression not accurate enough to fit the data in the long range. In order to preserve continuity full-range expressions have been used, accurate in the temperature interval $100 \div 10^5$. The fitting expression is generally given as a function T:

\begin{equation} K^d(T,T_v) = f(T;\{c_i(T_v)\}) \tag{11} \end{equation}

whose coefficients c_i are functions of T_v. The functions used are generally the sum of Arrhenius or of sigmoids:

\begin{equation} \sigma_f(x) = a \frac{e^{(x-c)/\ell}}{e^{(x-c)/\ell} + e^{-(x-c)/\ell}} \tag{12} \end{equation}

Conclusion

A novel mT model has been derived from accurate StS dynamical data. This is the first step toward a mT model of the entry in Ice Giants, including impurities already present in the atmosphere or evaporated from the vehicle surface. As in the traditional mT approaches, this model cannot take into account the departure from the Boltzmann distributions. However, corrections are possible, by adding an equation for the tail of the distributions [Colonna et al., 2008] to correct the rates with the contribution of highly-excited vibrational levels.

Acknowledgements

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References

[Bonelli et al., 2024] Bonelli, F., Ninni, D., Colonna, G., & Pascazio, G. (2024). "A finite-volume hybrid weno/central-difference shock capturing approach with detailed state-to-state kinetics for high-enthalpy flows," *Aeronautics and Astronautics*, p. 170.

[Guo et al., 2024] Guo, J., Wang, X., & Li, S. (2024). "Investigation of high enthalpy thermochemical nonequilibrium flow over spheres," Physics of Fluids, vol. 36, no. 1.

[Wang et al., 2023] Wang, X., Guo, J., Hong, Q., & Li, S. (2023). "High-fidelity state-to-state modeling of hypersonic flow over a double cone," Physics of Fluids, vol. 35, no. 11.

[Blanc et al., 2021] Blanc, M., Mandt, K., Mousis, O., André, N., Bouquet,

A., Charnoz, S., ... & Horizon 2061 team. (2021). "Science goals and mission objectives for the future exploration of ice giants systems: a horizon 2061 perspective," Space Science Reviews, vol. 217, pp. 1-59.

[Celiberto et al., 2023] Celiberto, R., Capitelli, M., Laricchiuta, A., Pietanza, L. D., & Colonna, G. (2023). "Advanced models for negative ion production in hydrogen ion sources," Physics and Applications of Hydrogen Negative Ion Sources, pp. 167-188. Springer.