Simulation of electronic excitation in transitional atmospheric entry flows.

J. Amorosetti(1), A. Bultel(1), S. Boccelli(2), T. Magin(2), J. Annaloro(3)

(1) CORIA, Saint-Etienne-du-Rouvray, France

(2) Von Karman Institute, Rhode-Saint-Genèse, Belgium

(3) CNES, Toulouse, France

Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modeling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

1. Testcase and baseline flow computation
2. Non-equilibrium effects

Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modeling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

1. Testcase and baseline flow computation
2. Non-equilibrium effects

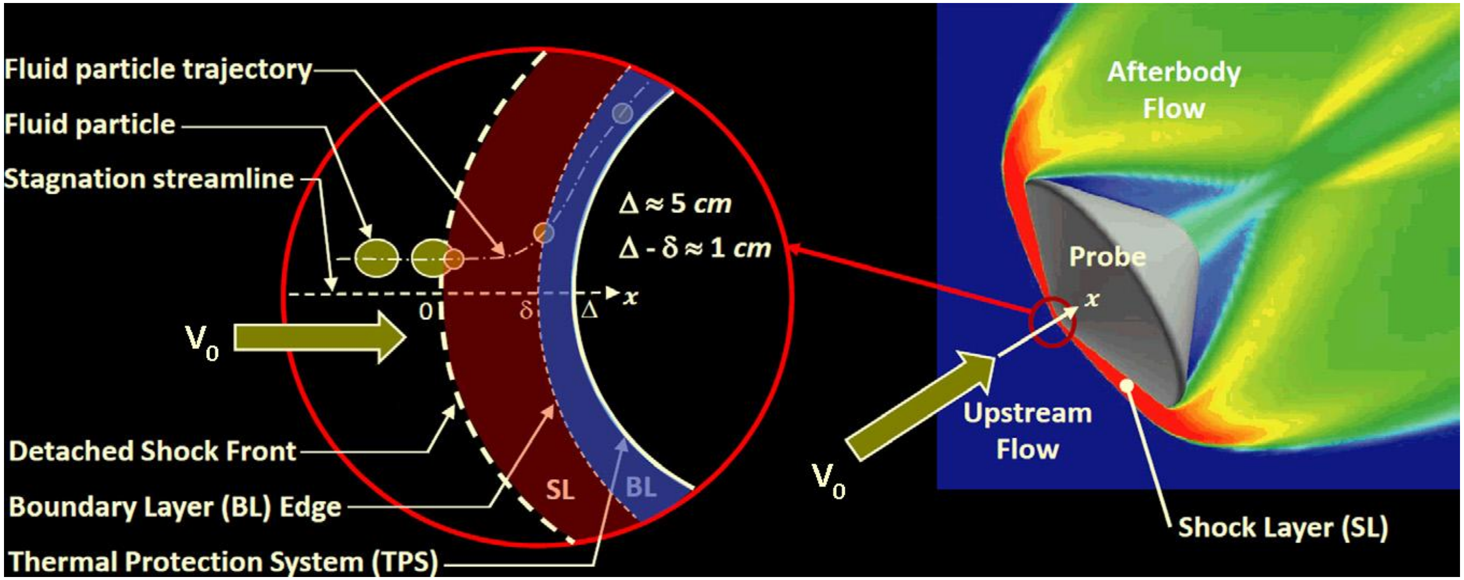
Atmospheric entry flows

Debris from Low Earth Orbit: $V_0 \approx 7$ - 8 km/s $M_0 \approx 25$

Survivability of fragments and trajectory

Size, number, impact zone ?

→ Need for reliable aerothermodynamic computations



Bultel et Annaloro, Plasma Sources Sci. Technol. 22 (2013).

Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modeling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

1. Testcase and baseline flow computation
2. Non-equilibrium effects

Utility of collisional-radiative modeling

Deriving thermo-chemical coupling models

Multi-temperature fluid models:

Equations for each energy mode *m* (e.g. translation, vibration, electronic) :

$$\frac{\partial}{\partial t}(\rho e^m) + \nabla \cdot (\rho e^m \boldsymbol{u}) + \nabla \cdot \boldsymbol{q}^m = \Omega^m + \mathscr{P}^m$$

- Coupling terms describing the coupling between modes $\boldsymbol{\Omega^m}$
- Nonequilibrium reaction rates $\mathbf{k(T_{tr}, T_{vib}, T_{el}, \ldots)}$: account for the strong influence of non-equilibrium distributions on chemical processes.

→ Improve empirical models

$$\boldsymbol{\Omega^{VT,diss}} = \sum_s \boldsymbol{e_s^{vib}\omega_s}$$

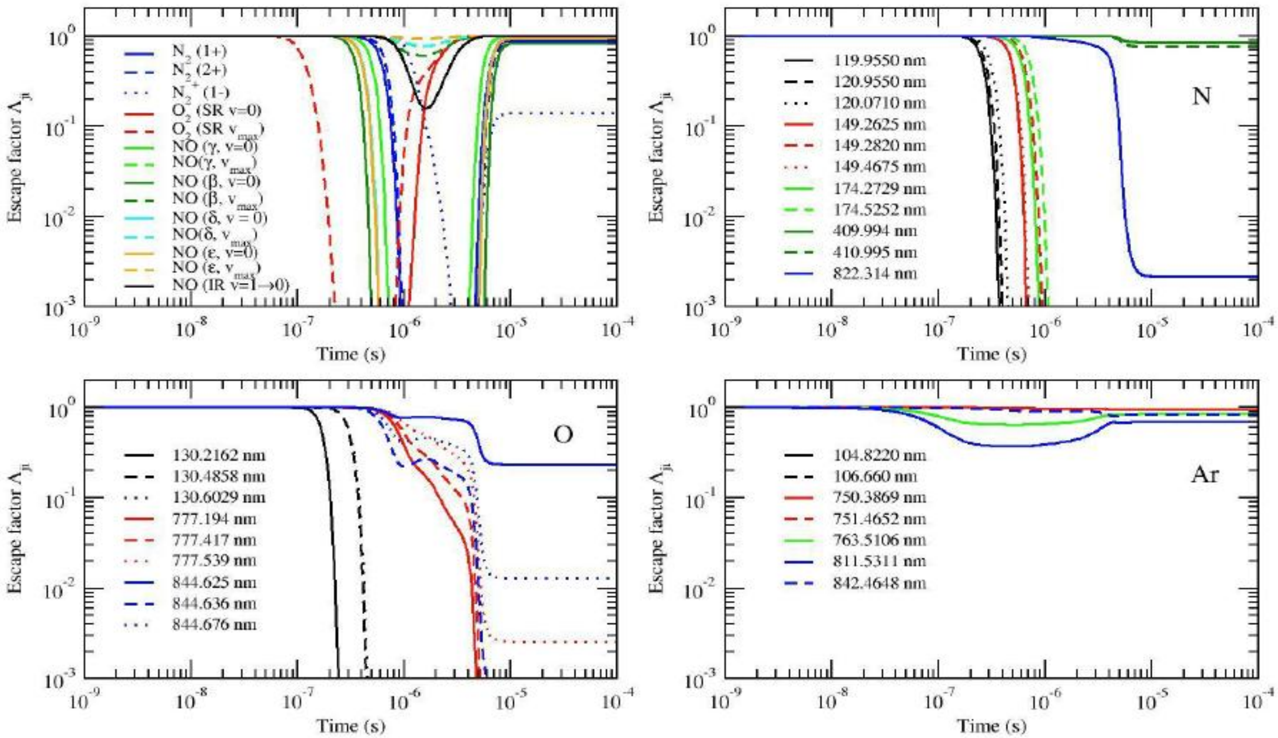
$$\boldsymbol{k^{diss}(T, T_{vib})} = \boldsymbol{k^{diss}(\sqrt{TT_{vib}})}$$

…

Utility of collisional-radiative modeling

Simulate Non-equilibrium radiation

- approximate treatment (escape factors) → source term $\mathcal{P}^m$



Annaloro and Bultel, Phys. Plasmas 21 (2014).

- accurate radiative transfer computations

Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modelling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

1. Testcase and baseline flow computation
2. Non-equilibrium effects

Peculiarities of transitional flows

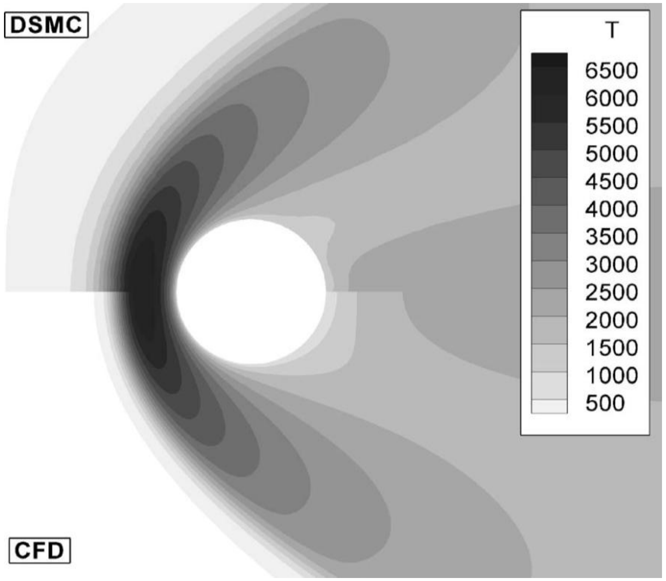
Rarefaction effects

High altitude (≈ 80 km) : $\mathbf{Kn} \approx \mathbf{0.001 - 0.1}$

$$Kn = \frac{\lambda}{L} \qquad \lambda_{HS} = \frac{1}{n\sqrt{2}\pi d^2}$$

- Diffuse shock
- Breakdown of behaviour laws (Newton / Fourier…)
- Velocity and temperature slip at the wall
- Non-equilibrium chemical rates

$$k(T) = \int_{x_0}^{\infty} x e^{-x} \sigma(x) dx$$



Lofthouse, Phys. Fluids 19 (2007).

Introduction

➢ Statistical fluctuations and trace species: $\mathbf{s_1, s_2}$ **with** $\mathbf{n(s_1) \ll n(s_2)}$

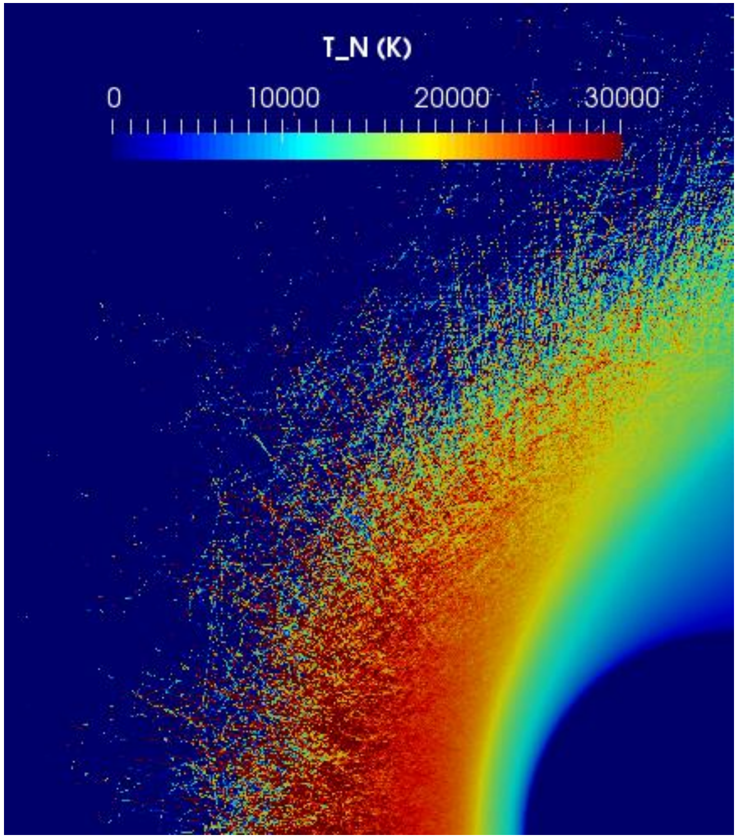
$$\propto \frac{1}{\sqrt{N_{samples}}}$$

Direct state-to-state computation:

- Prohibitive computational cost
- Waste of numerical ressources
- Uncertainty on cross sections

Weighting schemes:

- Handling of inelastic collisions and conservation of energy problematic
- Wide range of concentrations : weight separation ?
- Still uncertainty on cross sections



Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modelling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

1. Testcase and baseline flow computation
2. Non-equilibrium effects

Description of the CoRaM-Air model

CoRaM - Air

- 11 species, ≈ 400 levels
- State-to-sate for **electronic** mode (all species)
- ≈ 60000 elementary reactions

N_2 :	$X^1\Sigma_g^+$, $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'^3\Sigma_u^-$, $a'^1\Sigma_u^-$, $a^1\Pi_g$, $w^1\Delta_u$, $G^3\Delta_g$, $C^3\Pi_u$, $E^3\Sigma_g^+$
O_2 :	$X^3\Sigma_g^-$, $a^1\Delta_g$, $b^1\Sigma_g^+$, $c^1\Sigma_u^-$, $A'^3\Delta_u$, $A^3\Sigma_u^+$, $B^3\Sigma_u^-$, $f^1\Sigma_u^+$
NO :	$X^2\Pi$, $a^4\Pi$, $A^2\Sigma^+$, $B^2\Pi$, $b^4\Sigma^-$, $C^2\Pi$, $D^2\Sigma^+$, $B'^2\Delta$, $E^2\Sigma^+$, $F^2\Delta$
N_2^+ :	$X^2\Sigma_g^+$, $A^2\Pi_u$, $B^2\Sigma_u^+$, $a^4\Sigma_u^+$, $D^2\Pi_g$, $C^2\Sigma_u^+$
O_2^+ :	$X^2\Pi_g$, $a^4\Pi_u$, $A^2\Pi_u$, $B^4\Sigma_g^-$
NO^+ :	$X^1\Sigma^+$, $a^3\Sigma^+$, $b^3\Pi$, $W^3\Delta$, $b'^3\Sigma^-$, $A'^1\Sigma^+$, $W^1\Delta$, $A^1\Pi$
N :	${}^4S°_{3/2}$, ${}^2D°_{5/2}$, ${}^2D°_{3/2}$, ${}^2P°_{1/2}$, ...(177 levels)
O :	${}^3P_2$, ${}^3P_1$, ${}^3P_0$, ${}^1D_2$, ...(146 levels)
N^+ :	${}^3P_0$, ${}^3P_1$, ${}^3P_2$, ${}^1D_2$, ... (9 levels)
O^+ :	${}^4S°_{3/2}$, ${}^2D°_{5/2}$, ${}^2D°_{3/2}$, ${}^2P°_{3/2}$, ...(8 levels)

Description of the CoRaM-Air model

Elementary processes

- Inelastic collisions

$$A(i) + M \rightleftarrows A(i') + M$$
$$A(i) + B(j) \rightleftarrows A(i') + B(j')$$

- Chemical reactions

$$A(i) + B(j) \rightleftarrows C(k) + D(l)$$
$$A(i) + M \rightleftarrows C(k) + D(l) + M$$

Implementation in Mutation++ open-source library.

Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modelling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

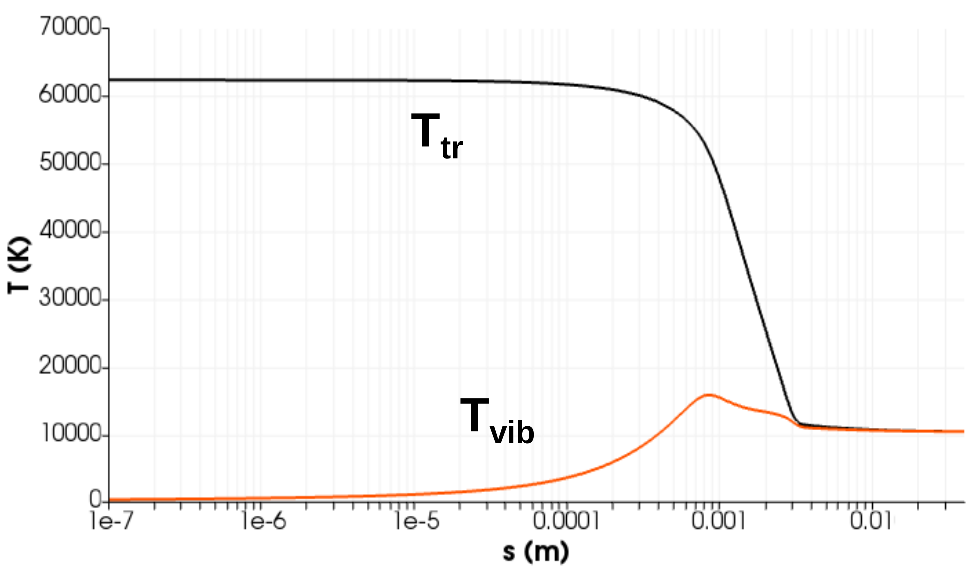
1. Testcase and baseline flow computation
2. Non-equilibrium effects

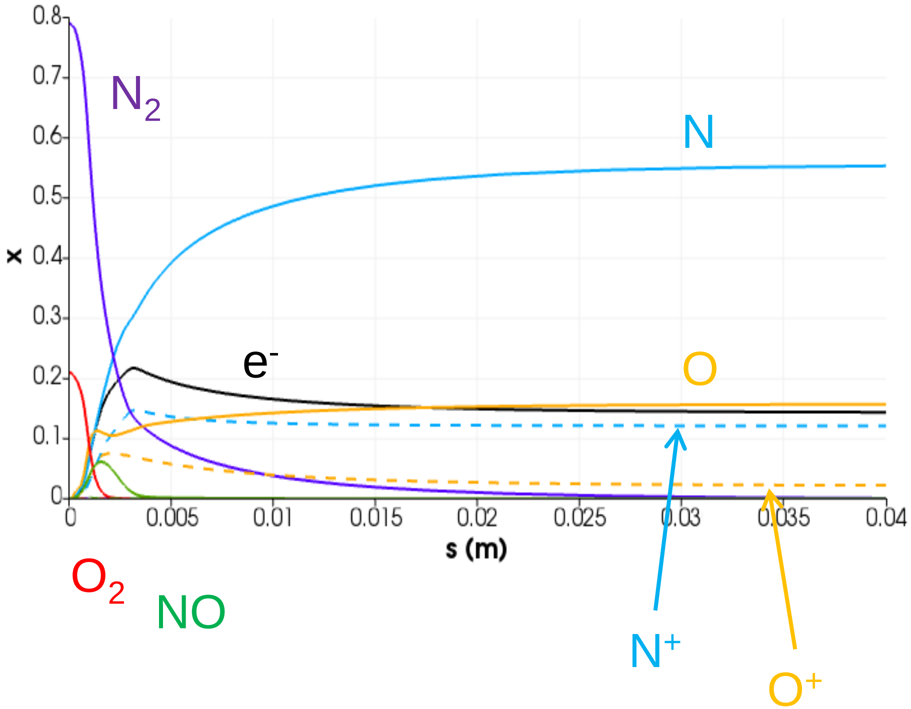
Hypersonic flow study

1D shock crossing computations (Euler T-Tv) ; FIRE-II conditions

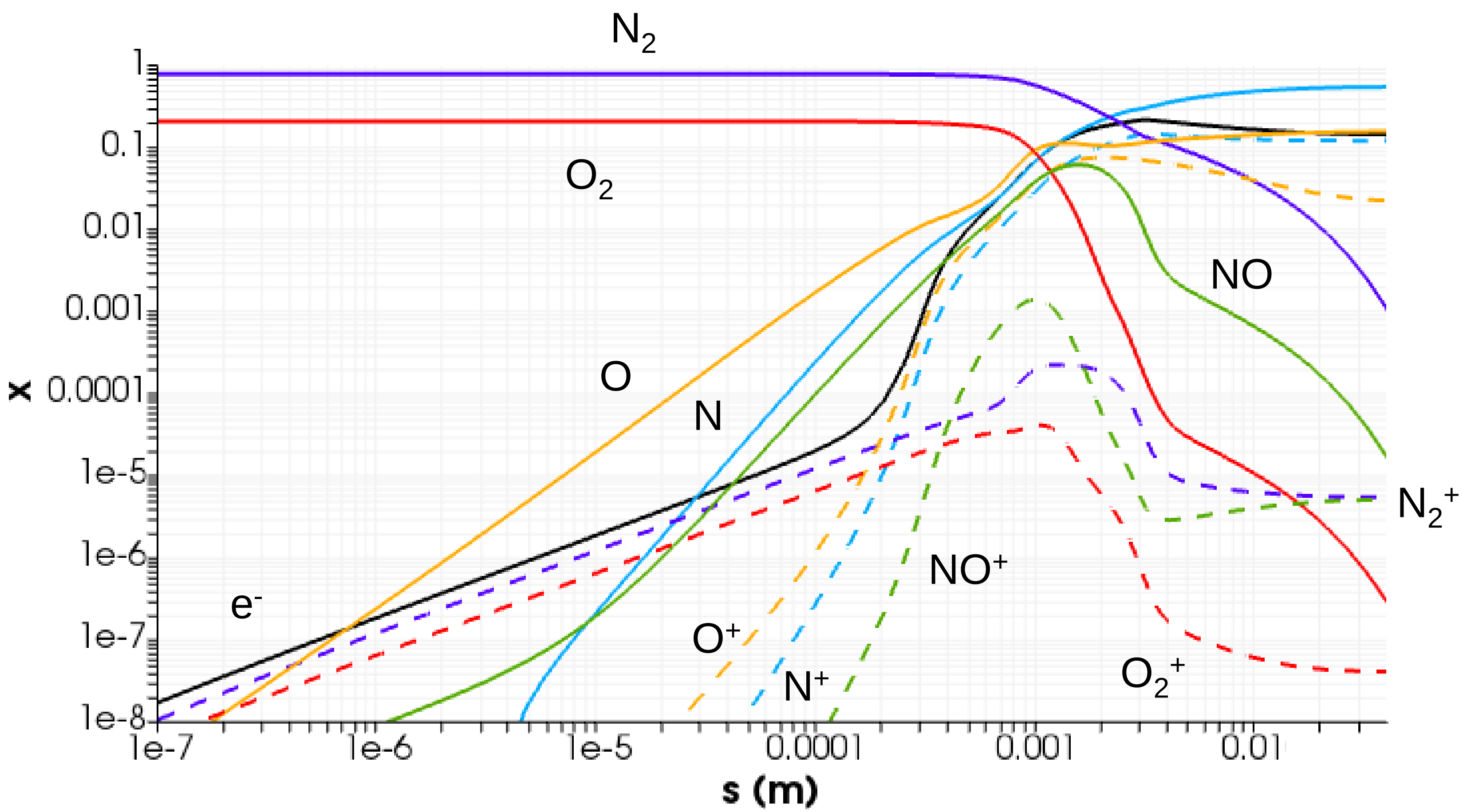
$T_{tr,\,0} = 195$ K $p_0 = 2$ Pa

$T_{tr,\,1} \approx 60000$ K



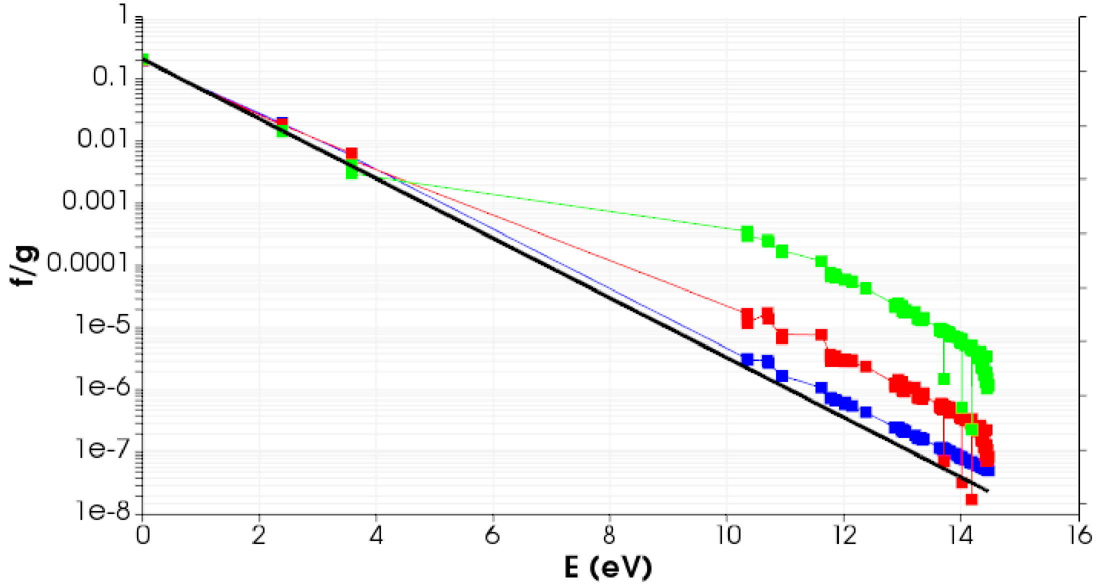


Hypersonic flow study



Hypersonic flow study

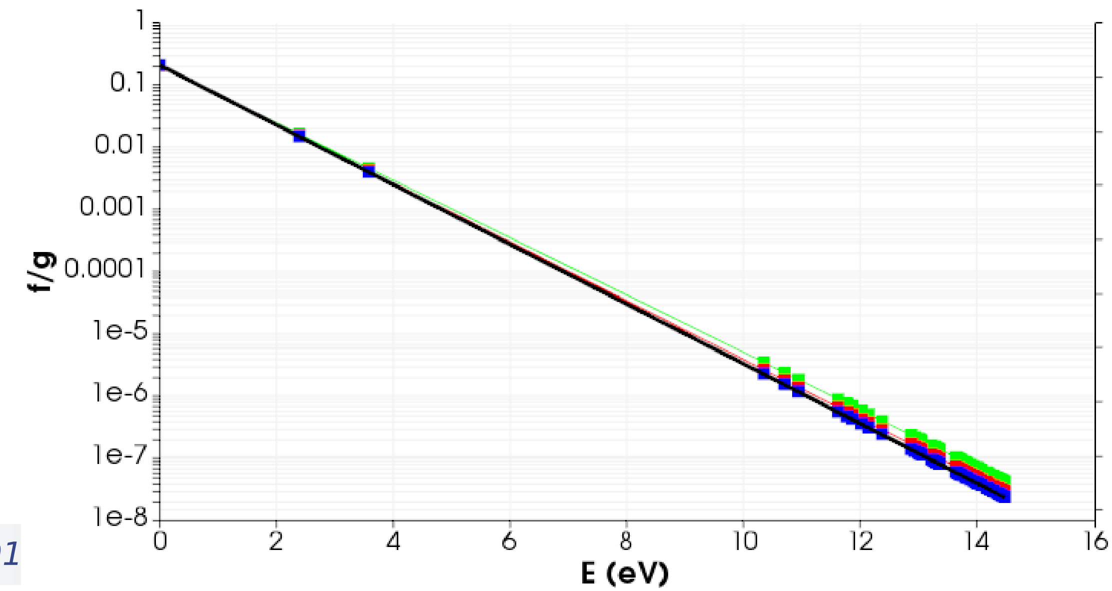
Nitrogen



$s = 5 \times 10^{-4}$ m

$s = 1 \times 10^{-3}$ m

$s = 3 \times 10^{-3}$ m



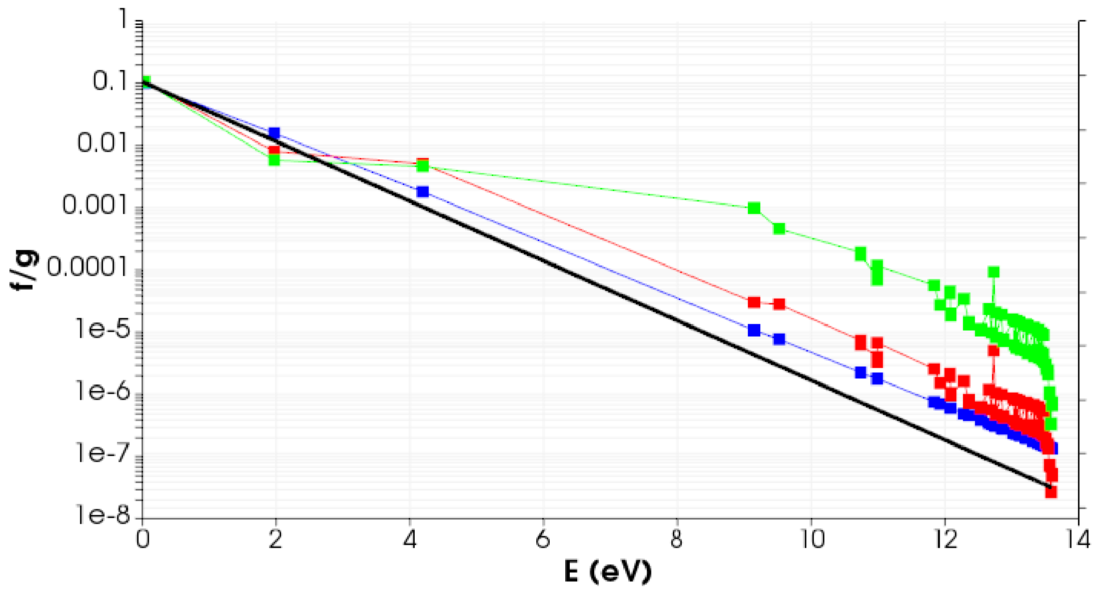
$s = 5 \times 10^{-3}$ m

$s = 1 \times 10^{-2}$ m

$s = 2 \times 10^{-2}$ m

Hypersonic flow study

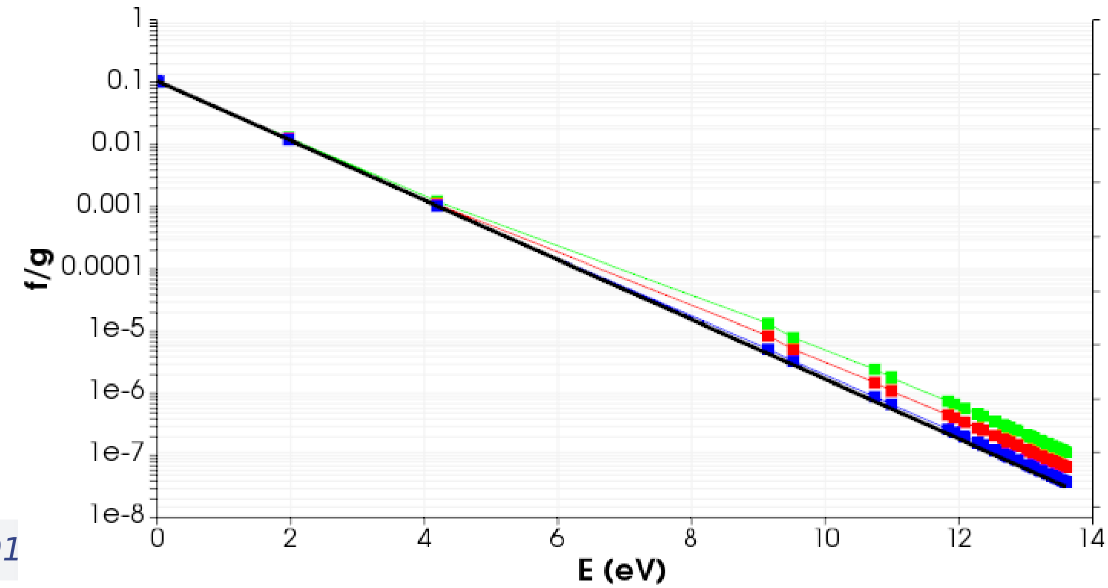
Oxygen



$s = 5 \times 10^{-4}$ m

$s = 1 \times 10^{-3}$ m

$s = 3 \times 10^{-3}$ m

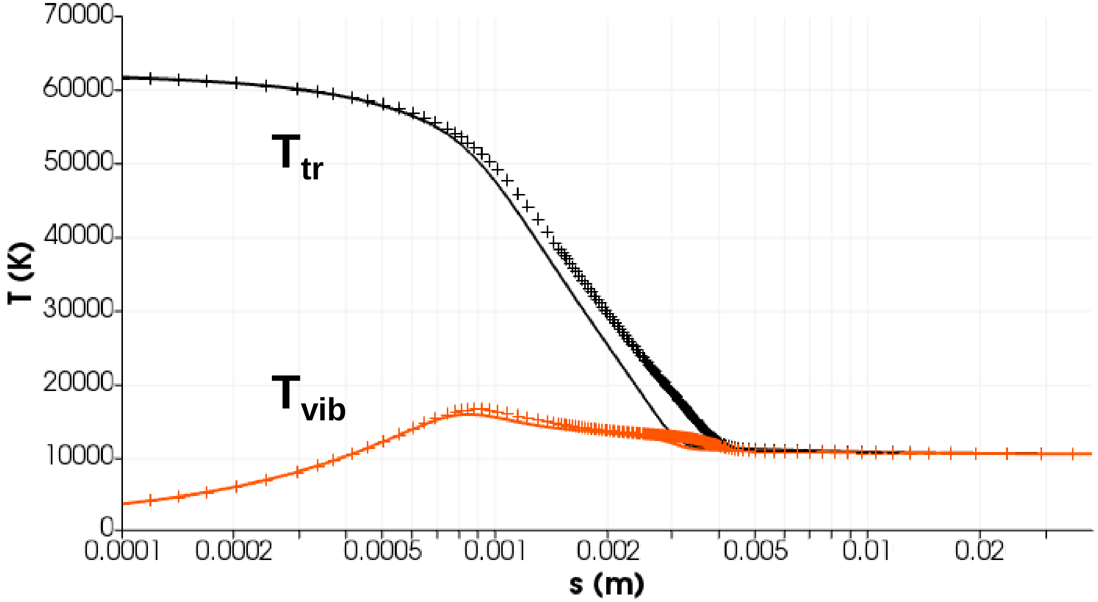


$s = 5 \times 10^{-3}$ m

$s = 1 \times 10^{-2}$ m

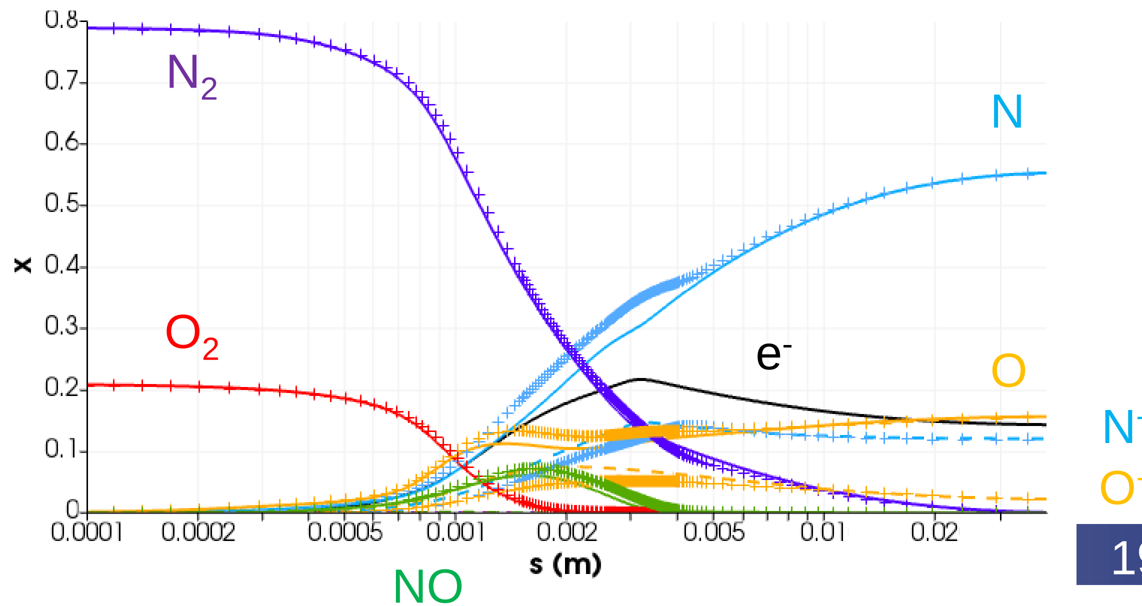
$s = 2 \times 10^{-2}$ m

Hypersonic flow study

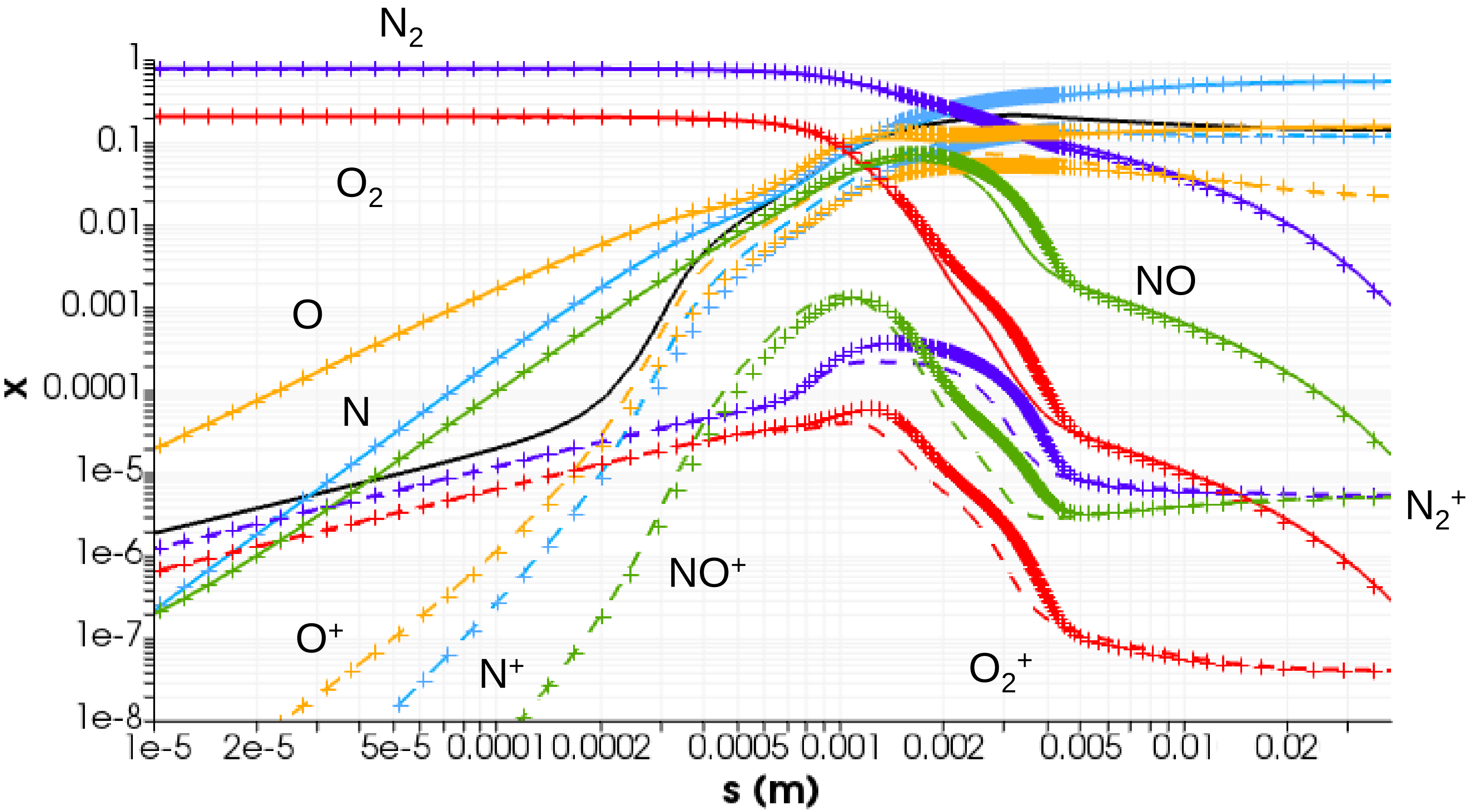


Comparison with reduced model

(grouped atomic levels)



Hypersonic flow study



Outline

I. Introduction

1. Context
2. Utility of collisional-radiative modelling
3. Peculiarities of transitional flows

II. State-to-state electronic excitation model

1. Description of the CoRaM-Air model
2. Hypersonic flow study (continuum regime)

III. Application to transitional entry flows

1. Testcase and baseline flow computation
2. Non-equilibrium effects

Numerical method

Lagrangian reactor approach

- Assume weak influence of the trace species on the flowfield
  → decoupled computation [1]

- Procedure:
  1) Perform a baseline simulation with only major species and chemical processes;
  2) Extract aerodynamic quantities $\mathbf{u(s)}$, $\boldsymbol{\rho}\mathbf{(s)}$, $\mathbf{T_m(s)}$, $\mathbf{x_i(s)}$ along one or more streamlines (**s** curvilinear abscissa, **i** species index, **m** internal energy mode);
  3) Solve the species mass conservation and the energy modes conservation equations along the streamlines with refined chemistry.

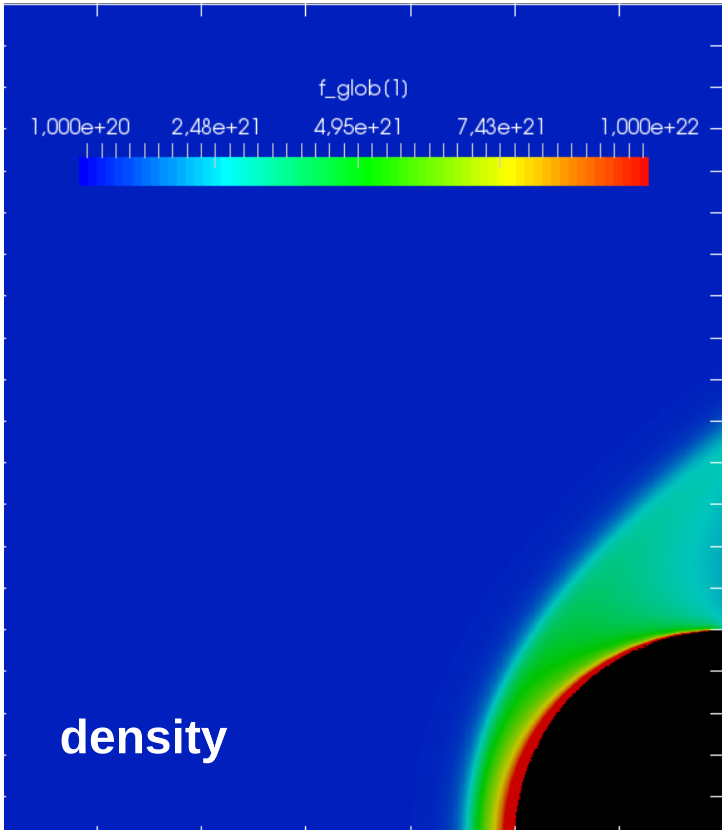
- Two-temperature T-Tv model

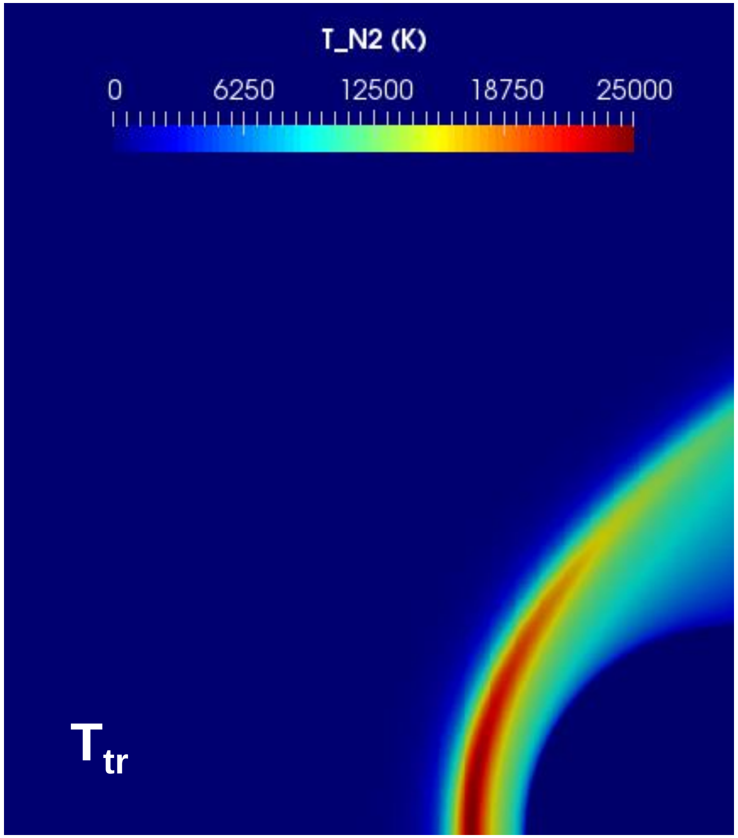
[1] ***Boccelli et al. Plasma Sources Sci. Technol. (2019).***

Baseline flow computation

- DSMC computation of 2D flow around a cylinder:

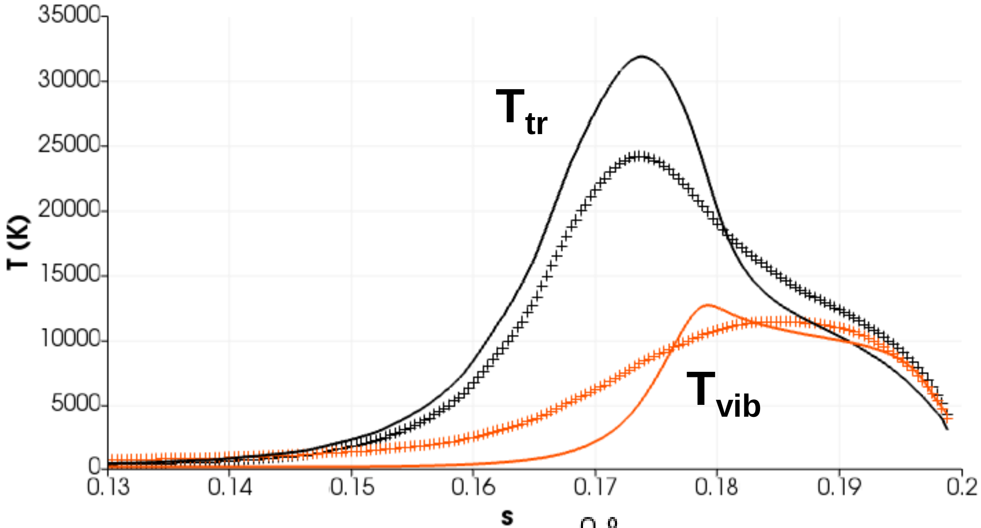
  $T_{tr,0} = 200$ K $p_0 = 1.38$ Pa   V = 7.5km/s   M = 25   Kn = 0.01



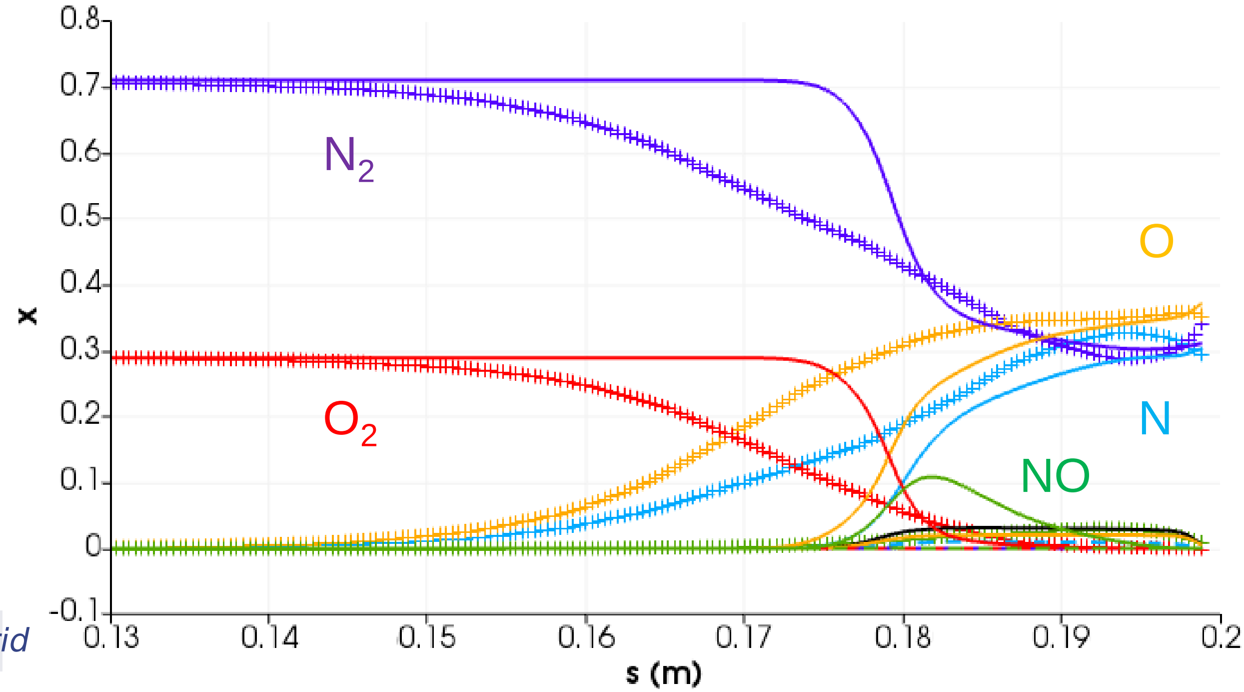


Outline

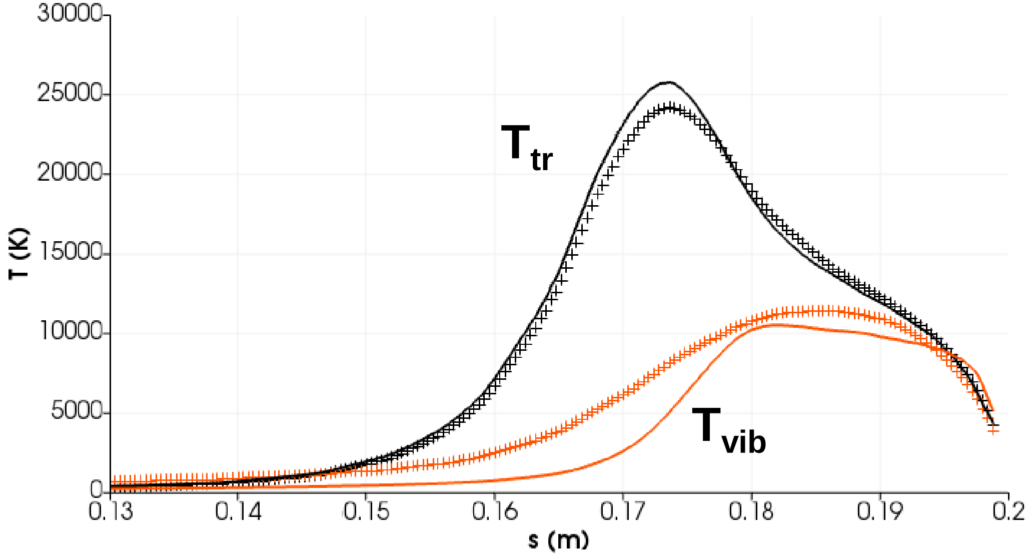
Non-equilibrium effects



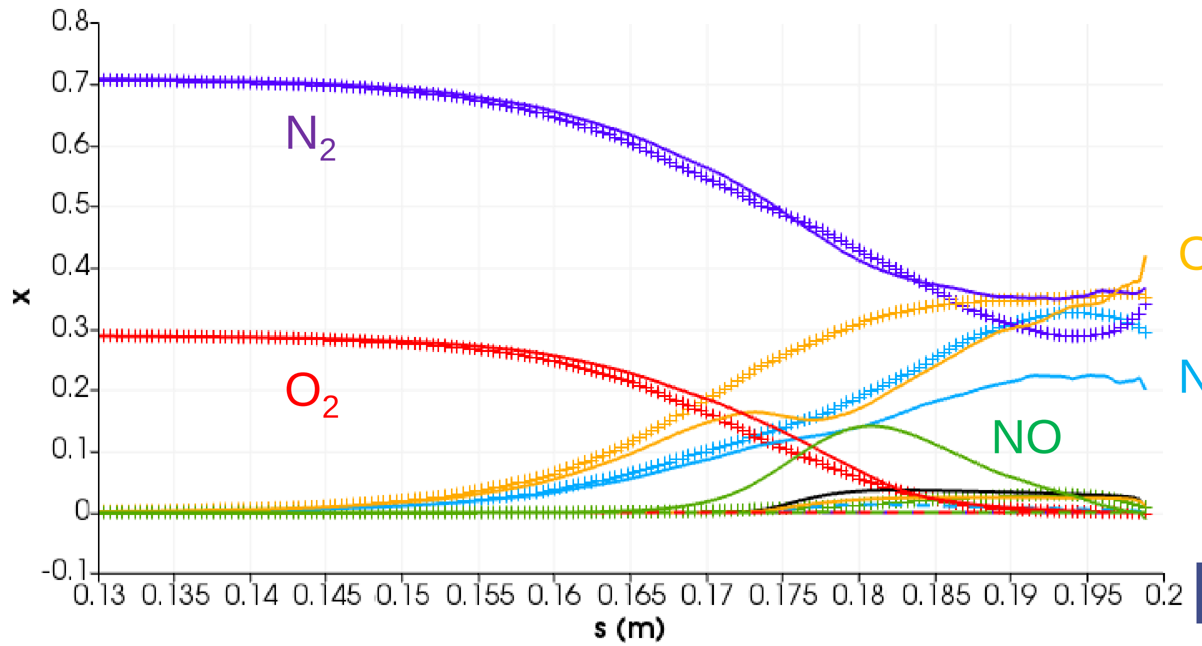
- Diffuse shock not recovered with continuum-based Lagrangian equations
- Strong effect of mass diffusion



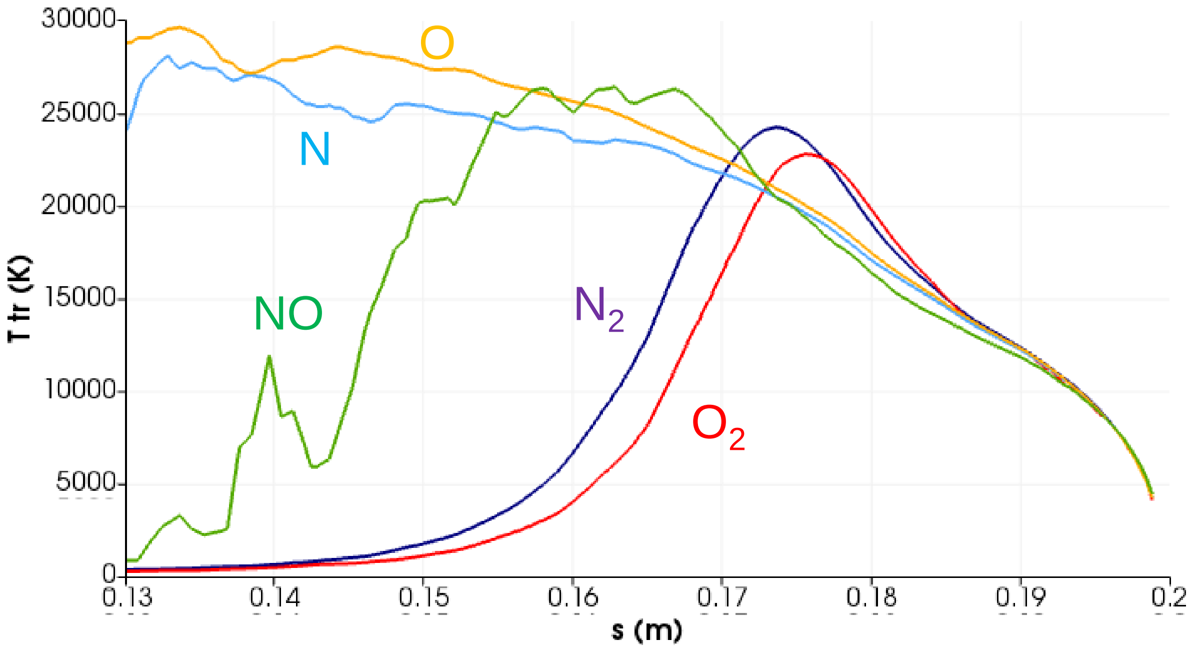
Non-equilibrium effects



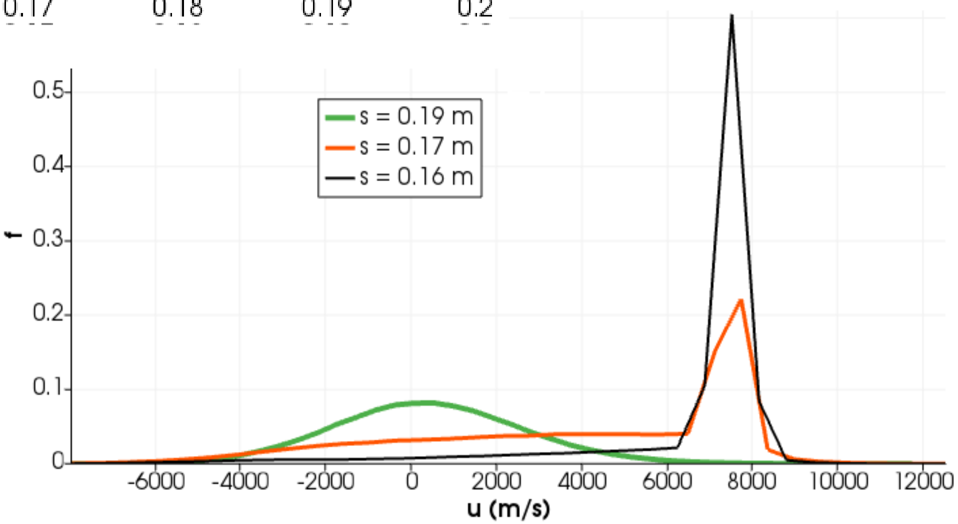
- Including an approximate source term to model the effect of mass diffusion along streamlines (estimated from baseline flow) improves the solution.



Non-equilibrium effects to be addressed



- Translational temperature depends on species



- Non-Maxwellian axial velocity distribution

Conclusion

- Collisional-radiative models provide valuable information to derive nonequilibrium chemical rates and thermo-chemical energy coupling terms for multi-temperature fluid models.

- State-to-state models are not suitable for direct implementation in DSMC due to the large number of species and their low mole fractions.

- Decoupled methods such as the Lagrangian reactor approach allow to use detailed CR models to compute excited species kinetics.

- Rarefaction / translational nonequilibrium effects still need to be addressed in order to achieve meaningful results when dealing with transitional flows.