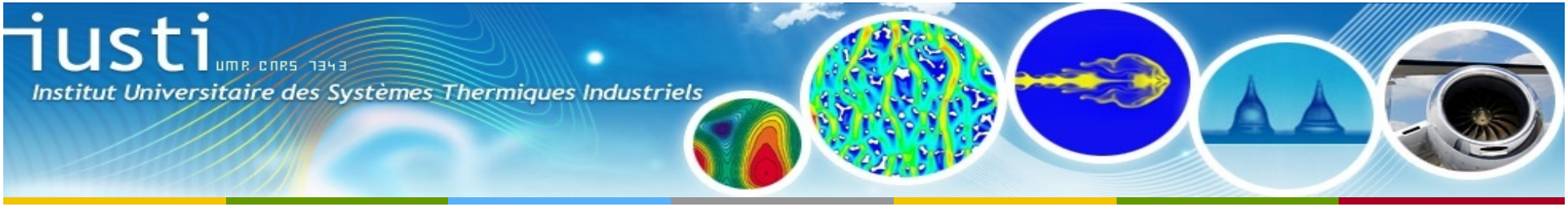


iusti UMR 7343 — Aix*Marseille université — cnrs — coria COMPLEXE DE RECHERCHE INTERPROFESSIONNEL EN AEROTHERMOCHIMIE

Simulation des Ecoulements de Plasmas hors-Equilibre Thermodynamique Local Application aux Entrées Atmosphériques Planétaires

Marie-Claude DRUGUET

Laboratoire IUSTI – CNRS UMR 4373 – Aix-Marseille Université
Marseille (France)

Arnaud BULTEL

Laboratoire CORIA – CNRS UMR 6614 – Université Normandie
St Etienne du Rouvray (France)

Re-entry and hypersonic aerothermodynamics :

➢ some of the issues :

- Hypersonic flow
- Strong shock wave

→

- Transfer from kinetic to thermal energy
- Structure of the aerothermodynamic flow field
- Shock layer thickness / shock interactions – pressure loads

MARS entry

- Convective and radiative heat fluxes - thermal loads
- Radiation of the plasma (Mars components) depends on

↓

- Composition of the plasma in the shock layer (molecules, atoms, electrons, ions)
- Chemical processes

↓

- Gas in thermodynamical non-equilibrium state
- Vibrational excitation of the molecules
- Electronic state of each particle

↔

- Ablation
- Couplings :
  - noneq. flow / radiation
  - noneq. flow / ablation
  - radiation / ablation

Re-entry and hypersonic plasma aerothermodynamics :

➢ Reconstruct the flow-field and the aerothermodynamic loads towards a space probe when it enters a planetary atmosphere

- ✓ pressure loads – shock interactions
- ✓ thermal loads – **convective and radiative heat fluxes**

- ✓ chemical composition
- ✓ thermodynamical state

} of the plasma

Assumptions for plasma flows:

- Plasma issued from the atmosphere behind the shock wave
- Continous gas, Laminar flow
- Local Non-equilibrium State :
  - ✓ vibrational excitation of the molecules : Boltzmann distrib
  - ✓ dissociation of the molecules
  - ✓ (electronic excitation of the species)
  - ✓ (ionization of the species)
  - ✓ chemical composition (ns)
  - ✓ thermodynamical state (nv)

Mars

Species	Vibrational energy
CO_2	$e^V_{CO_2}(1), e^V_{CO_2}(2), e^V_{CO_2}(3)$
C_2	$e^V_{C_2}$
N_2	$e^V_{N_2}$
O_2	$e^V_{O_2}$
CN	e^V_{CN}
CO	e^V_{CO}
NO	e^V_{NO}
C	-
N	-
O	-

Nitrogen

Species	Vibrational energy	(Electronic energy)
N_2	$e^V_{N_2}$	$(e^L_{N_2})$
N	-	(e^L_N)

Outline

- Equations
- CFD code (PINENS – IUSTI)
  - Double-cone flow
- Radiative transfers
  - ExoMars probe into CO_2-N_2
- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
- Concluding remarks

Conservative Equations for plasma flows:

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s(\mathbf{V} + \tilde{\mathbf{V}}_s)) = \omega_s^C \qquad s = 1, \ldots, n_s \quad (e^-)$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V} + p\bar{\bar{I}} - \bar{\bar{\tau}}) = 0$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot ((\rho e + p)\mathbf{V} - \bar{\bar{\tau}}\mathbf{V} + \mathbf{q}) = 0$$

$$\frac{\partial \rho_v e_v^V}{\partial t} + \nabla \cdot (\rho_v e_v^V (\mathbf{V} + \tilde{\mathbf{V}}_v) + \mathbf{q}_v^V) = \omega_v^V \qquad v = 1, \ldots, n_v$$

$$\left(\frac{\partial \rho_e e_e^E}{\partial t} + \nabla \cdot ((\rho_e e_e^E + p_e)(\mathbf{V} + \tilde{\mathbf{V}}_e) + \mathbf{q}_e^E) = \omega_e^E \qquad e^- \right)$$

$$\mathbf{q} = \mathbf{q^T} + \mathbf{q^C} + \mathbf{q^V} + \mathbf{q^E} \qquad \mathbf{q}^C = \sum_{s=1}^{ns} \mathbf{q}_s^C \quad \text{and} \quad \mathbf{q}^V = \sum_{v=1}^{nv} \mathbf{q}_v^V \quad \text{and} \quad \mathbf{q}^E \equiv \mathbf{q}_e^E$$

$$\omega_v^V = \omega_v^C e_v^V + Q_v^{V-T} + Q_v^{V-V} (+ Q_v^{V-E}) \qquad v = 1, \ldots n_v$$

$$(\omega_e^E = \omega_e^C e_e^E + Q^{E-T} + \sum_{v=1}^{n_v} Q_v^{E-V} \qquad e^- \qquad \textbf{TBC})$$

Equation of state for a plasma:

- Links the non-conserved variables (T, p,…) to the conserved variables

$$\rho e = \sum_{s\neq e}^{n_s} \rho_s c_{v_s}(T)T + \frac{1}{2}\sum_{s\neq e}^{n_s} \rho_s \mathbf{V}^2 + \sum_{s\neq e}^{n_s} \rho_s h_s^0 + \sum_{v=1}^{n_v} \rho_v e_v^V + \sum_{s\neq e}^{n_s} \rho_s e_s^L + \rho_e e_e^E$$

Translational-rotational specific heats

$$c_{v_s}^T = \frac{3}{2}\frac{\mathcal{R}}{M_s}$$

$$c_{v_s}^R = \begin{cases} \dfrac{\mathcal{R}}{M_s} & \text{for } s = 1,\ldots,n_v \\ 0 & \text{otherwise} \end{cases}$$

$$c_{v_s} = c_{v_s}^T + c_{v_s}^R$$

$$c_{p_s} = c_{v_s} + \frac{\mathcal{R}}{M_s}$$

Capitelli / Bultel

$$c_{p_s}(T) = (a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 + a_6 T^6)/T^2$$

Vibrational specific heat

$$c_{v_v}^V = \frac{\partial e_v^V}{\partial T_v^V}$$

Equation of state for a plasma:

- Inverse the equation of state to obtain T : iterative process

$$\rho e = \sum_{s\neq e}^{n_s} \rho_s c_{v_s}(T)T + \frac{1}{2}\sum_{s\neq e}^{n_s} \rho_s \mathbf{V}^2 + \sum_{s\neq e}^{n_s} \rho_s h_s^0 + \sum_{v=1}^{n_v} \rho_v e_v^V + \sum_{s\neq e}^{n_s} \rho_s e_s^L + \rho_e e_e^E$$

- Inverse the formula of vibrational energy to obtain the vibrational temperature :

$$\rho_v e_v^V = \frac{\rho_v R_v \theta_v^V}{\exp\left(\frac{\theta_v^V}{T_v^V}\right) - 1}$$

- Inverse the expression of translational energy of electrons to obtain the electron temperature

$$\rho_e e_e^E = \rho_e c_{v_e}(T_e)T_e + \frac{1}{2}\rho_e \mathbf{V}^2$$

- Compute the pressure with the formulae

$$p = \sum_{s\neq e}^{n_s} \rho_s \frac{\mathcal{R}}{M_s} T + p_e \qquad \text{and} \qquad p_e = \rho_e \frac{\mathcal{R}}{M_e} T_e$$

Equation of state for a plasma:

- Inverse the equation of state to obtain T :

$$\rho e = \sum_{s\neq e}^{n_s} \rho_s c_{v_s}(T)T + \frac{1}{2}\sum_{s\neq e}^{n_s} \rho_s \mathbf{V}^2 + \sum_{s\neq e}^{n_s} \rho_s h_s^0 + \sum_{v=1}^{n_v} \rho_v e_v^V + \sum_{s\neq e}^{n_s} \rho_s e_s^L + \rho_e e_e^E$$

- Determine the electronic energy of the species

$$e_s^L = R_s \frac{\sum_{i=1}^{\infty} g_{i_s} \theta_{i_s}^L \exp(-\frac{\theta_{i_s}^L}{T_e})}{\sum_{i=0}^{\infty} g_{i_s} \exp(-\frac{\theta_{i_s}^L}{T_e})}$$

Species	$\theta_0^L(K)$	$\theta_1^L(K)$	g_{0_s}	g_{1_s}
N_2		71642	1	3
O_2		11341	3	2
N		27665	9	10
O		22831	9	5

- All the formulae regarding the electron translational energy and the electronic excitation of the species are taken from G. Candler PhD thesis (1988)

Shear stresses, heat fluxes, diffusive fluxes (transport) :

- Shear stresses : proportional to the 1st derivatives of velocity V

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \lambda\frac{\partial u_k}{\partial x_k}\delta_{ij} \qquad \lambda = -\frac{2}{3}\mu$$

Viscosity coefficient :
Blottner (1971) curve fit $\mu_s = 0.1\exp[(A_s \ln T + B_s)\ln T + C_s], \quad (\text{in kg/ms})$

Wilke's (1950) semi-empirical mixing rule $\mu = \sum_s \frac{X_s\mu_s}{\phi_s}$

where $X_s = Y_s\frac{M}{M_s}$ and $Y_s = \frac{\rho_s}{\rho}$ and $\frac{1}{M} = \sum_s \frac{Y_s}{M_s}$

$$\phi_s = \sum_{r\neq e} X_r \frac{\left[1+\sqrt{\frac{\mu_s}{\mu_r}}\left(\frac{M_r}{M_s}\right)^{1/4}\right]^2}{\sqrt{8\left(1+\frac{M_s}{M_r}\right)}}$$

Shear stresses, heat fluxes, diffusive fluxes (transport) :

- Heat fluxes : Fourier law

$$\begin{aligned} \mathbf{q}^{\mathrm{T}} &= -\kappa^{TR}\nabla T \\ \mathbf{q}_e^E &= -\kappa_e^E \nabla T_e \quad (= 0 \text{ in this work}) \\ \mathbf{q}_v^V &= -\kappa_v^V \nabla T_v^V \end{aligned}$$

Translational-Rotational thermal conductivities : derived from an Eucken relation (Vincenti-Kruger (1965)) :

$$\kappa_s^{TR} = \mu_s\left(\frac{5}{2}c_{v_s}^T + c_{v_s}^R\right)$$

Wilke's semi-empirical mixing rule :

$$\kappa^{TR} = \sum_s \frac{X_s \kappa_s^{TR}}{\phi_s}$$

Vibrational thermal conductivity :

$$\kappa_v^V = \mu_v c_{v_v}^V$$

Shear stresses, heat fluxes, diffusive fluxes (transport) :

- Diffusive fluxes :
  - ✓ Those due to p and T gradients : negligible
  - ✓ Diffusion velocity of each component within the gas mixture is proportional to the sole gradient of the mass fraction
  - ✓ Additional assumption of binary diffusion where the species s diffuses into a similar mixture :

$$\rho_s \tilde{\mathbf{V}}_s = -\rho \mathcal{D}_s \nabla Y_s$$

  - ✓ Also assumed that the neutral species have the same diffusion coefficient and the ions have a double diffusion coefficient because of an existence of an electric field
  - ✓ The electron diffusion coefficient also derived from Lee

$$\mathcal{D}_e = M_e \frac{\sum_{s=ions} \rho_s \mathcal{D}_s / M_s}{\sum_{s=ions} \rho_s}$$

Conservative Equations for plasma flows:

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s(\mathbf{V} + \tilde{\mathbf{V}}_s)) = \omega_s^C \qquad s = 1, \ldots, n_s \quad (e^-)$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V} + p\bar{\bar{I}} - \bar{\bar{\tau}}) = 0$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot ((\rho e + p)\mathbf{V} - \bar{\bar{\tau}}\mathbf{V} + \mathbf{q}) = 0$$

$$\frac{\partial \rho_v e_v^V}{\partial t} + \nabla \cdot (\rho_v e_v^V (\mathbf{V} + \tilde{\mathbf{V}}_v) + \mathbf{q}_v^V) = \omega_v^V \qquad v = 1, \ldots, n_v$$

$$\left(\frac{\partial \rho_e e_e^E}{\partial t} + \nabla \cdot ((\rho_e e_e^E + p_e)(\mathbf{V} + \tilde{\mathbf{V}}_e) + \mathbf{q}_e^E) = \omega_e^E \qquad e^- \right)$$

$$\mathbf{q} = \mathbf{q}^{\mathbf{T}} + \mathbf{q}^{\mathbf{C}} + \mathbf{q}^{\mathbf{V}} + \mathbf{q}^{\mathbf{E}} \qquad \mathbf{q}^C = \sum_{s=1}^{ns} \mathbf{q}_s^C \quad \text{and} \quad \mathbf{q}^V = \sum_{v=1}^{nv} \mathbf{q}_v^V \quad \text{and} \quad \mathbf{q}^E \equiv \mathbf{q}_e^E$$

$$\omega_v^V = \omega_v^C e_v^V + Q_v^{V-T} + Q_v^{V-V}(+Q_v^{V-E}) \qquad v = 1, \ldots n_v$$

$$(\omega_e^E = \omega_e^C e_e^E + Q^{E-T} + \sum_{v=1}^{n_v} Q_v^{E-V} \qquad e^- \qquad \textbf{TBC})$$

Energy exchanges :

- Vibration-Translation exchanges at “low temperatures” :
  - ✓ Landau-Teller formulation from Millikan and While where it is assumed that the vibrational level of a molecule can change by only one quantum level at a time – harmonic oscillator :

$$Q_v^{V-T} = \rho_v \frac{e_v^V(T) - e_v^V}{\tau_v^{V-T}} = \frac{E_v^V(T) - E_v^V}{\tau_v^{V-T}}$$

$$\tau_v^{V-T(LT)} = \frac{\sum_{r \neq e} X_r}{\sum_{r \neq e} X_r / \tau_{vr}^{V-T(LT)}}$$

$$p\tau_{vr}^{V-T(LT)} = \exp[A_{vr}(T^{-1/3} - 0.015\mu_{vr}^{1/4}) - 18.42], \quad p \text{ in atm}$$

- At high temperatures, the rate of energy exchanges is unrealistically large due to the overprediction of the collision cross-section
- Park suggested an additional limiting cross section rate that limits relaxation time at high temperatures :

$$\tau_v^{corr} = 10^{-21}\left(\frac{50,000}{T}\right)^2 \quad m^2$$

$$\tau_v^{V-T} = \tau_v^{V-T(LT)} + \tau_v^{corr}$$

Energy exchanges :

- Vibration-Vibration exchanges : Stupochenko model revisited by S. Pascal and R. Brun

$$Q_{vw}^{V-V} = \frac{1}{\tau_{vw}^{V-V}}\left[\frac{1}{\rho R\theta_w^V}\left\{E_w^V(E_v^V+\rho_v R_v\theta_v^V)\exp\left(\frac{\theta_w^V-\theta_v^V}{T}\right)+E_v^V(E_w^V+\rho_w R_w\theta_w^V)\right\}\right]$$
$$= \frac{1}{p\tau_{vw}^{V-V}}\left[\frac{T}{\theta_w^V}\left\{E_w^V(E_v^V+\rho_v R_v\theta_v^V)\exp\left(\frac{\theta_w^V-\theta_v^V}{T}\right)+E_v^V(E_w^V+\rho_w R_w\theta_w^V)\right\}\right]$$

with $$Q_{wv}^{V-V} = -Q_{vw}^{V-V}$$

and $$\frac{1}{p\,\tau_{vw}^{V-V}} = \frac{4.482\times10^{-17}}{k_B}T^{-2/3}\frac{\pi^2}{\sqrt{\widetilde{\mu_{vw}}}}\frac{\theta_v^V\theta_w^V}{(\theta_w^V-\theta_v^V)^2}\frac{\alpha_{\Delta_{vw}}^{13/6}}{\alpha_{vw}\alpha_{wv}}\frac{\exp\left(\frac{\theta_v^V-\theta_w^V}{2T}\right)}{\exp\left[\frac{3}{2}\left(\frac{\alpha_{\Delta_{vw}}}{T}\right)^{1/3}\right]} \qquad [Pa^{-1}s^{-1}]$$

Several other models available in the literature
Comparisons were made in the early 90's

Energy exchanges :

➢ Electron-Translation exchanges

According to Candler (1988), the energy transfer rate between the heavy-particle and electron translational modes is derived from Lee (1985)

$$Q^{E-T} = 3\rho_e \mathcal{R}(T - T_e)\sqrt{\frac{8\mathcal{R}T_e}{\pi M_e}}\sum_{s\neq e}\frac{\rho_s \mathcal{N}_{\mathcal{A}}}{M_s^2}\sigma_{es}$$

For electron-ion interactions, the effective Coulomb cross-section is also given by Lee

$$\sigma_{e,ions} = \frac{8\pi}{27}\frac{e^4}{k_b^2 T_e^2}\ln\left[1 + \frac{9k_B^3 T_e^3}{4\pi N_e e^6}\right]$$

$$\sigma_{e,neutral} = 10^{-20} m^2$$

This mechanism causes the heating of the electron translational mode just behind the shock wave where the difference $(T - T_e)$ is large

Energy exchanges :

➢ Electron-Vibration exchanges :

According to Candler (1988), the coupling between the electron translational mode and the vibrational modes of the molecules is weak, except for the nitrogen molecule

$$Q_v^{E-V} = \rho_e \frac{M_v}{M_e} \frac{e_v^V(T_e) - e_v^V}{\tau_{ev}^{E-V}}, \quad \text{for } v = N_2$$

Lee derived an expression for the rate of electron-vibrational energy transfer by solving the system of master equations that accounts for transitions of multiple levels. A curve-fit of this expression is

$$\log(p_e \tau_{ev}^{E-V}) = \begin{cases} 7.50\,(\log T_e)^2 - 57.0\,\log T_e + 98.70, & \text{for } T_e < 7000K \\ 2.36\,(\log T_e)^2 - 17.9\,\log T_e + 24.35, & \text{for } T_e > 7000K \end{cases}$$

A plot of this function shows that the relaxation time is lowest near 7,000 K that corresponds to the strong resonance between the electron and vibrational modes

Source terms for chemical species mass conservation :

Every chemical reaction may be written as

$$\sum_{s=1}^{n_s} \nu'_{s,r} A_s \underset{k_r^b}{\overset{k_r^f}{\rightleftharpoons}} \sum_{s=1}^{n_s} \nu''_{s,r} A_s, \qquad r = 1, \ldots, n_r$$

where the forward and backward rates for each process are written

$$k_r^f(T) = C_r^f T^{\eta_r^f} \exp\left(-\frac{\theta_r^f}{T}\right)$$

$$k_r^b(T) = C_r^b T^{\eta_r^b} \exp\left(-\frac{\theta_r^b}{T}\right)$$

Several models are available in the literature (Park, Dunn-Kang, Gupta-Yos,…).

The chemical source term for each species mass conservation equation is then

$$\omega_s^C = M_s \sum_{r=1}^{n_r} (\nu'_{s,r} - \nu''_{s,r}) \left[-k_r^f \prod_{j=1}^{n_s} \left(\frac{\rho_j}{M_j}\right)^{\nu'_{s,r}} + k_r^b \prod_{j=1}^{n_s} \left(\frac{\rho_j}{M_j}\right)^{\nu''_{s,r}} \right], \qquad s = 1, \ldots, n_s$$

Outline

- Equations
- CFD code (PINENS – IUSTI)
  - Double-cone flow
- Radiative transfers
  - ExoMars probe into CO_2-N_2
- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
- Concluding remarks

CFD code PINENS :

PINENS : Parallel Implicit NonEquilibrium Navier-Stokes code

- finite volume on structured grid
- 2D / axi-symmetric computations
- shock capturing schemes
  - approximate Riemann solvers (LF, Roe, HLL, HLLC,…)
  - entropy fix to avoid carbuncle phenomenon (H-correction)
- reconstruction at the cell interfaces : TVD schemes
  - van Leer, van Albada, minmod, superbee…
  - 2^{nd} order accuracy in space
- 1^{st} or 2^{nd} order accuracy in time (stationary or time-dependent)

- implicit time integration (DPLR)
- parallel (MPI)

CFD code PINENS :

Flow, thermodynamics and transport properties modeling:

- Laminar flow, continous gas
- Thermodynamics data base
- Viscosities :
  - single species:Blottner, collision integrals (Séror, Palmer-Wright)
  - gas mixtures : mixing rules of Wilke, Armaly-Sutton, Mason-Saxena, Gupta-Yos,...
- Thermal conductivities :
  - single species : collision integrals, Palmer-Wright, Séror, Monchick,..
  - vibrational thermal conductivities : Pascal
- Diffusion coefficients :
  - single species : Eucken, collision integrals,…

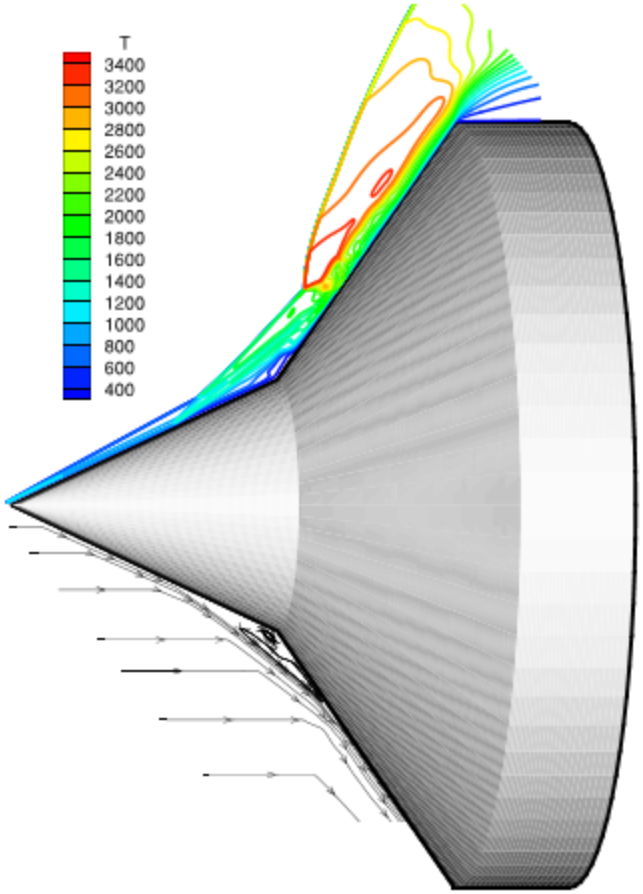
Applications : Flow past a double-cone (25-55 deg – sharp nose)

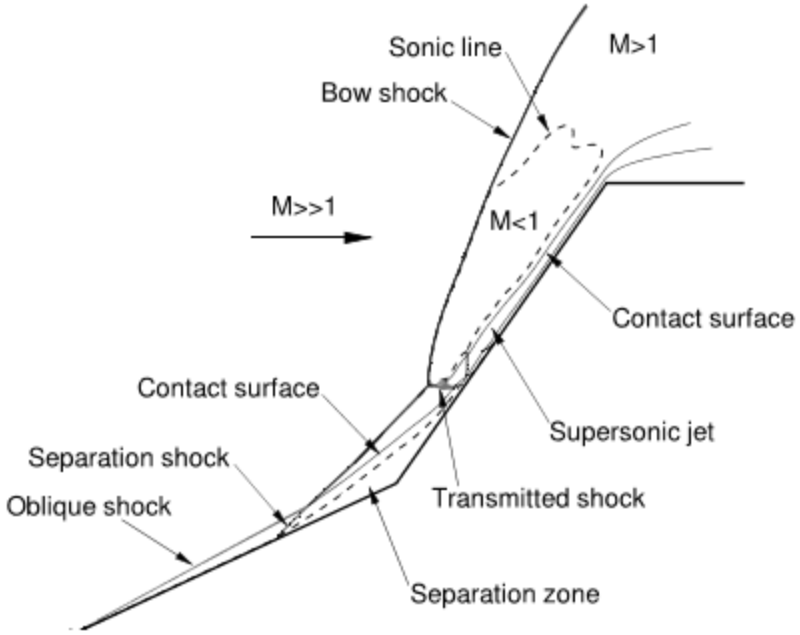
- History of double-cone flow simulations :
- Original motivation : validation of high-enthalpy chemistry models
- Framework : NATO RTO Working group 10 – Code validation
- Initially : blind comparison of simulation and data
- General good prediction : separation zone, pressure variation, heat transfer at the double cone surface
- Low-enthalpy case with pure Nitrogen and small degree of dissociation

Case	Run 35
M_∞	11.30
Re_m	133000 m^{-1}
T_∞	138.89 K
T_wall	296.11 K
ρ_∞	0.5515 $\mathrm{g/m}^3$
u_∞	2712.7 m/s

Applications : Flow past a double-cone (25-55 deg – sharp nose)

Flow characteristics

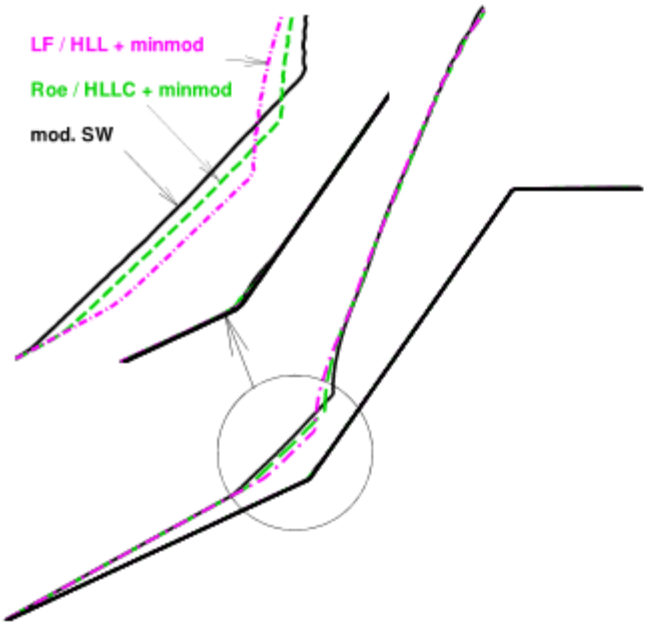




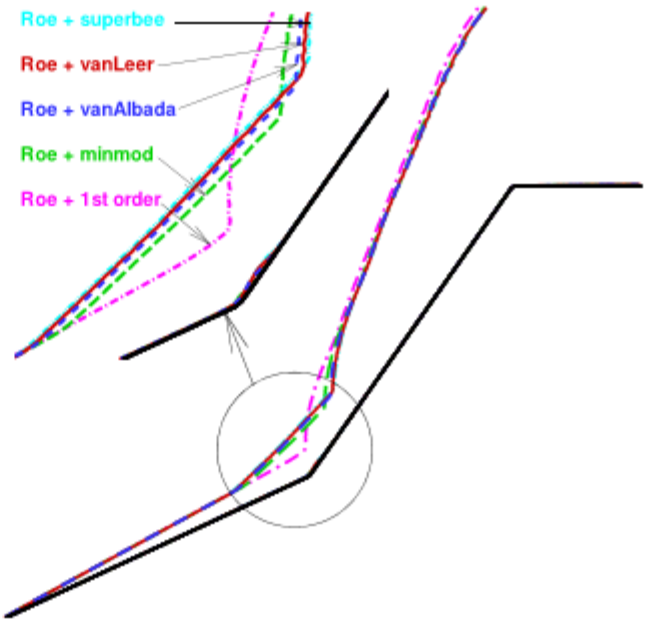
Applications : Flow past a double-cone (25-55 deg – sharp nose)

Effects of numerics (on a coarse grid)

different flux evaluation schemes



different slope limiters

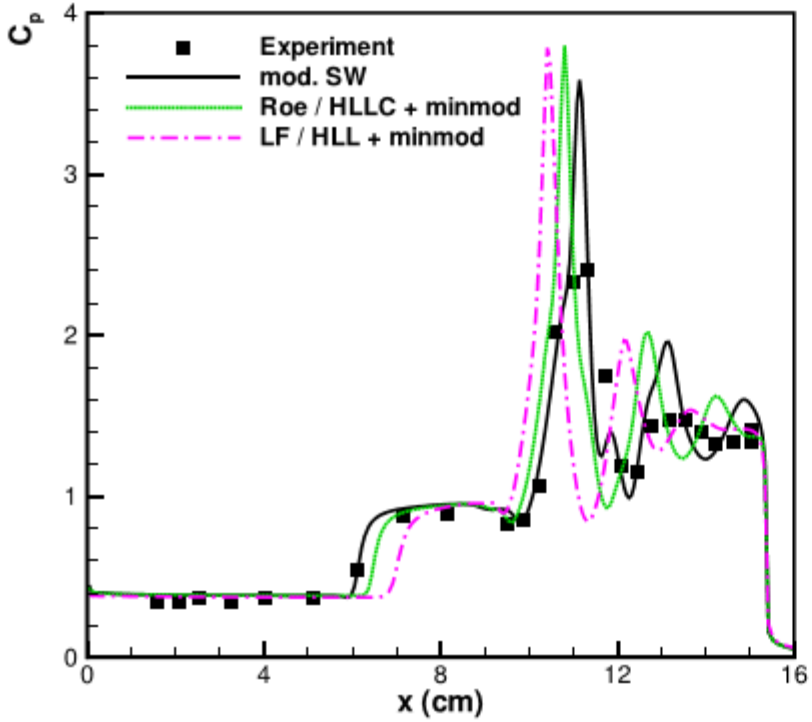


Temperature contours

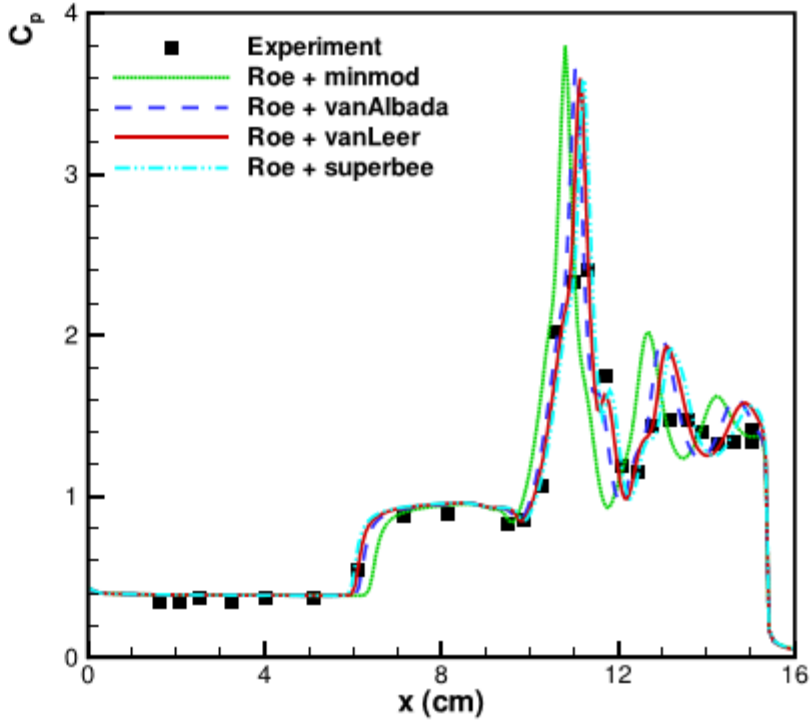
Applications : Flow past a double-cone (25-55 deg – sharp nose)

Effects of numerics (on a coarse grid)

different flux evaluation schemes



different slope limiters

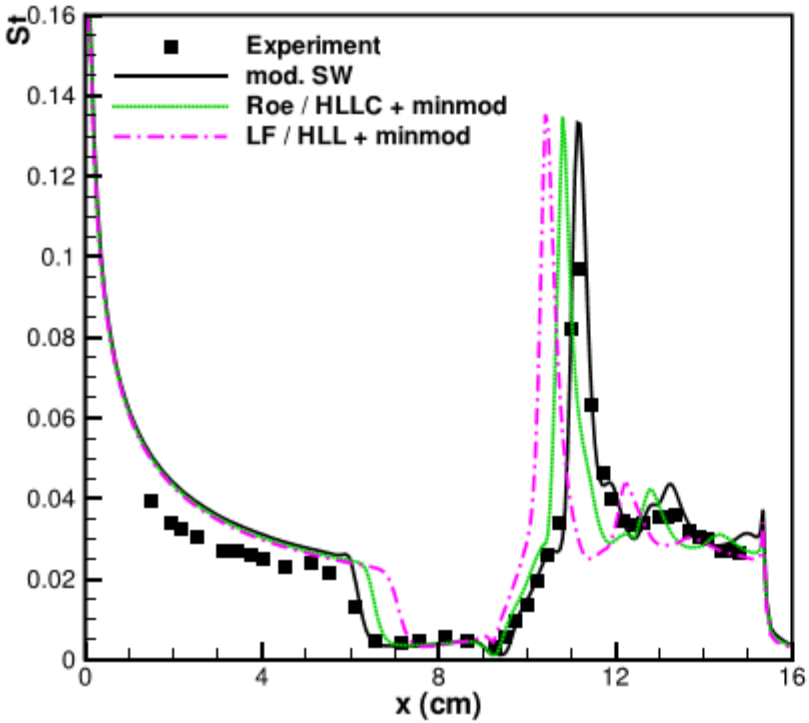


Surface pressure coefficients

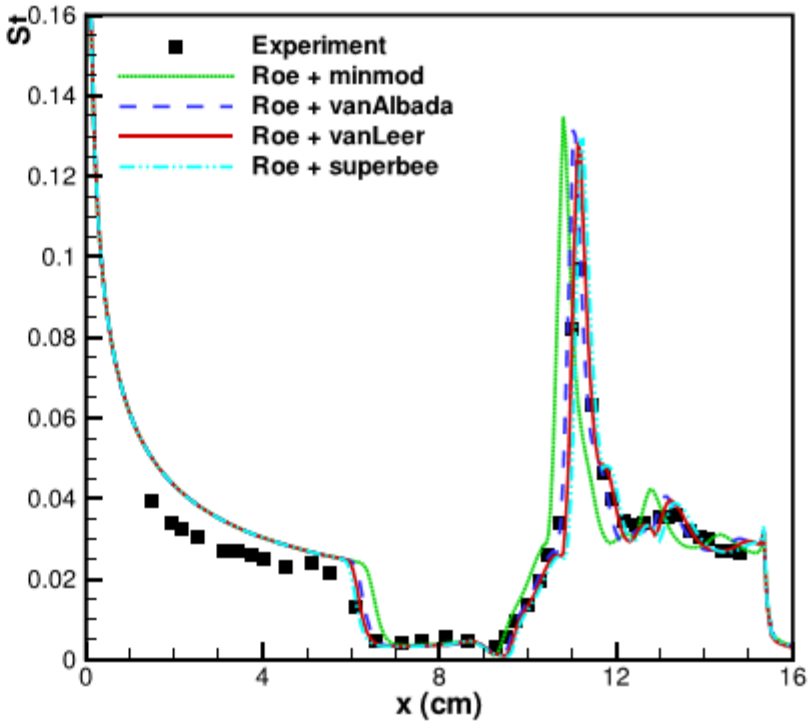
Applications : Flow past a double-cone (25-55 deg – sharp nose)

Effects of numerics (on a coarse grid)

different flux evaluation schemes



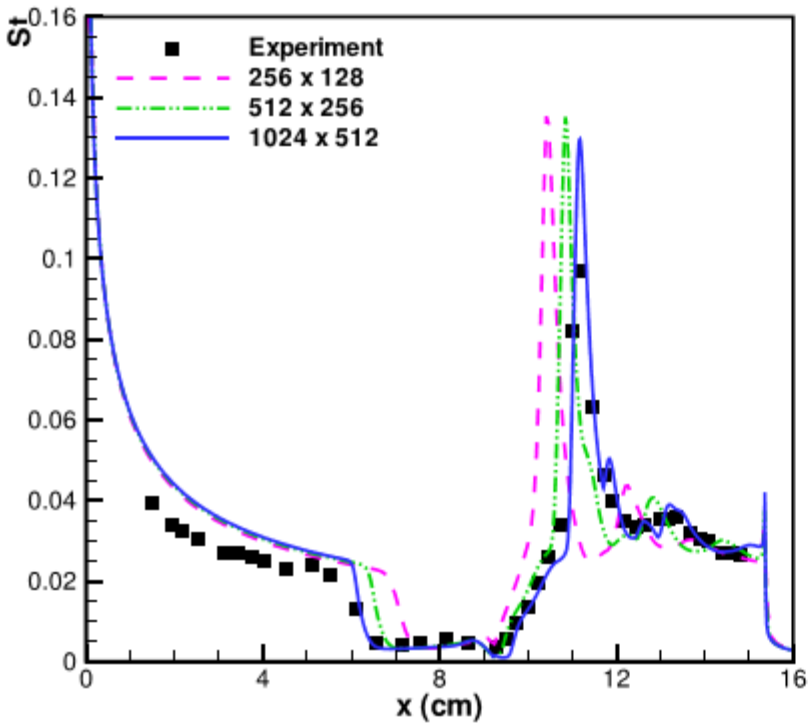
different slope limiters



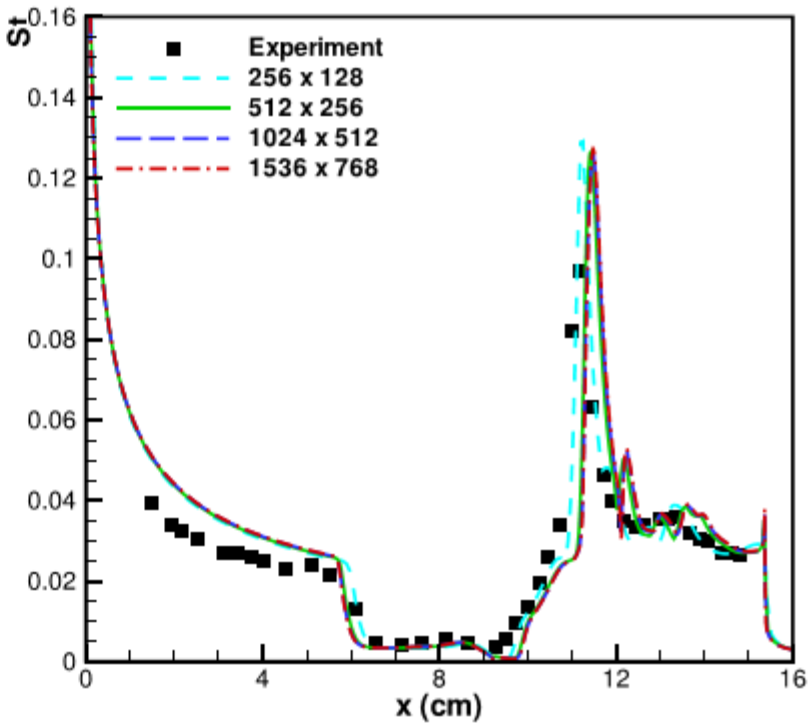
Heat transfer rates

Applications : Flow past a double-cone (25-55 deg – sharp nose)

Effects of numerics: Grid refinement



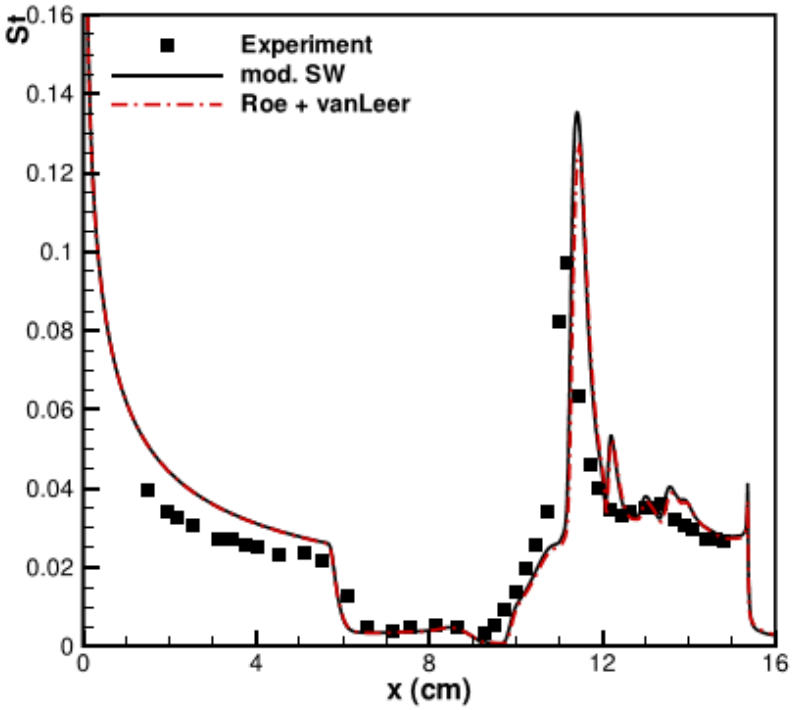
Lax-Friedrichs
minmod slope limiter



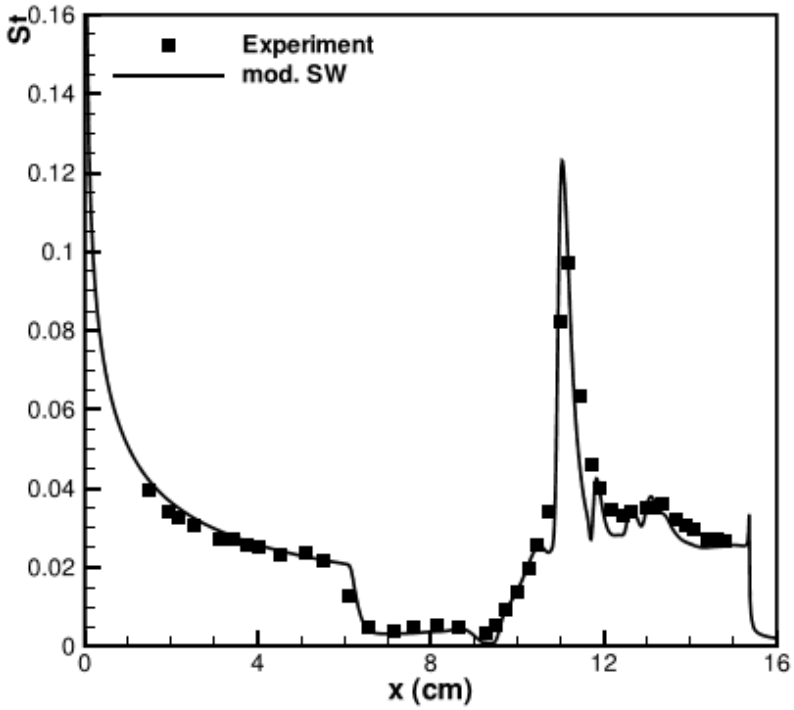
Roe
superbee slope limiter

Applications : Flow past a double-cone (25-55 deg – sharp nose)

Effects of numerics on a fine grid, with our best schemes, and with full physical modeling included



Full physical modeling NOT included



Full physical modeling included

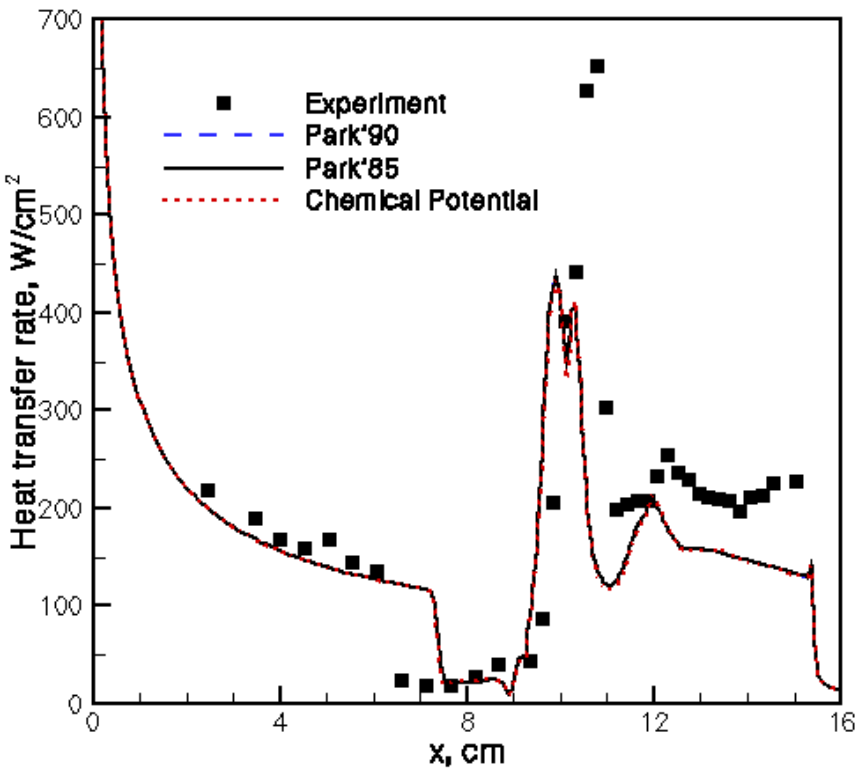
Applications : Flow past a double-cone (25-55 deg – sharp nose)

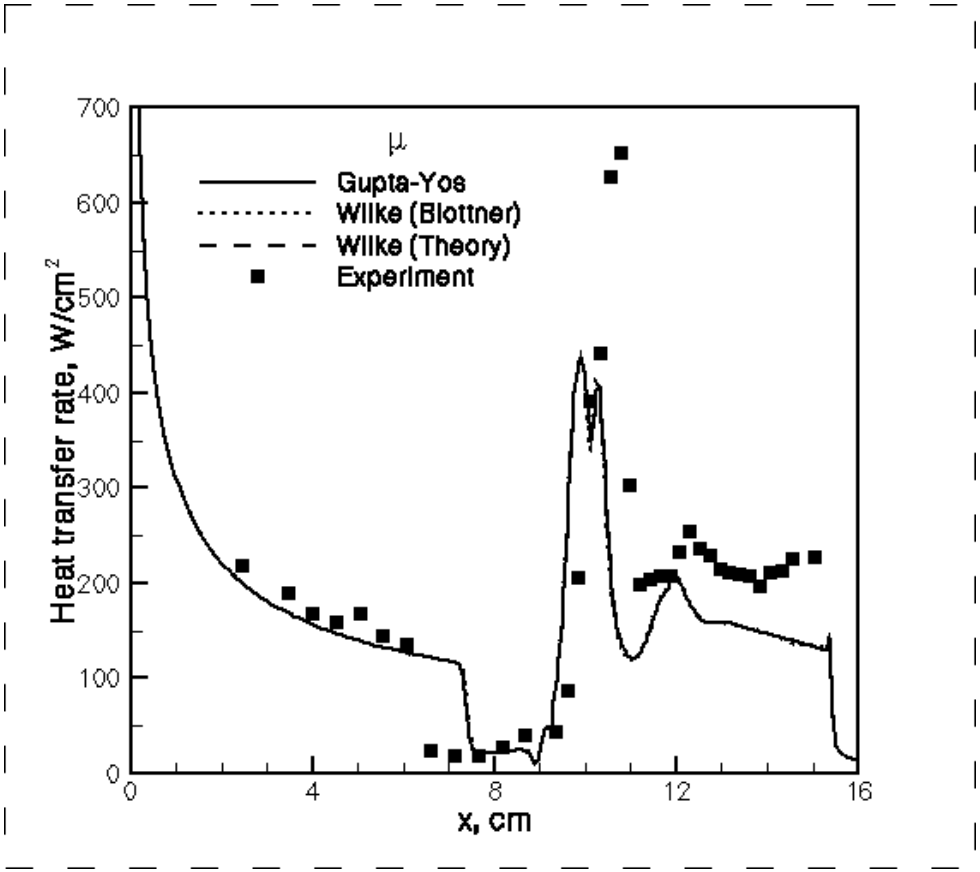
- What about the high-enthalpy case with air and large degree of dissociation (Run 43) ?
- Conditions at the exit of the shock tunnel (M. Holden) where the double-cone model is placed
  - ➢ Freestream conditions for the double cone simulations

Case	Run 43
T_∞	576.0 K
$T^V_{N_2,\infty} = T^V_{O_2,\infty}$	576.0 K
$c_{N_2,\infty}$	0.73704
$c_{O_2,\infty}$	0.17160
$c_{NO,\infty}$	0.06477
$c_{N,\infty}$	0.00000
$c_{O,\infty}$	0.02659
ρ_∞	2.134×10^{-3} kg/m^3
u_∞	4218.1 m/s
T_w	296.2 K
M_∞	8.87
Re_∞	306,600 m^{-1}

Applications : Flow past a double-cone (25-55 deg – sharp nose)

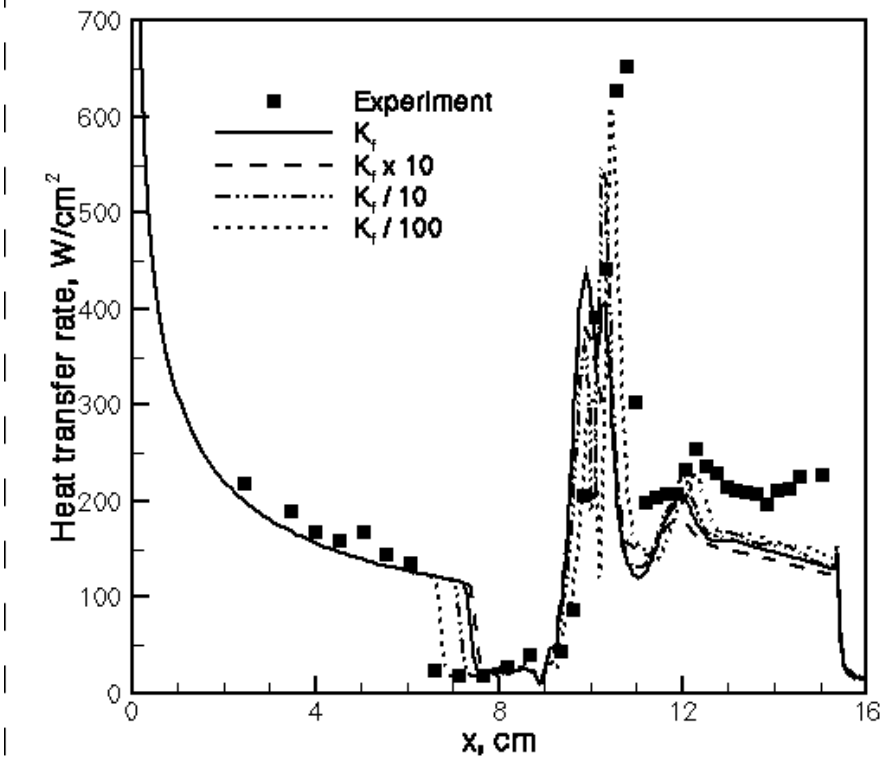
High-enthalpy case with air (Run 43)

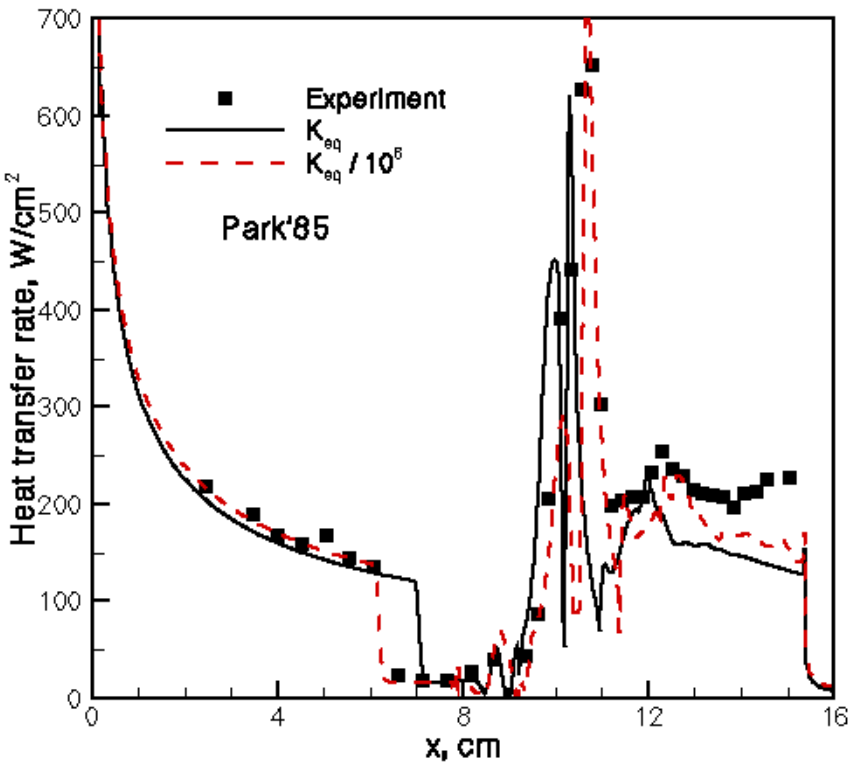




Applications : Flow past a double-cone (25-55 deg – sharp nose)

High-enthalpy case with air (Run 43) – Results 2005





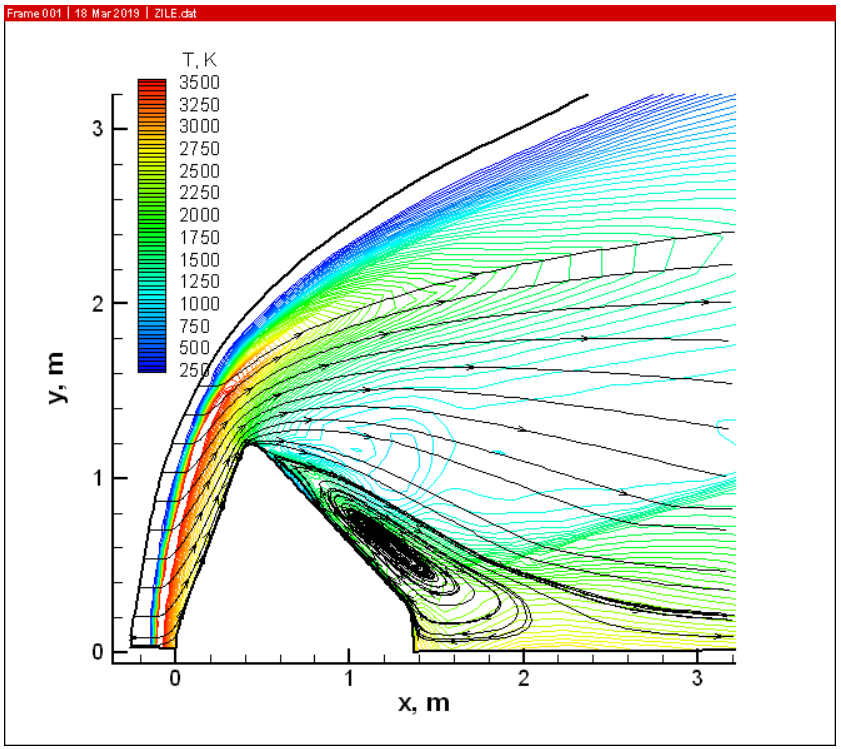
In 2025, pb not yet resolved (Tom Schwartzentruber, ISSW35) !

Outline

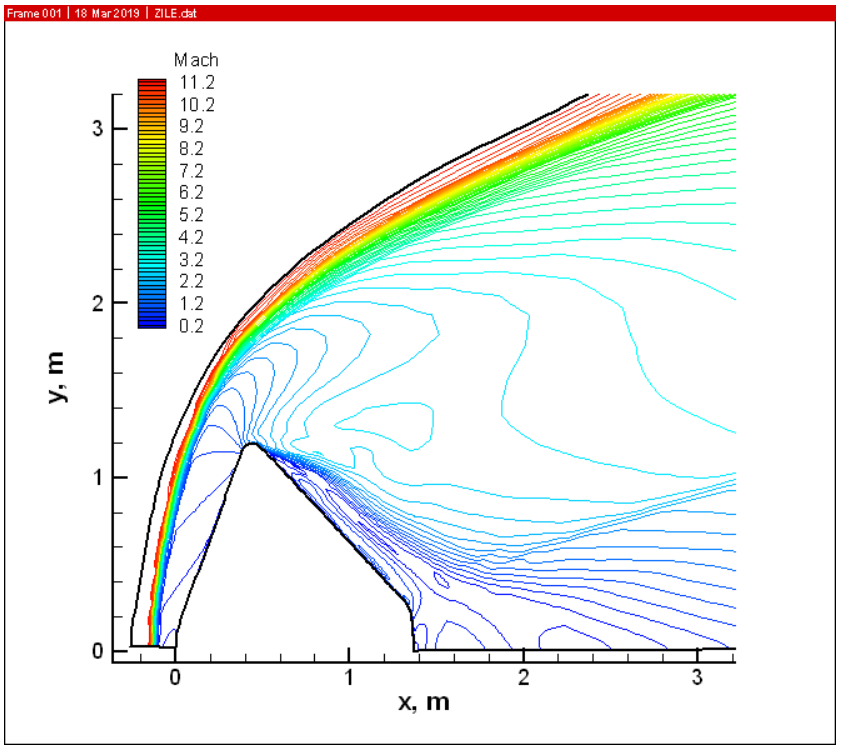
- Equations
- CFD code (PINENS – IUSTI)
  - Double-cone flow
- Radiative transfers
  - ExoMars probe into CO_2-N_2
- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
- Concluding remarks

Chemically reacting CO_2-N_2 flow over the ExoMars probe at Mach 11 (kinetics model from CORIA) :

Temperature contours



Mach number contours



Solution not yet steady in the wake

Flow past the Exomars probe in a CO_2-N_2 environment - Mach 11

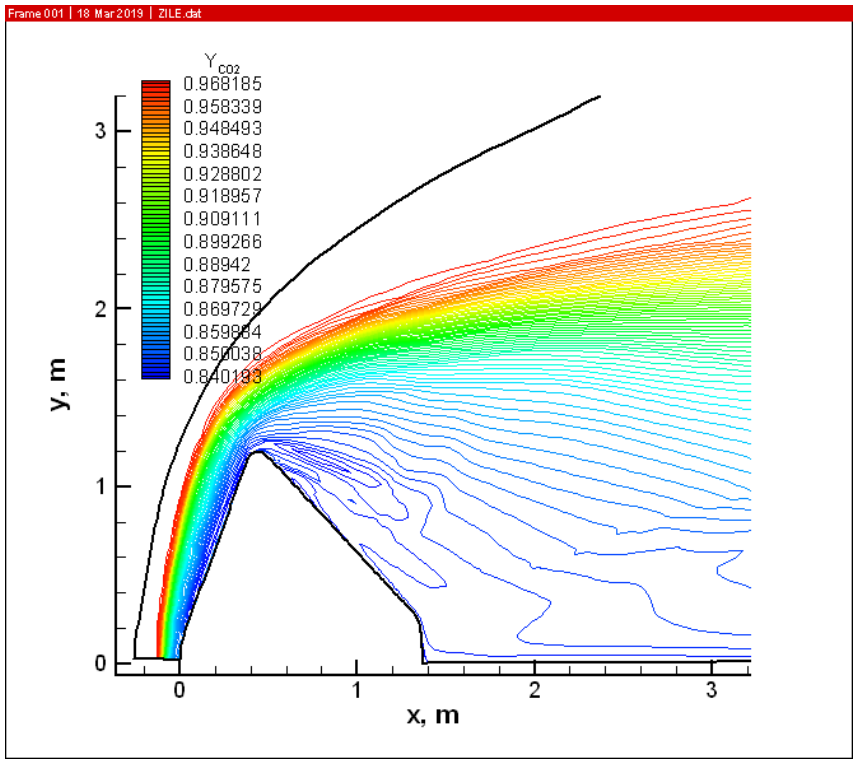
➢ to reconstruct the measured radiative fluxes (ICOTOM)

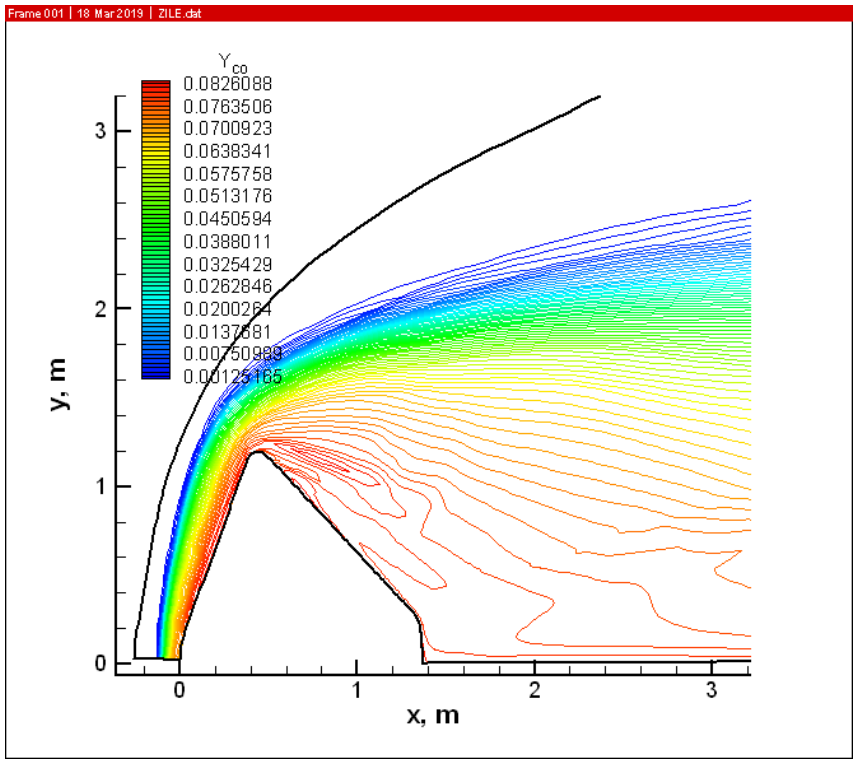
Chemically reacting gas **(kinetics model from CORIA)**

- 128x045 : grid cell numbers in i and j directions
- Mars09 : 9 species s : $CO_2(1)$, $CO_2(2)$, $CO_2(3)$, N_2, O_2, CO, C, N ,O
- nvh06 : 6 vibrating molecules v : $CO_2(1)$, $CO_2(2)$, $CO_2(3)$, N_2, O_2, CO
- kinetics model with 14 reactions (7 dissociation, 7 exchange reactions)
- Tw=1500 K on the front shield, and 500 K on the back cover
- C2V0 : active chemistry, non-active vibration

Chemically reacting CO_2-N_2 flow over the ExoMars probe at Mach 11 (kinetics model from CORIA) :

CO_2 and CO contours





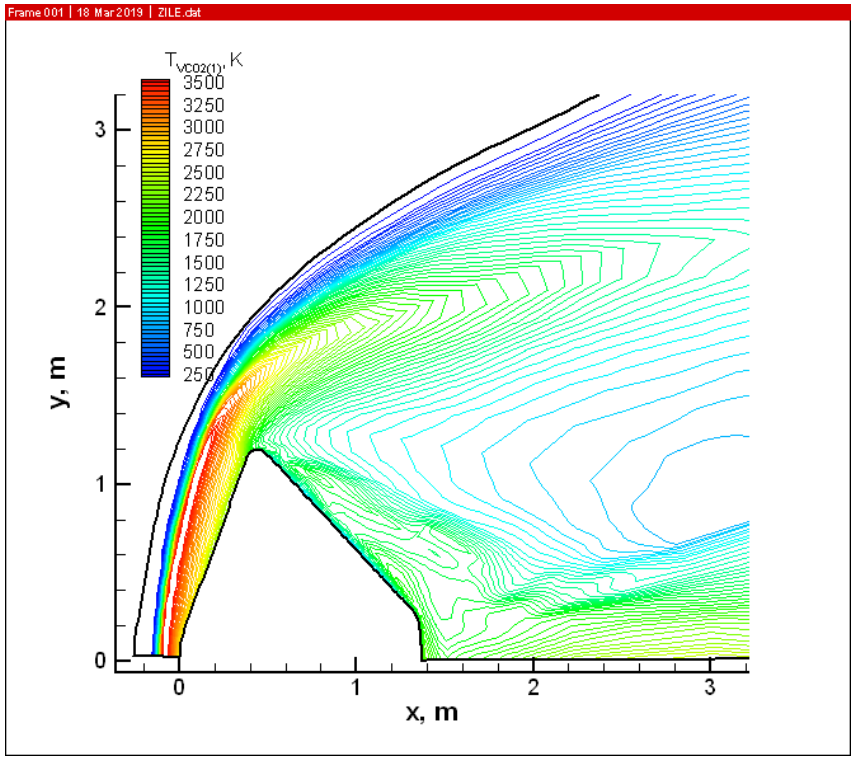
Solution not yet steady in the wake

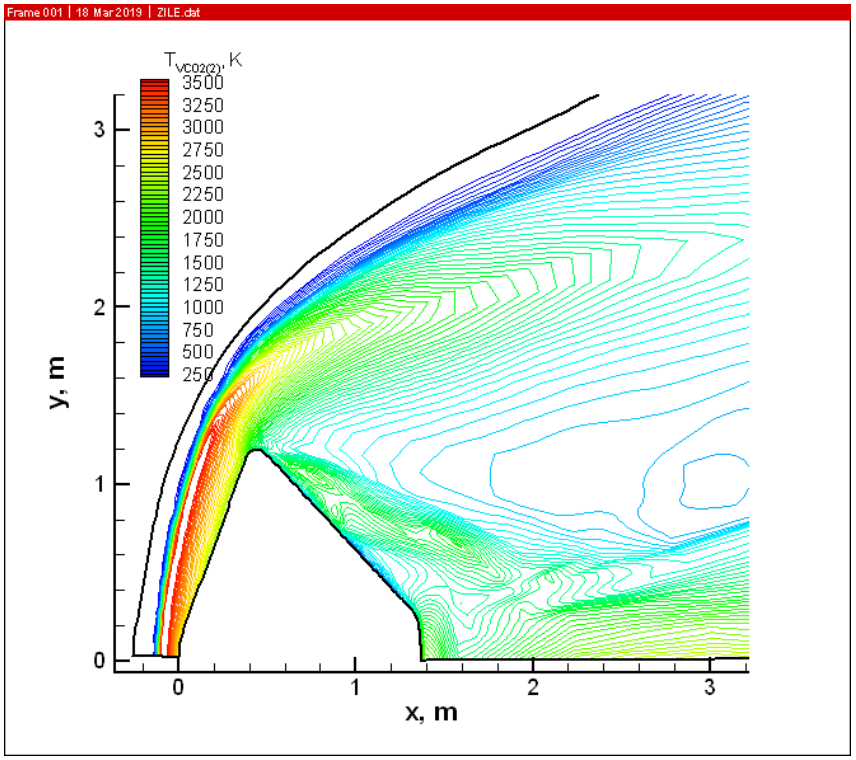
Chemically reacting and vibrationally excited gas (flow-field not yet steady in the wake)

- 128x045 : grid cell numbers in i and j directions
- Mars09 : 9 species s : $CO_2(1)$, $CO_2(2)$, $CO_2(3)$, N_2, O_2, CO, C, N ,O
- nvh06 : 6 vibrating molecules v : $CO_2(1)$, $CO_2(2)$, $CO_2(3)$, N_2, O_2, CO
- kinetics model with 14 reactions (7 dissociation, 7 exchange reactions)
- Tw=1500 K on the front shield, and 500 K on the back cover
- C2V2 : active chemistry, and active vibrational relaxation

Chemically reacting and nonequilibrium vibration CO_2-N_2 flow over the ExoMars probe at Mach 11 :

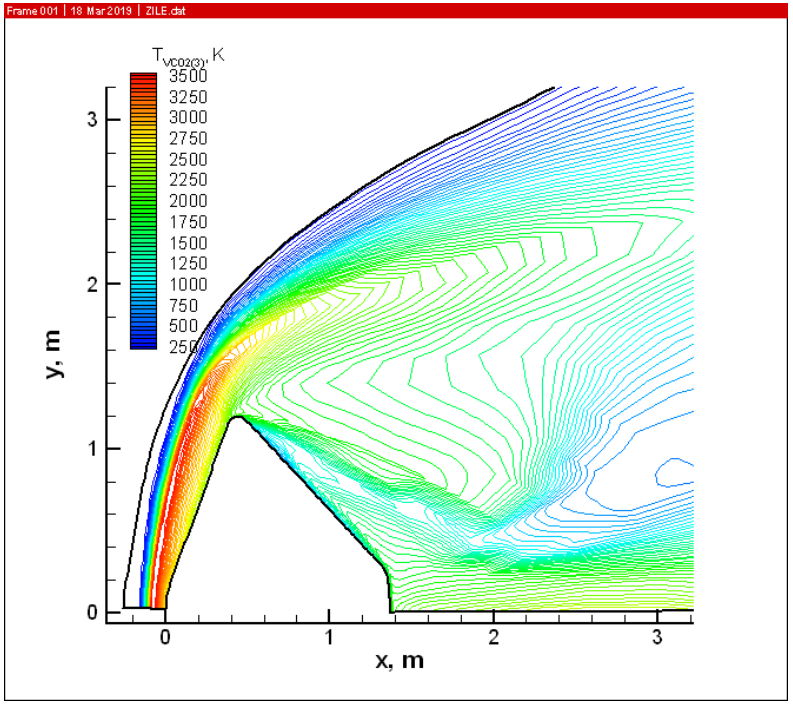
CO_2(1) and CO_2 (2) vibrational temperature contours

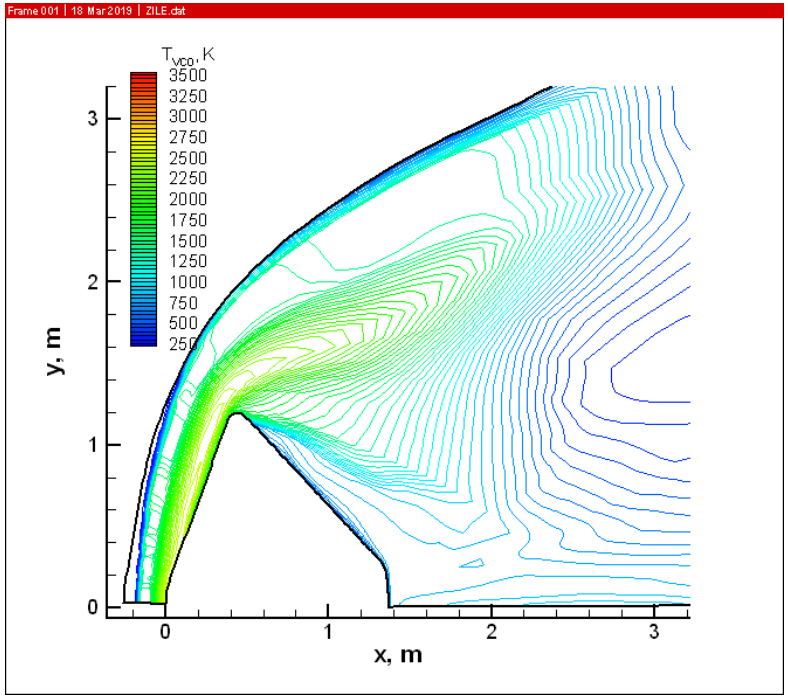




Chemically reacting and nonequilibrium vibration CO_2-N_2 flow over the ExoMars probe at Mach 11 :

CO_2(3) and CO vibrational temperature contours

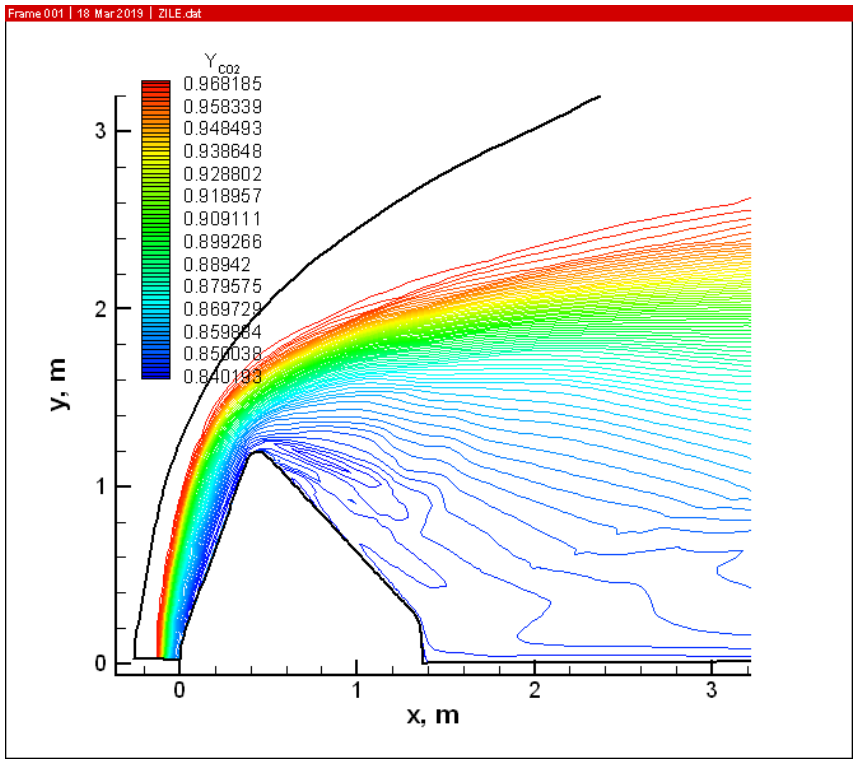


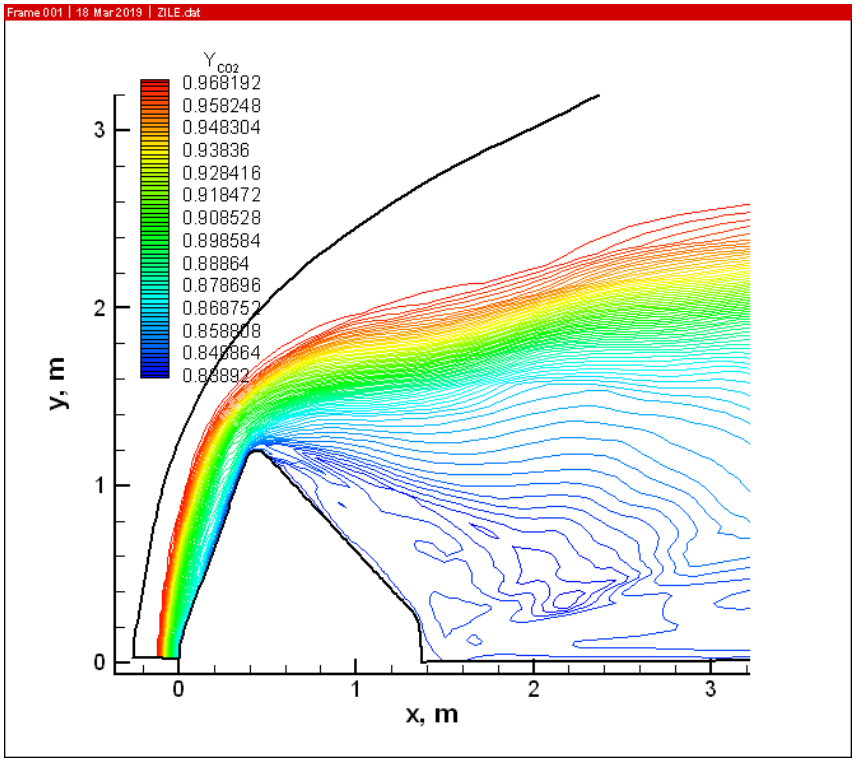


Chemically reacting and nonequilibrium vibration CO_2-N_2 flow over the ExoMars probe at Mach 11 :

Left : chemistry only

Right : chemistry and vibration

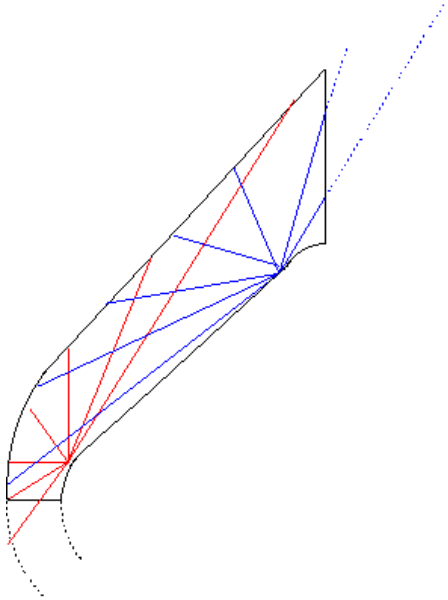




CO_2 contours

Radiation transport modeling :

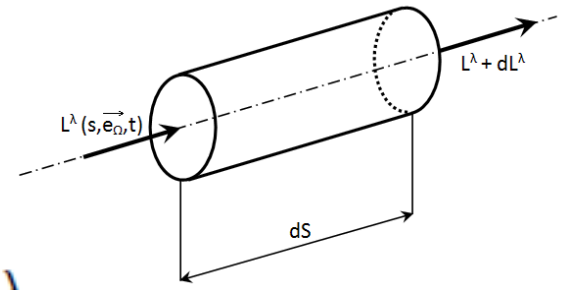
Ray tracing method in PINENS code



• Divide the half space in front of the heat shield in solid angles held on equally spread rays

• Write and solve the radiative transfer equation (RTE) along each ray and for each wavelength

$$\frac{dL^\lambda}{ds} = \varepsilon^\lambda - \kappa^\lambda L^\lambda$$



• Compute the radiative flux

$$q_R = \mathbf{q_R} \cdot \mathbf{n} = \int_0^{+\infty} \left(\int_{2\pi} L^\lambda(r_{wall}, \mathbf{s})\ \mathbf{s}.\mathbf{n}\ d\Omega \right) d\lambda$$

• No flow-radiation coupling for now

High-temperature gas radiation modeling :

Line-by-line spectral code (PASTIS, P. Boubert at CORIA) :

- Atoms : Ar, Ar+, C, C+, H, D, N, N+, O, O+, Al, Al+, Al++, Si, Si+, Si++, W, W+, W++, Be, Be+, Be++, He
- Molecular systems :
  - C_2 Phillips, C_2 Swan, C_2 Deslandres-dAzumbuja, C_2 Fox-Herberg, C_2 Mulliken
  - CH (AX), CH (BX), CH (CX)
  - CN Violet, CN Red, CN Leblanc
  - CO et CO_2 rovibrational (CDSD4000 database)
  - CO Cameron, CO (4e positive), CO (3e positive), CO Angstrom, CO Asundi, CO Triplet, CO Herman
  - CO+ Comet tail, CO+ (1er negative), CO+ Baldet-Johnson…

High-temperature gas radiation modeling :

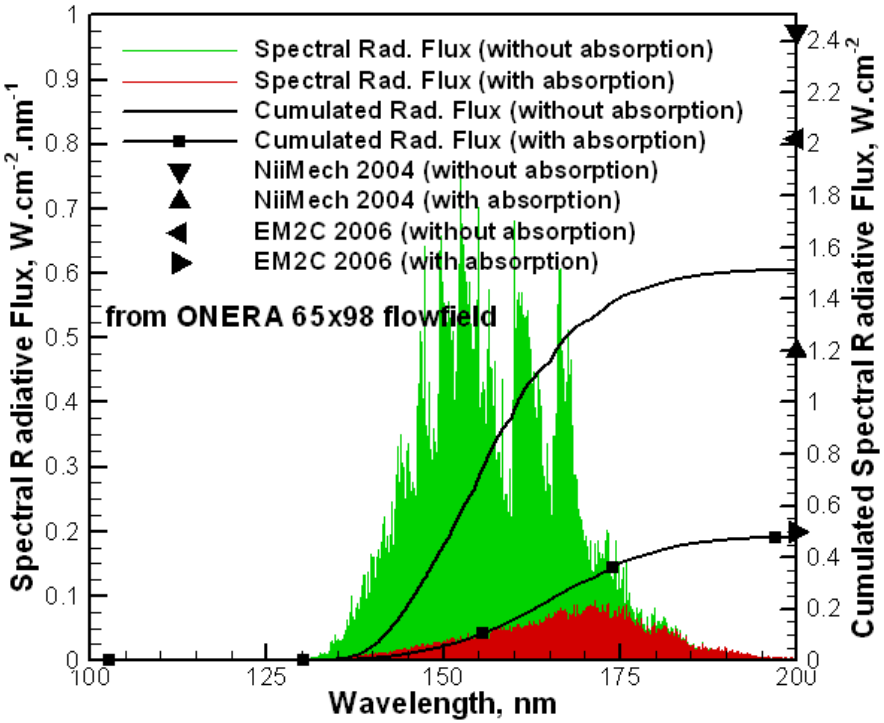
Spectral code PASTIS

- Molecular systems (continued) :
  - N_2 Herman, N_2 (1er positive), N_2 (2e positive), N_2 Lyman-Birge-Hopfield, N2 Birge-Hopfield1, N_2 Birge-Hopfield2, N_2 Worley-Jenkins, N_2 Worley, N_2 Carroll-Yoshino
  - N_2+ Meinel, N_2+ (1er negative), N_2+ (2e negative),
  - NO gamma, NO beta, NO epsilon

- For discharge and combustion issues : NH, OH

Radiation transport modeling :

Spectral and cumulated radiative heat flux



- at the stagnation point of the flow around a blunt body
- optically thin gas (green) vs. absorbing gas (red)
- discrepancies between radiative flux predictions
- radiative fluxes strongly depend gas composition and thermodynamical state

Outline

- Equations
- CFD code (PINENS – IUSTI)
  - Double-cone flow
- Radiative transfer modeling
  - ExoMars probe into CO_2-N_2
- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
- Concluding remarks

Re-entry and hypersonic aerothermodynamics

So far :

- **Global** chemical **kinetics** models for gas mixtures
  (Park, Dunn-Kang, Gupta-Yos,…)

- **Multi-temperature** models for the vibrational / electronic relaxation (Landau-Teller, Millikan & White, Treanor & Marrone)

- **Limits** of global models
  - most of them suppose that the molecules dissociate at the same rate, whatever the vibrational level they are on

  - suppose that the distribution of the vibrational energy on the various levels follows a Boltzmann distribution

Re-entry and hypersonic aerothermodynamics

Now :

- **Collisional-Radiative (CR)** models are developed
  - to overcome the limits of the global models, both for reacting and radiating gases
  - the elementary vibrational specific data are obtained either
    - by a Quasi-Classical Trajectory (QCT) method (Capitelli, 2004)
    - or experimentally on the 1st vib. levels, then extrapolated by means of the SSH theory
- Collisional Radiative Models (CoRaM) :
  - developed at CORIA by Arnaud Bultel and his colleagues
  - for various gases :
    - Nitrogen : CoRaM-N_2
    - Air : CoRaM-Air
    - Mars : CoRaM-Mars

Chemical kinetics modeling :

• CoRaM models implemented in a 1D code for simulating reactive gas flow across a normal shock solved with a Rankine-Hugoniot method

• We now want to predict the aerothermodynamic state of a reacting gas in a **2D or axi-symmetric flow field with detailed kinetics models :**

- implement detailed kinetics models into a CFD code
- challenging
- start with simple configurations and a simple gas : **Nitrogen**

Chemical kinetics modeling :

CoRaM-N_2 → reduced → vibrational-state specific model

- **neutral** species : N_2 (X,v=0,…67) , N(X)
  → 69 pseudo-species
- 6817 processes :
  - VT exchanges through molecular impact (67, VT-m)
    $N_2(X,v) + M \leftrightarrow N_2(X,v') + M$
  - VV exchanges through molecular impact (4489, VV-m)
    $N_2(X,v) + N_2(X,w) \leftrightarrow N_2(X,v+1) + N_2(X,w-1)$
  - VT by molec. impact leading to dissociation(1, VT-m-D)
    $N_2(X,v) + M \leftrightarrow N + N + M$
  - VV leading to dissociation (67, VV-m-D)
  - VT by atomic impact (2125, VT-a)
  - VT by atomic impact leading to dissociation (68, VT-a-D)

Chemical kinetics modeling :

Navier-Stokes equations for N_2,N mixtures :

- Global kinetics / multi-temperature models (N_2,N):

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s(\mathbf{V} + \tilde{\mathbf{V}}_s)) = \omega_s^C, \qquad s = 1, \ldots, n_s \qquad n_s = 2$$

$$\frac{\partial \rho_v e_v^V}{\partial t} + \nabla \cdot (\rho_v e_v^V (\mathbf{V} + \tilde{\mathbf{V}}_v) + \mathbf{q}_v^V) = \omega_v^V, \qquad v = 1, \ldots, n_v \qquad n_v = 1$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V} - \bar{\bar{\sigma}}) = 0$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{V} - \bar{\bar{\sigma}}\mathbf{V} + \mathbf{q}) = 0$$

→ 6 transport equations

- Detailed kinetics model (N_2(X,v),N(X)):

$$\frac{\partial \rho_{sv}}{\partial t} + \nabla \cdot (\rho_{sv}(\mathbf{V} + \tilde{\mathbf{V}}_{sv})) = \omega_{sv}^C, \qquad sv = 1, \ldots, n_{sv} \qquad n_{sv} = 69$$

→ 72 transport equations

Outline

- Equations
- CFD code (PINENS – IUSTI)
  - Double-cone flow
- Radiative transfer modeling
  - ExoMars probe into CO_2-N_2
- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
    - Population densities along the stagnation streamline
    - Boltzmann diagrams
    - Comparison global / detailed kinetics models
- Concluding remarks

Nitrogen flow over a sphere at Mach 30 :

- one-meter radius sphere
- flow conditions (FIRE II flight conditions):
  - Pressure : 54 Pa
  - Temperature : 274 K
  - Velocity : 10.6 km/s
  - Gas composition : 100% of N_2 (X,v=0)
- axisymmetric, laminar, viscous flow
- sphere surface : fixed temperature : 1500 K
  non catalytic
- transport coefficients : basic models presented earlier

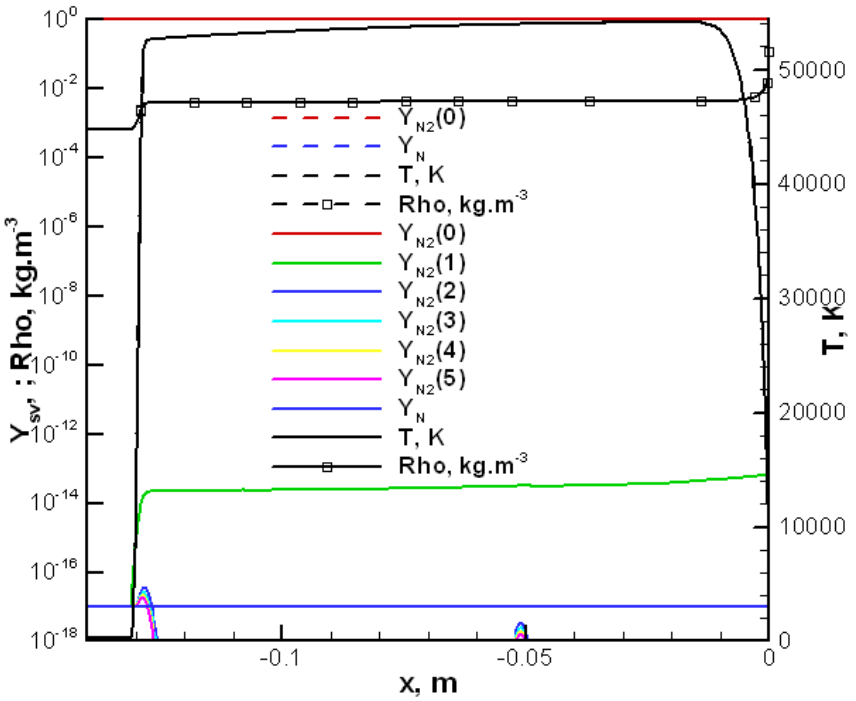
- vibrational-state specific model :
  - 69 pseudo-species : N_2 (X,v=0,…67) , N(X)
  - 6817 processes :

Elementary processes	Process number
vibration–vibration under molecular impact (VV-m)	4489
vibration–translation under molecular impact (VT-m)	67
vibration–translation under molecular impact leading to dissociation (VT-m-D)	1
vibration–vibration under molecular impact leading to dissociation (VV-m-D)	67
vibration–translation under atomic impact (VT-a)	2125
vibration–translation under atomic impact leading to dissociation (VT-a-D)	68

N_2 flow over a sphere at Mach 30 with a vib. specific model :

VV by molecular impact → 4489 reactions
(VV-m)

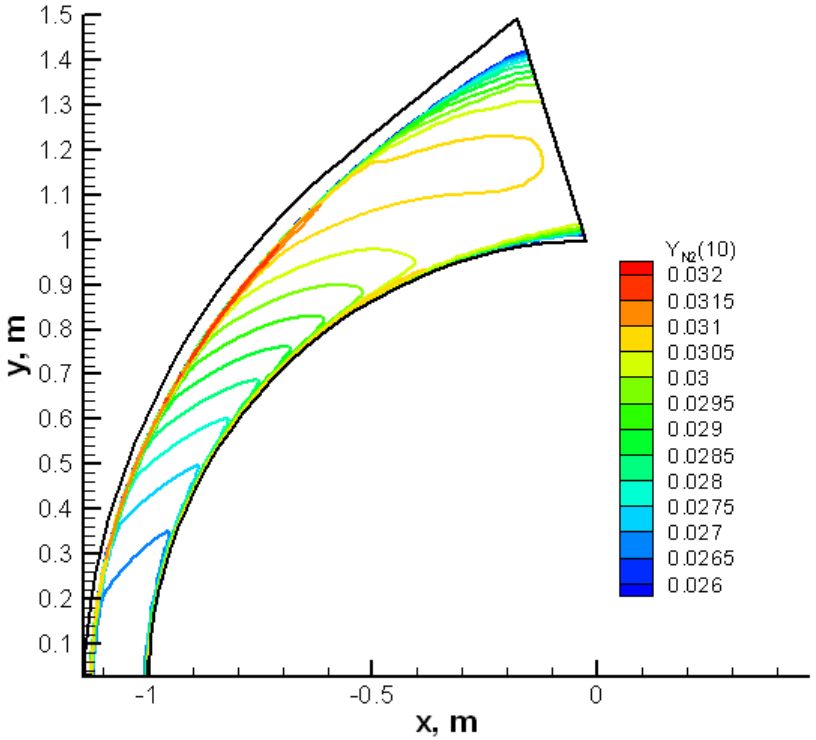
T and Ys along the stagnation line



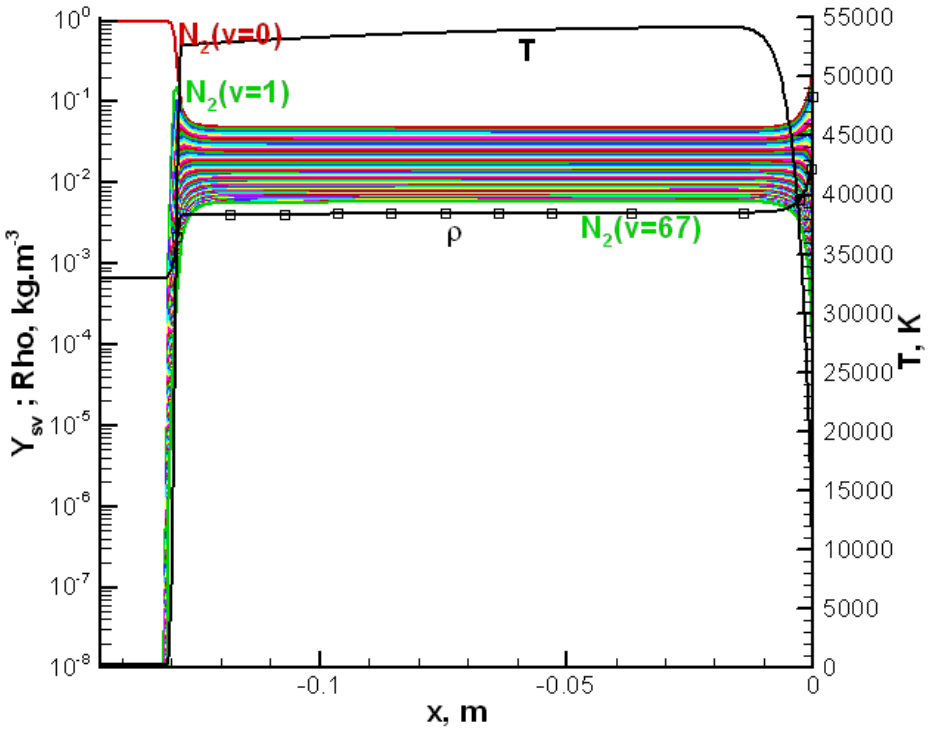
insignificant effect
of VV exchanges on the
$N_2(X,v)$ density populations
in this particular flow test case
(compression flow)…

N_2 flow over a sphere at Mach 30 with a vib. specific model :

VT by molecular impact → 67 reactions
(VT-m)



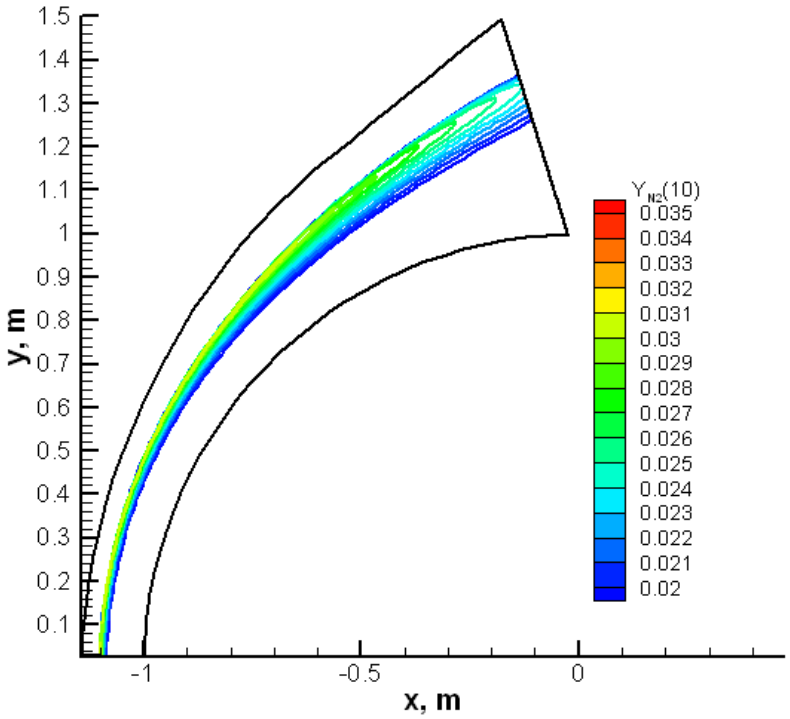
N_2(X, v=10) contours



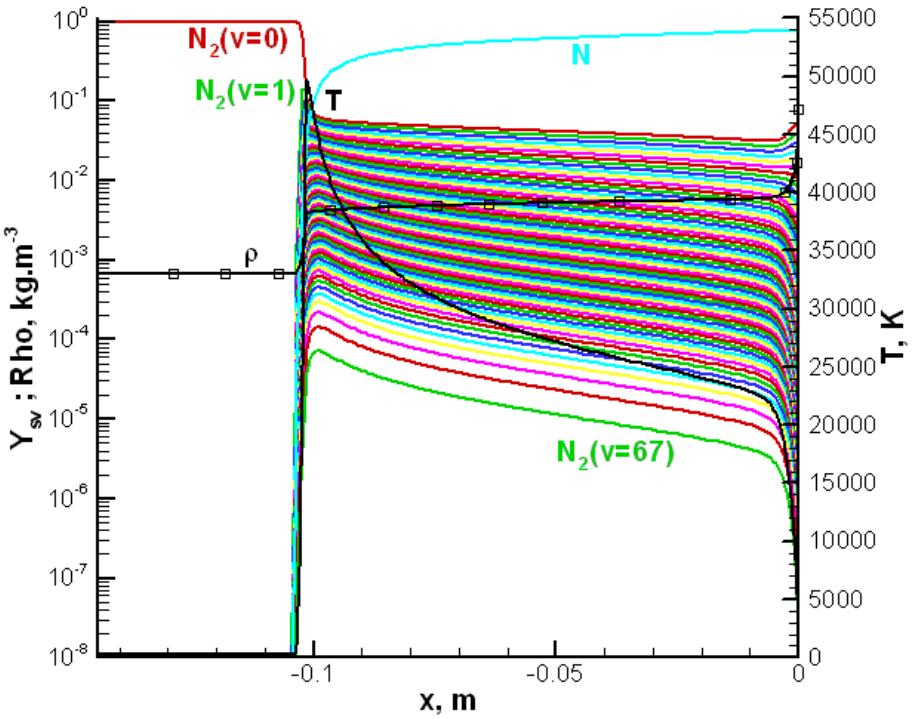
T and Ys along the stagnation line

N_2 flow over a sphere at Mach 30 with a vib. specific model :

VT by molecular impact + dissociation → 68 reactions
(VT-m) + (VT-m-D)



N_2(X, v=10) contours



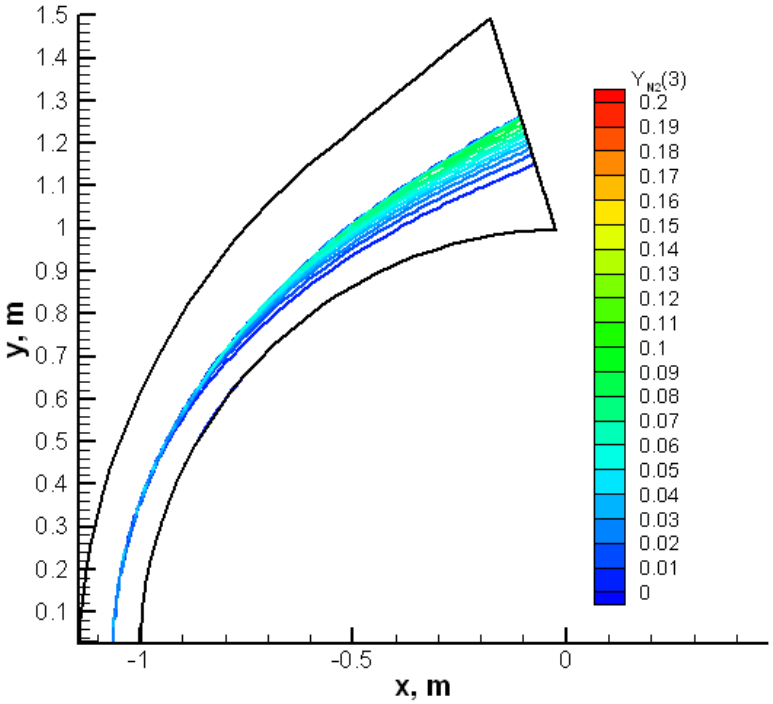
T and Ys along the stagnation line

N_2 flow over a sphere at Mach 30 with a vib. specific model :

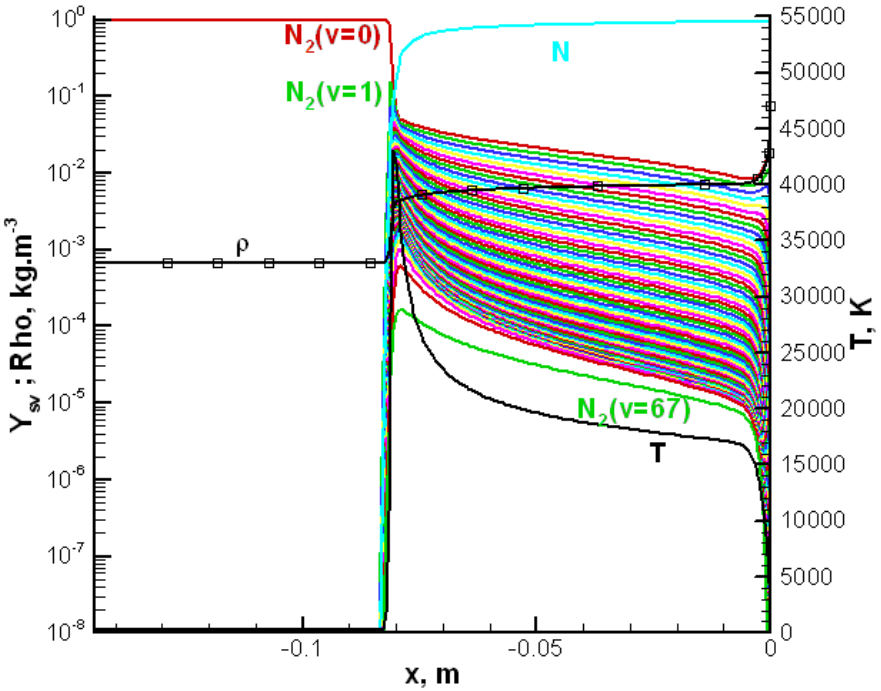
VT and VV by molecular impact + dissociation

+ VT by atomic impact → 2260 reactions

(VT-m) + (VT-m-D) + (VV-m-D) + (VT-a)



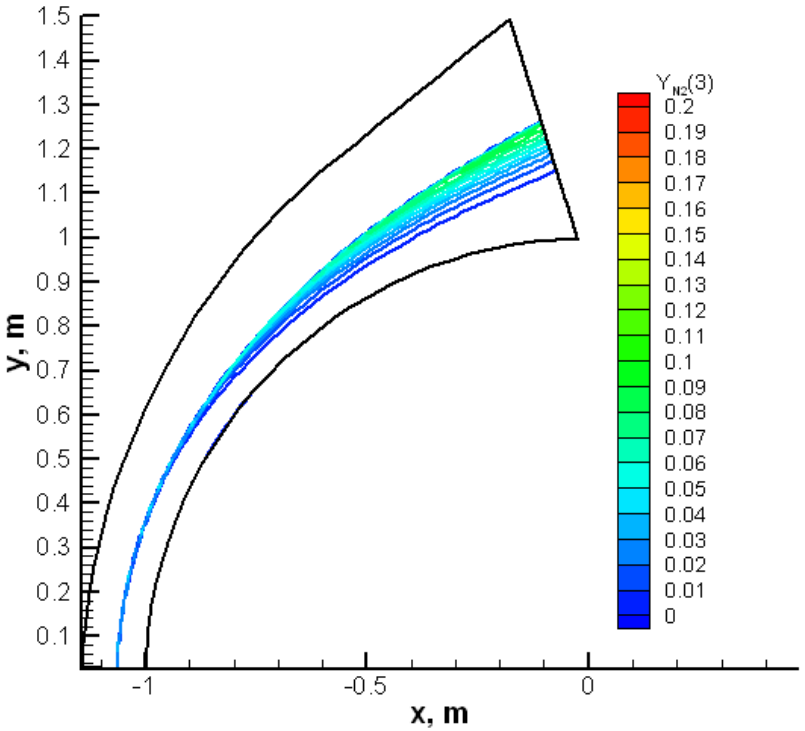
$N_2(X, v=3)$ contours

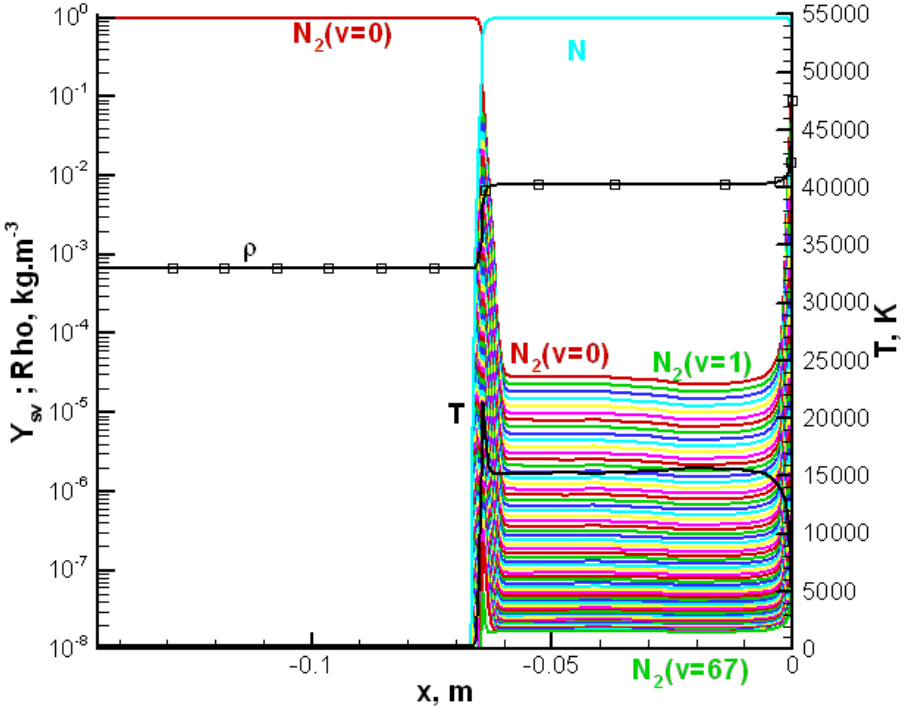


T and Ys along the stagnation line

N_2 flow over a sphere at Mach 30 with a vib. specific model :

VT and VV by molecular impact + dissociation
+ VT by atomic impact + dissociation → 2328 reactions
(VT-m) + (VT-m-D) + (VV-m-D) + (VT-a) + (VT-a-D)





N_2(X, v=3) contours

T and Ys along the stagnation line

Outline

- Equations

- CFD code (PINENS – IUSTI)
  - Double-cone flow

- Radiative transfer modeling
  - ExoMars probe into CO_2-N_2

- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
    - Population densities along the stagnation streamline
    - Boltzmann diagrams
    - Comparison global / detailed kinetics models

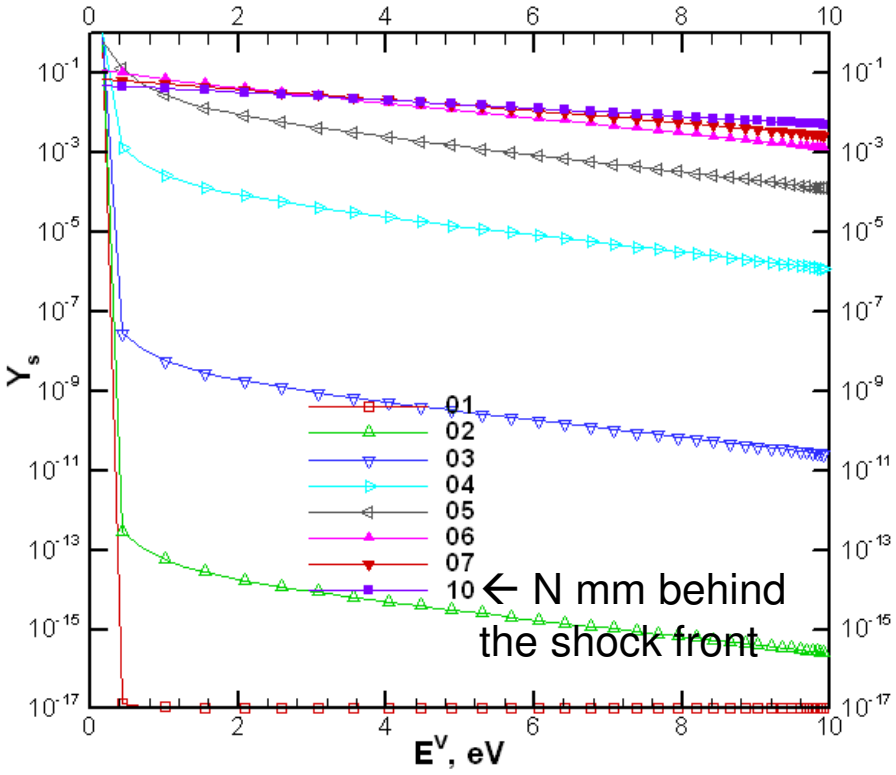
- Concluding remarks

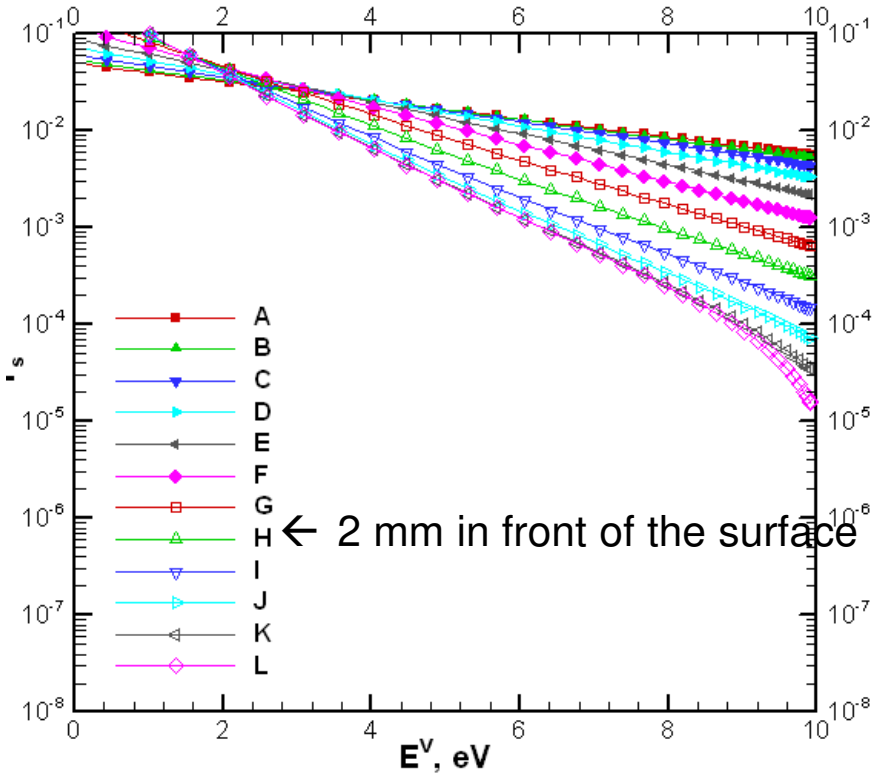
Boltzmann distribution ?

67 processes (VT-m)

Behind the shock front

In the boundary layer

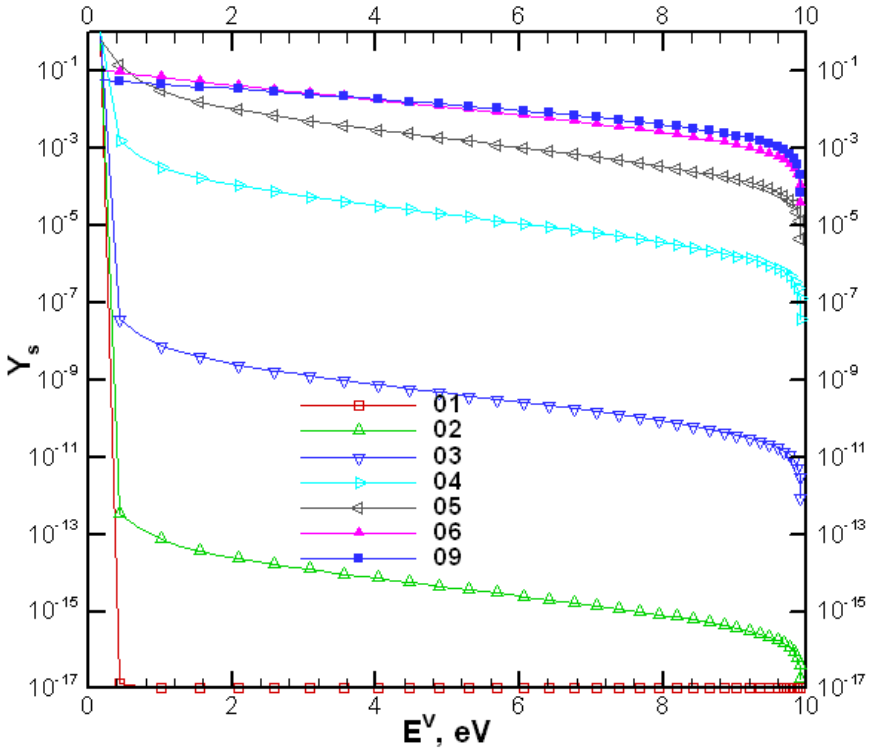




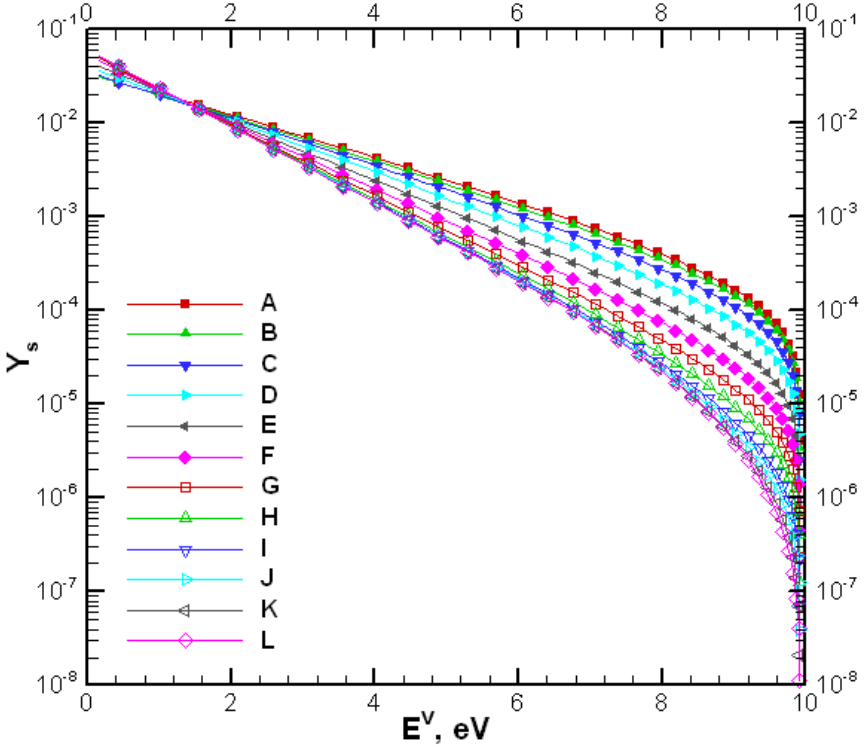
Boltzmann distribution ?

68 processes (VT-m) + (VT-m-D)

Behind the shock front



In the boundary layer

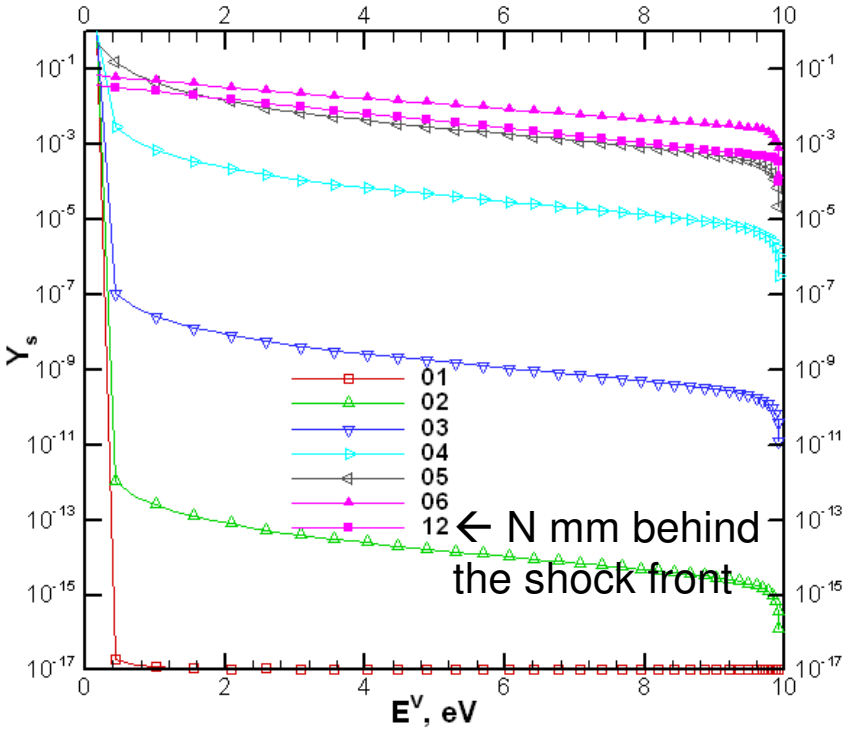


Boltzmann distribution not reached

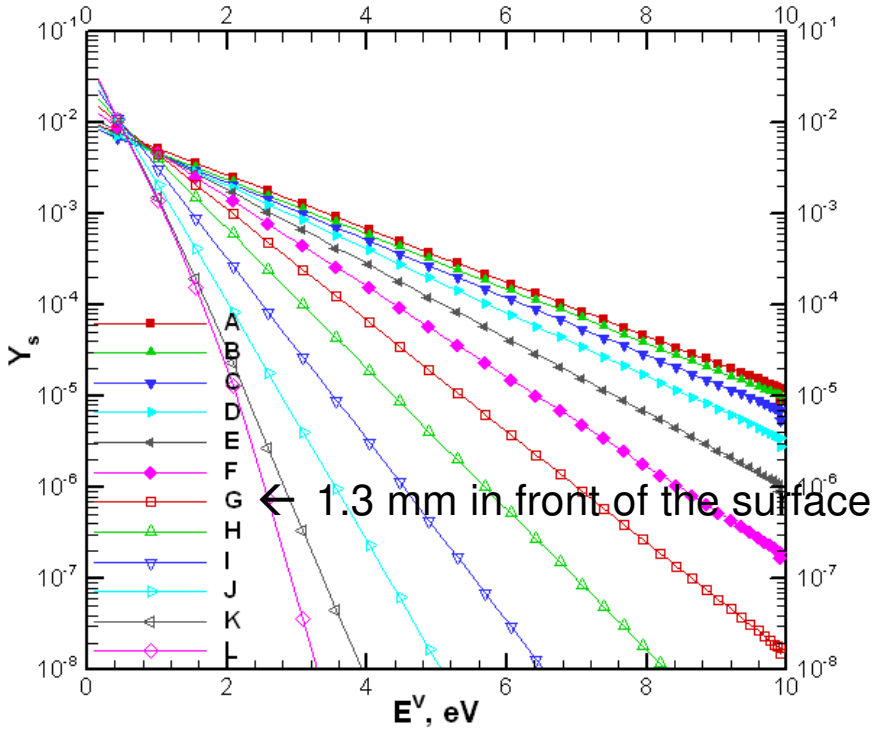
Boltzmann distribution ?

2260 processes: (VT-m) + (VT-m-D) + (VV-m-D) + (VT-a)

Behind the shock front



In the boundary layer



Boltzmann distribution reached only outside of the SW and the BL

Outline

- Equations

- CFD code (PINENS – IUSTI)
  - Double-cone flow

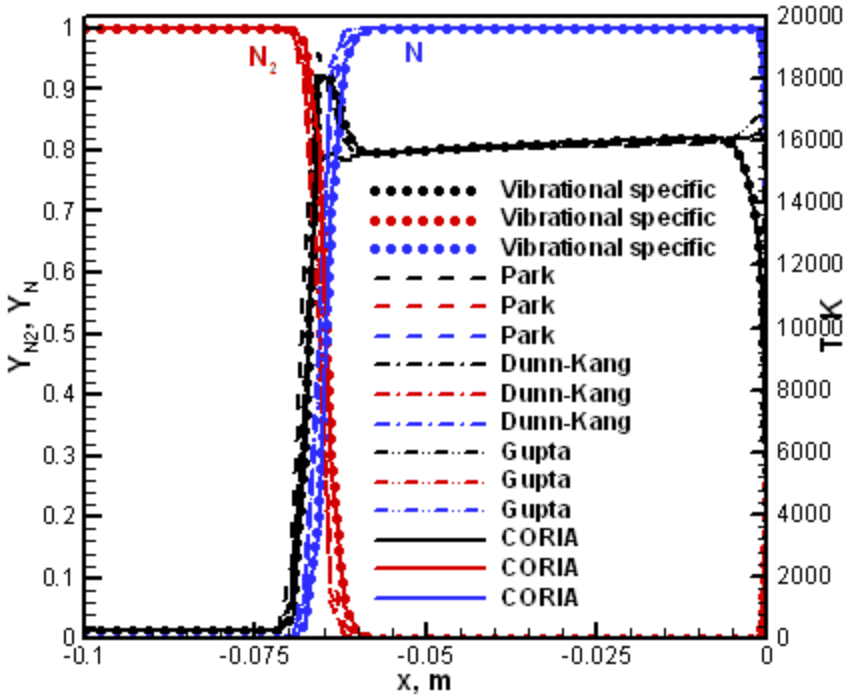
- Radiative transfer modeling
  - ExoMars probe into CO_2-N_2

- Detailed chemical kinetics modeling (CoRaM – CORIA)
  - Sphere into $N_2(v)$
    - Population densities along the stagnation streamline
    - Boltzmann diagrams
    - Comparison global / detailed kinetics models

- Concluding remarks

Comparison of flow fields obtained with global and detailed models:

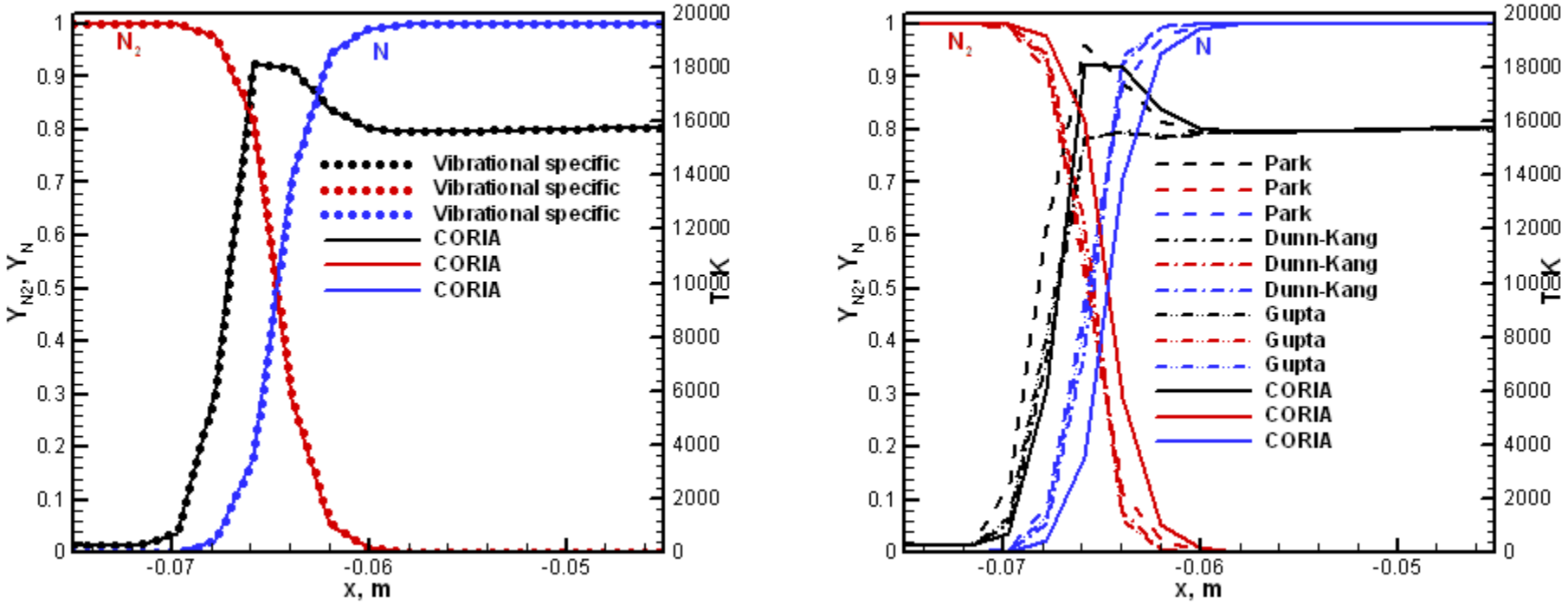
Global models for kinetic rates (2 reactions : dissociation of N_2)
vs. Vibrational specific model (6817 reactions)



T and Ys along the stagnation line

Comparison of flow fields obtained with global and detailed models:

Global models for kinetic rates (2 reactions : dissociation of N_2)
vs. Vibrational specific model (6817 reactions)



T and Ys along the stagnation line

N_2 flow over a sphere with a vib. specific model :

Other flight entry conditions :

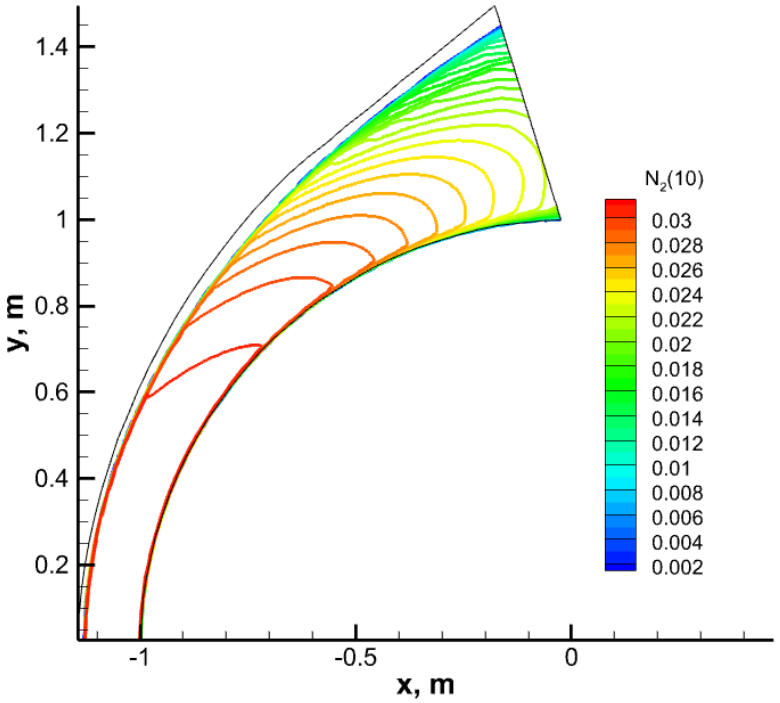
Time, s	Altitude, km	Velocity, km/s	Density, kg/m^3	T_∞, K	T_w, K
1637.5	67.05	11.25	1.47×10^{-4}	228	1030
1642.66	53.86	10.56	7.17×10^{-4}	273	480 → 1500
1648	42.14	8.30	3.00×10^{-3}	267	1560
1651	37.19	6.19	6.05×10^{-3}	253	1060

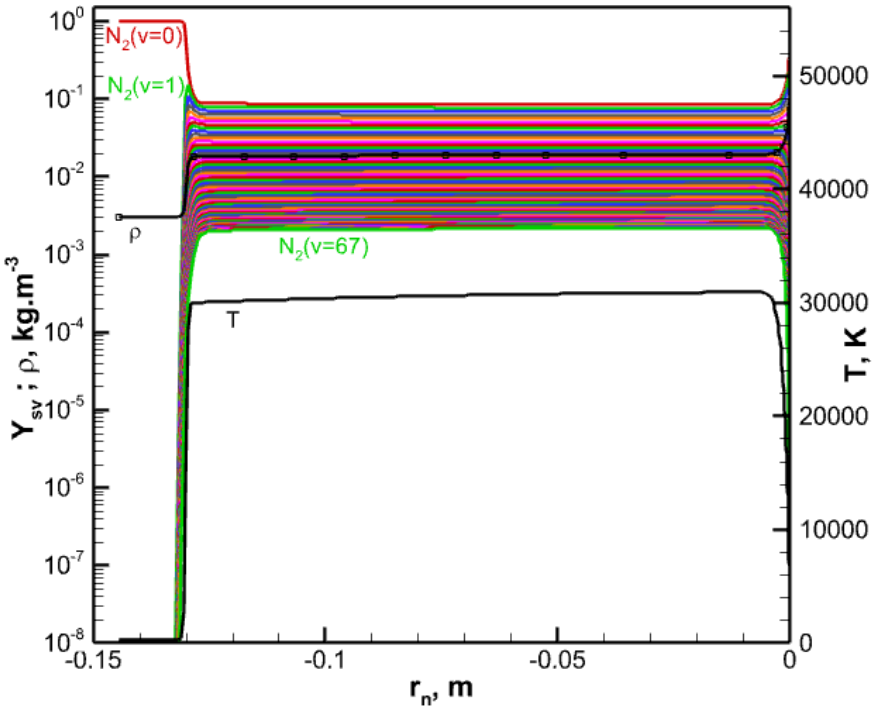
Atmosphere = 100% N_2(v=0)

Chemical kinetics : 69 pseudo-species : N_2(v=0,67), N

N_2 flow over a sphere at Mach 24 with a vib. specific model :

67 (VT-m) processes





N_2(v=10) contours

T and Ys along the stagnation line

N_2 flow over a sphere at Mach 24 with a vib. specific model :

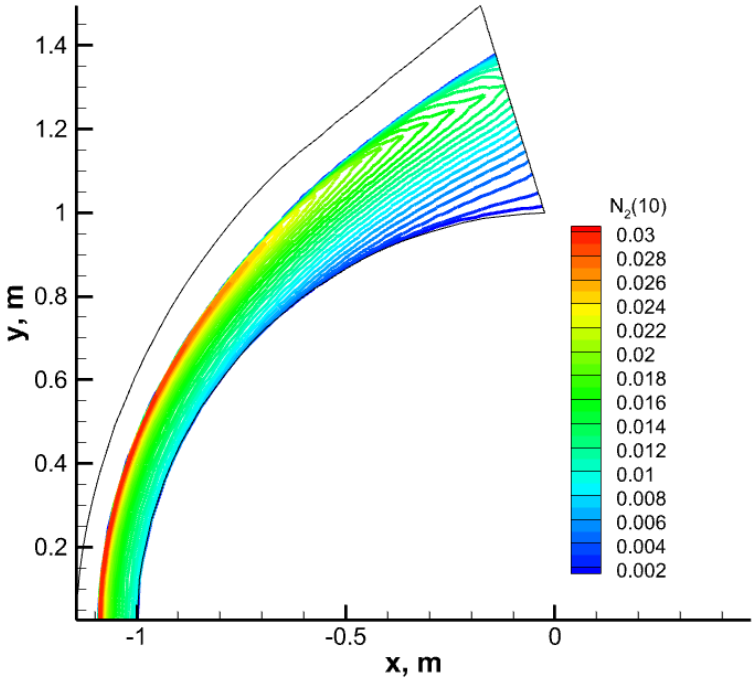
+ 4489 (VV-m) processes

No significant effect on the $N_2(v)$ density populations
in this particular flow test case
(compression flow)…

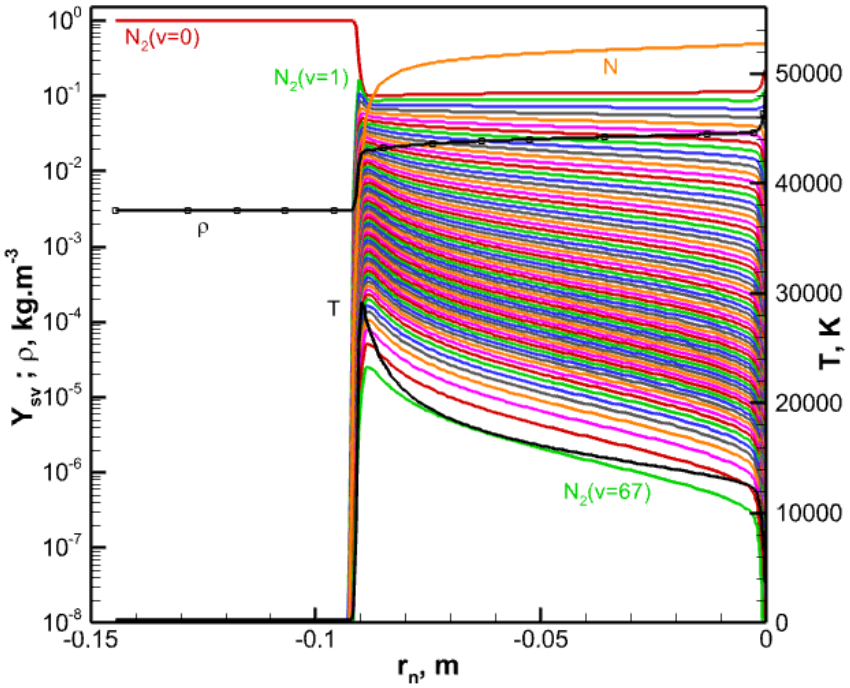
→ the 4489 (VV-m) processes will be ignored for the rest of the study

N_2 flow over a sphere at Mach 24 with a vib. specific model :

67(VT-m) + 1(VT-m-D) → 68 reactions



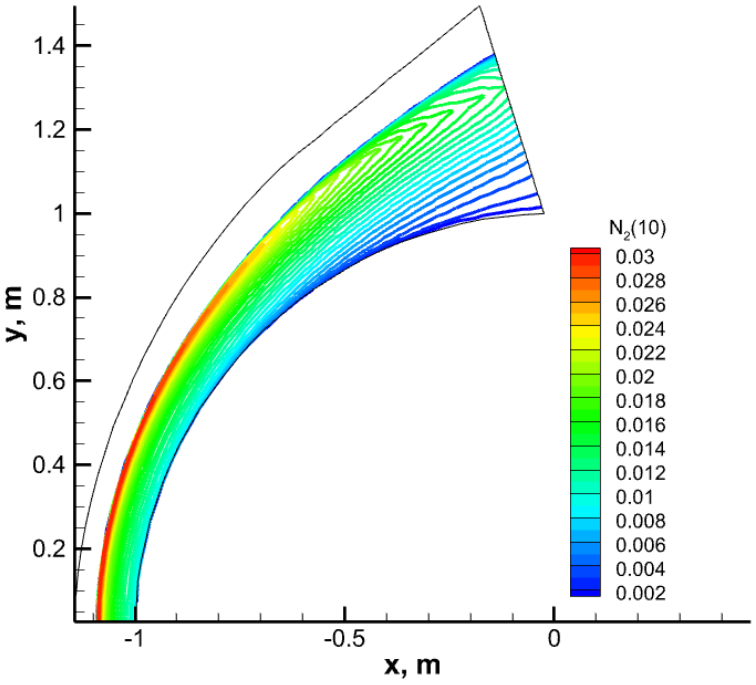
N_2(v=10) contours



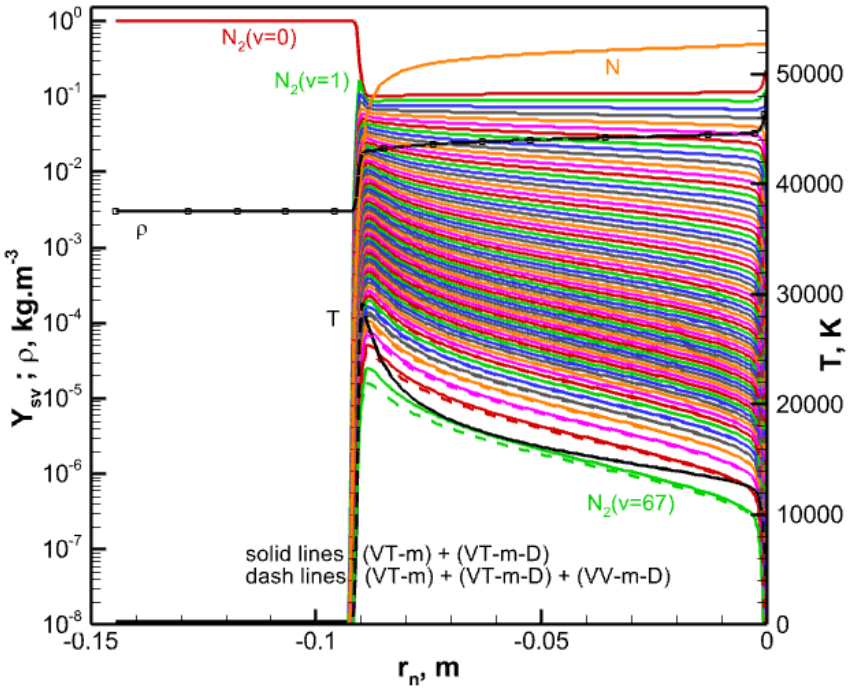
T and Ys along the stagnation line

N_2 flow over a sphere at Mach 24 with a vib. specific model :

67(VT-m) + 1(VT-m-D) + 67(VV-m-D) → 135 reactions



N_2(v=10) contours

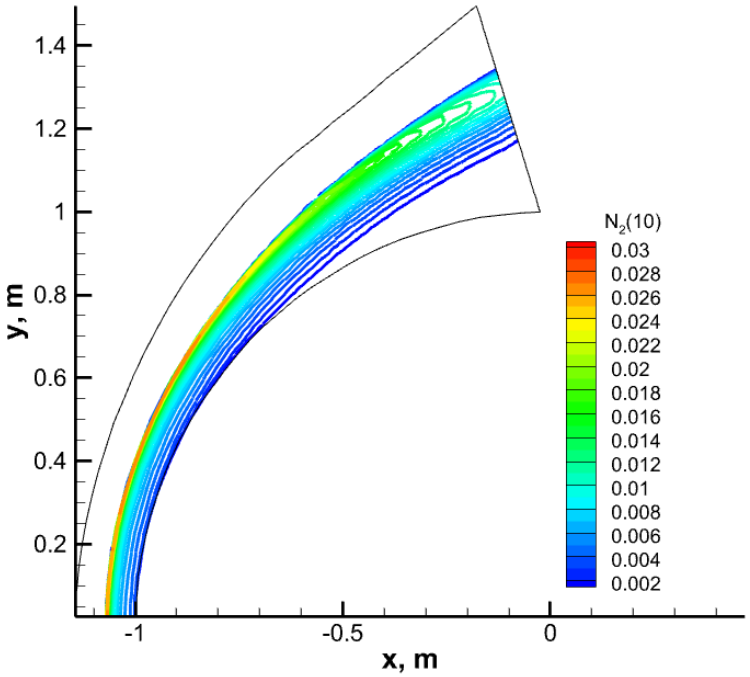


T and Ys along the stagnation line

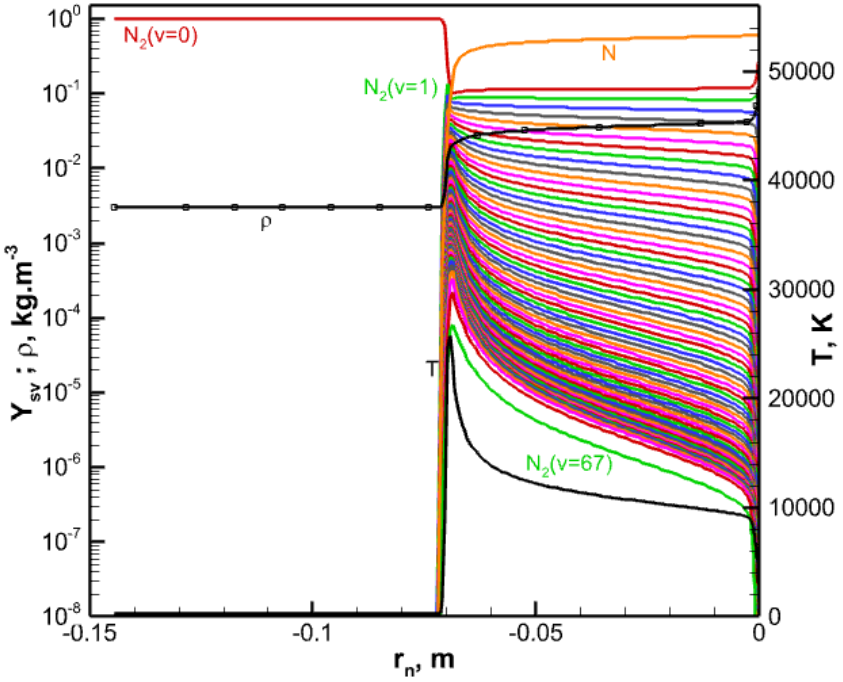
N_2 flow over a sphere at Mach 24 with a vib. specific model :

67(VT-m) + 1(VT-m-D) + 67(VV-m-D) + 2125(VT-a)

→ 2260 reactions



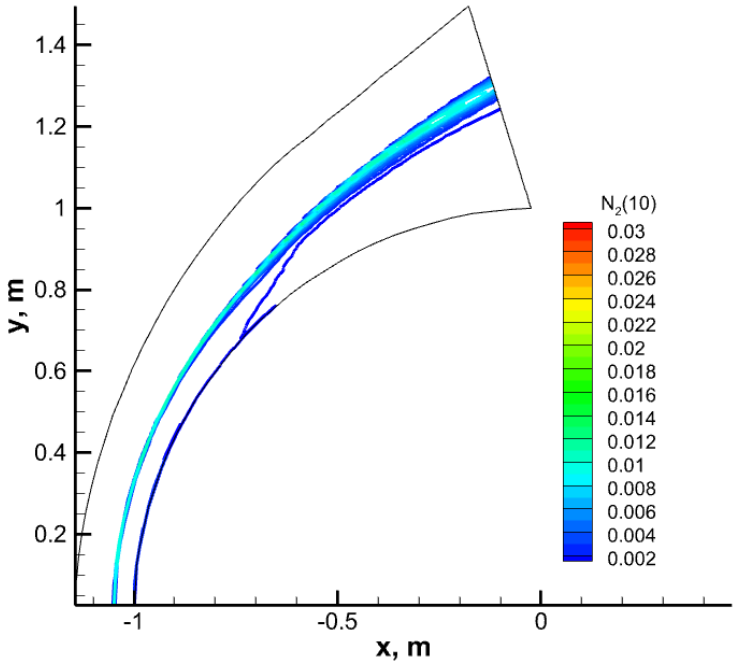
N_2(v=10) contours



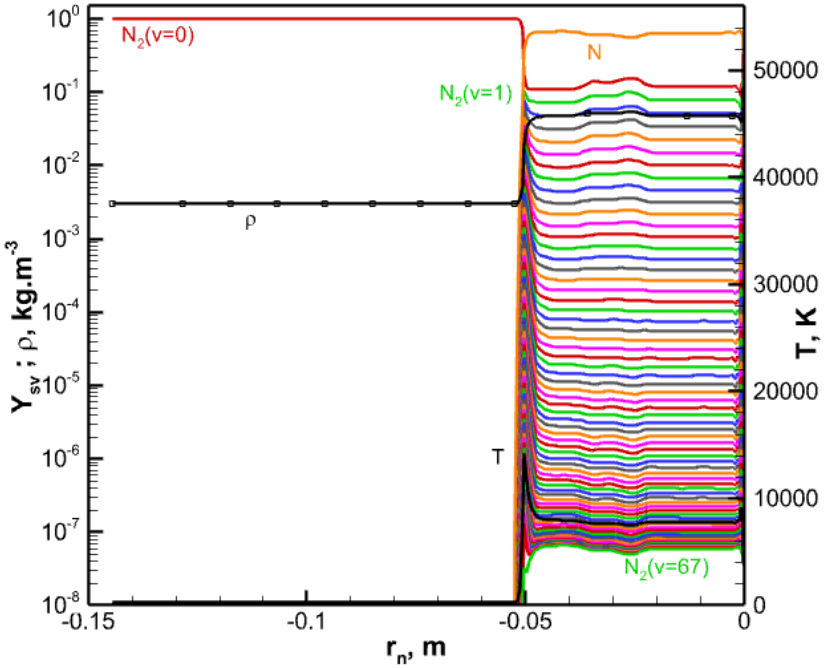
T and Ys along the stagnation line

N_2 flow over a sphere at Mach 24 with a vib. specific model :

67(VT-m) + 1(VT-m-D) + 67(VV-m-D) + 2125(VT-a) + 68(VT-a-D)
→ 2328 reactions



N_2(v=10) contours

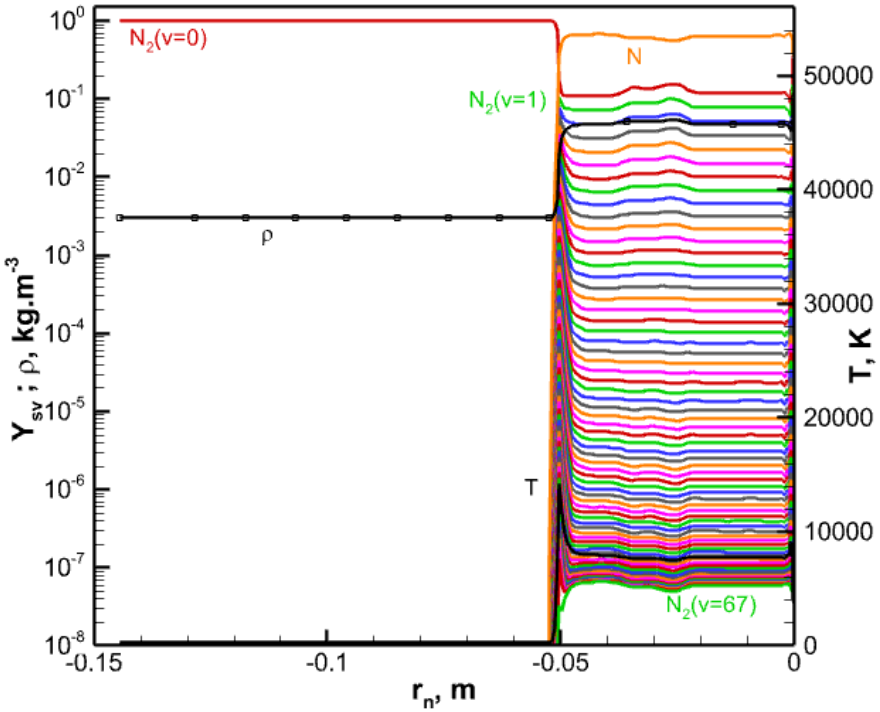


T and Ys along the stagnation line

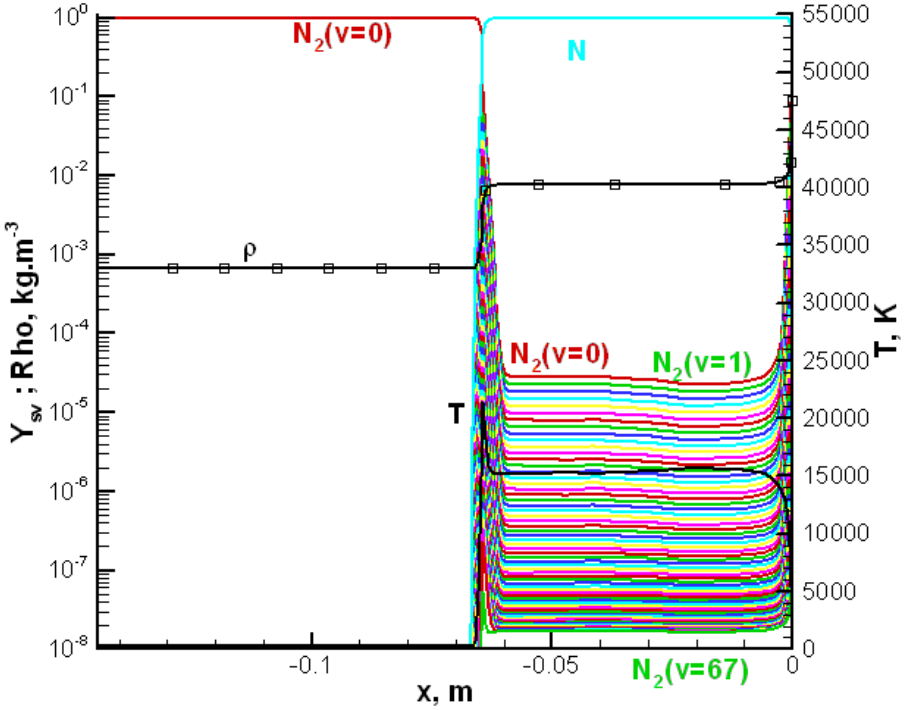
67(VT-m) + 1(VT-m-D) + 67(VV-m-D) + 2125(VT-a) + 68(VT-a-D)

Comparison

V=8 km/s



V=10.6 km/s



T and Ys along the stagnation line

N_2 flow over a sphere with a vibrational-state specific model :

Other flight entry conditions :

Time, s	Altitude, km	Velocity, km/s	Density, kg/m^3	T_∞, K	T_w, K
1637.5	67.05	11.25	1.47×10^{-4}	228	1030
1642.66	53.86	10.56	7.17×10^{-4}	273	480 → 1500
1648	42.14	8.30	3.00×10^{-3}	267	1560
1651	37.19	6.19	6.05×10^{-3}	253	1060

Atmosphere = 100% N_2(v=0)
Chemical kinetics : 69 pseudo-species : N_2(v=0,67), N

• **successfully implemented** a vibrational-state specific model into PINENS code (based on shock capturing method)

→ simple gas mixture : N_2 (X,v=0,…67), N(X)

→ 69 (pseudo-)species

→ more than 6800 reactions

• showed the **effect of** each group of VT and VV exchanges and dissociation **processes** on the vibrational level population densities in the shock layer

• showed when and where the **Boltzmann distribution** is reached

• compared results obtained with **detailed** (vibrational specific model) and **global** models (Park, Dunn-Kang, Gupta-Yos,…)

Global summary :

• Conservative equations for plasma flows, in atmospheric entry conditions

• 3 application cases computed with the PINENS code :

- Double-cone flow : not yet resolved. Freestream conditions (that are the exit conditions of the shock tunnel nozzle) need to be better defined. Not an easy task
- ExoMars probe entry into a Mars-like atmosphere (CO_2-N_2) : computation of the radiative transfer. Not an easy task either
- Entry into a nitrogen atmosphere simulated with a vibrational-state specific model

Acknowledgement :

- This work was performed using the HPC resources from mesocentre Aix-Marseille University

Thank you for your attention