Modélisation et simulation numérique des écoulements plasmas

Applications hypersoniques

Thierry Magin

Aeronautics and Aerospace Department
von Karman Institute for Fluid Dynamics, Belgium

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- Collaborators who contributed to the results presented
  - **Benjamin Graille** (Laboratoire de Mathématiques d'Orsay)
  - **Alejandro Alvarez Laguna, Anne Bourdon, Pietro Congedo, Vincent Giovangigli, Olivier Lemaitre**, **Marc Massot**, & **Teddy Pichard** (Ecole Polytechnique)
  - **Federico Bariselli, Anatole Berger, Stefano Boccelli, Michele Capriati, Anabel del Val, Bruno Dias, Giuseppe Gangemi, Pedro Jorge, Damien Le Quang, Pietro Parodi,** & **Alessandro Turchi** (von Karman Institute)

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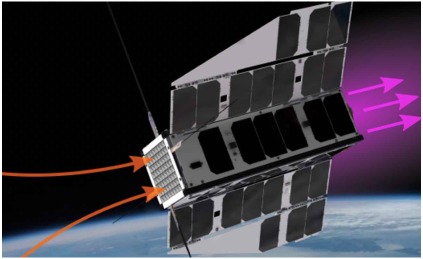
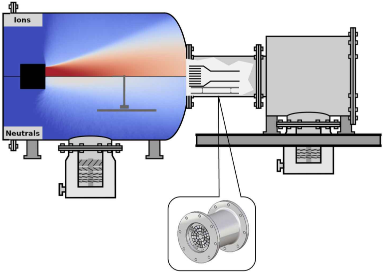
Developing disruptive technology for hypersonics

- Hypersonics
  - Fight within planetary atmosphere at Mach > 5
- Challenges for fluid models and numerical methods
  - Multiscale and multiphysics problem
  - Calibration and validation of computational models



Air Breathing Electric Propulsion concept for Very Low Earth Orbit observation

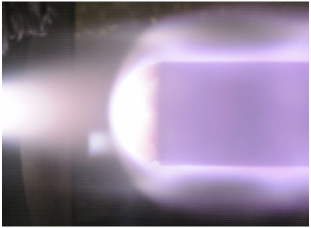


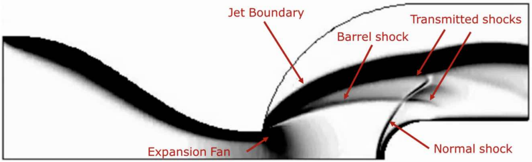
VKI Drag-on low density plasma facility [Jorge, Parodi, LeQuang, M., RGD32 2022]

‘Aerothermochemistry” coined by von Kármán in 1950’s

> *“With the advent of jet propulsion, it became necessary to broaden the field of aerodynamics to include problems which before were treated mostly by physical chemists. . .”* Theodore von Kármán, 1958

- Some open problems
  - Fluid models for thermo-chemical nonequilibrium
  - High-order methods for hypersonic flows
  - Efficient solvers for 3D plasma sheath



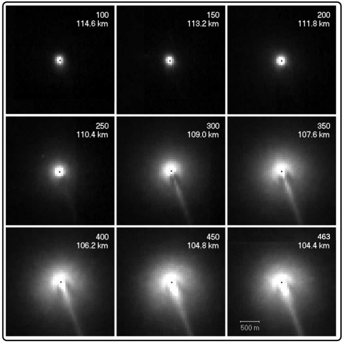


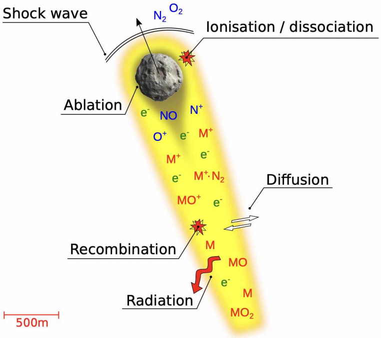
[Capriati, Turchi, Congedo, M., 9th EUCASS 2022]

Under-expanded air jet over catalytic probe in VKI Plasmatron

Fluid models beyond Navier-Stokes. . .

- Kinetic theory allows us to
  - Describe plasmas in the rarefied regime
  - Derive asymptotic fluid solutions





[Bariselli, Boccelli, Dias, Hubin, M., Astronomy & Astrophysics 2020]

Meteors can be detected by scattering of electromagnetic waves by electrons in rarefied trail

Outline

Simulation of plasma sheath

Reactive collision operator

Calibration of models

Outline

Simulation of plasma sheath

Reactive collision operator

Calibration of models

Dimensional analysis for plasmas [Petit, Darrozes 1975]

- 2 kinetic temporal scales based on common mean-free-path l^0

$$t_{\mathrm{e}}^0 = \frac{l^0}{V_{\mathrm{e}}^0}, \qquad t_h^0 = \frac{l^0}{V_h^0} = \frac{1}{\varepsilon} t_{\mathrm{e}}^0 \quad \text{with} \quad \varepsilon = \frac{V_h^0}{V_{\mathrm{e}}^0} = \sqrt{\frac{m_{\mathrm{e}}}{m_h}}$$

- 1 macroscopic temporal scale based on macroscopic length L^0

$$t^0 = \frac{L^0}{V_h^0} = \frac{1}{Kn} t_h^0 \quad \text{with} \quad Kn = \frac{l^0}{L^0}$$

- Hall parameter governed by magnetic field strength b

$$\beta_{\mathrm{e}} = \frac{q^0 B^0}{m_{\mathrm{e}}^0} t_{\mathrm{e}}^0$$

Nondimensional form and scaling of Boltzmann eq.

- Electrons: e

$$\partial_t f_{\mathrm{e}} + \frac{1}{\varepsilon}\boldsymbol{c}_{\mathrm{e}}\cdot\boldsymbol{\partial_x} f_{\mathrm{e}} + \frac{\beta_{\mathrm{e}}}{\varepsilon Kn} q_e \boldsymbol{c}_{\mathrm{e}}\wedge\boldsymbol{B}\cdot\boldsymbol{\partial}_{\boldsymbol{c}_{\mathrm{e}}} f_{\mathrm{e}} + \frac{1}{\varepsilon} q_e \boldsymbol{E}\cdot\boldsymbol{\partial}_{\boldsymbol{c}_{\mathrm{e}}} f_{\mathrm{e}} = \frac{1}{\varepsilon Kn}\mathcal{J}_{\mathrm{e}}$$

- Heavy particles: $i \in \mathrm{H}$

$$\partial_t f_i + \boldsymbol{c}_i\cdot\boldsymbol{\partial_x} f_i + \frac{\varepsilon\beta_{\mathrm{e}}}{Kn}\frac{q_i}{m_i}\boldsymbol{c}_i\wedge\boldsymbol{B}\cdot\boldsymbol{\partial}_{\boldsymbol{c}_i} f_i + \frac{q_i}{m_i}\boldsymbol{E}\cdot\boldsymbol{\partial}_{\boldsymbol{c}_i} f_i = \frac{1}{Kn}\mathcal{J}_i$$

- Multiscale assympotic analysis with entangled parabolic and hyperbolic scalings [Graille, M., Massot 2009]

$$\varepsilon = Kn \quad \text{and} \quad \beta_{\mathrm{e}} = \varepsilon^{1-b}$$

  - **Electrons**: low Mach number regime [Bardos, Golse, Levermore, 1991]
  - **Heavy particles**: compressible gas dynamics regime [Goudon, Jabin, Vasseur, 2005]

Electron heavy-particle collision dynamics

- The collision operators read

$$\begin{aligned} \mathcal{J}_{\mathrm{e}} &= \mathcal{J}_{\mathrm{ee}}(f_{\mathrm{e}}, f_{\mathrm{e}}) + \sum_{j\in \mathrm{H}} \mathcal{J}_{\mathrm{e}j}(f_{\mathrm{e}}, f_j) \\ \mathcal{J}_i &= \frac{1}{\varepsilon}\mathcal{J}_{i\mathrm{e}}(f_i, f_{\mathrm{e}}) + \sum_{j\in \mathrm{H}} \mathcal{J}_{ij}(f_i, f_j), \quad i \in \mathrm{H} \end{aligned}$$

- Momentum conservation in terms of the peculiar velocities

$$\begin{aligned} \boldsymbol{C}_i' &= \frac{\varepsilon}{m_i+\varepsilon^2}\boldsymbol{C}_{\mathrm{e}} + \frac{\varepsilon}{m_i+\varepsilon^2}\boldsymbol{C}_i + s\frac{\varepsilon}{m_i+\varepsilon^2}|\varepsilon\,\boldsymbol{C}_i - \boldsymbol{C}_{\mathrm{e}}|\,\boldsymbol{\omega}, \qquad i \in \mathrm{H} \\ \boldsymbol{C}_{\mathrm{e}}' &= \frac{\varepsilon^2}{m_i+\varepsilon^2}\boldsymbol{C}_{\mathrm{e}} + \frac{\varepsilon m_i}{m_i+\varepsilon^2}\boldsymbol{C}_i - s\frac{m_i}{m_i+\varepsilon^2}|\varepsilon\,\boldsymbol{C}_i - \boldsymbol{C}_{\mathrm{e}}|\,\boldsymbol{\omega} \end{aligned}$$

  - Heavy-particle reference frame

$$\boldsymbol{C}_{\mathrm{e}} = \boldsymbol{c}_{\mathrm{e}} - \varepsilon\boldsymbol{v}_h, \qquad \boldsymbol{C}_i = \boldsymbol{c}_i - \boldsymbol{v}_h, \quad i \in \mathrm{H}$$

  - Relative velocity after collision of direction $\boldsymbol{\omega} = s\frac{\varepsilon\boldsymbol{C}_i' - \boldsymbol{C}_{\mathrm{e}}'}{|\varepsilon\boldsymbol{C}_i' - \boldsymbol{C}_{\mathrm{e}}'|}$
  - Where $s = +1$ for $\mathcal{J}_{i\mathrm{e}}$, $i \in \mathrm{H}$, or $s = -1$ for $\mathcal{J}_{\mathrm{e}i}$, $i \in \mathrm{H}$

Expansion of crossed collision operators

- Introducing the relative velocity vector $\gamma_{\mathrm{e}} = \frac{\varepsilon \boldsymbol{C}_i - \boldsymbol{C}_{\mathrm{e}}}{(1+\varepsilon^2/m_i)^{1/2}}$, the crossed collision operator $\mathcal{J}_{i\mathrm{e}}$, $i \in \mathrm{H}$, is defined as

$$\mathcal{J}_{i\mathrm{e}}(f_i, f_{\mathrm{e}}) = \int \sigma_{ie}\Big(|\gamma_{\mathrm{e}}|^2, \boldsymbol{\omega}\cdot\frac{\gamma_{\mathrm{e}}}{|\gamma_{\mathrm{e}}|}\Big)\,|\varepsilon \boldsymbol{C}_i - \boldsymbol{C}_{\mathrm{e}}|\Big[f_i(\boldsymbol{C}_i')f_{\mathrm{e}}(\boldsymbol{C}_{\mathrm{e}}') - f_i(\boldsymbol{C}_i)f_{\mathrm{e}}(\boldsymbol{C}_{\mathrm{e}})\Big]\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}\boldsymbol{C}_{\mathrm{e}}$$

Theorem 1 (Degond, Lucquin 1996, Graille, M., Massot 2009)
$\mathcal{J}_{i\mathrm{e}}$, $i \in \mathrm{H}$, can be expanded in the form:

$$\boxed{\mathcal{J}_{i\mathrm{e}}(f_i, f_{\mathrm{e}})(\boldsymbol{C}_i) = \varepsilon\mathcal{J}^1_{i\mathrm{e}}(f_i, f_{\mathrm{e}})(\boldsymbol{C}_i) + \varepsilon^2\mathcal{J}^2_{i\mathrm{e}}(f_i, f_{\mathrm{e}})(\boldsymbol{C}_i) + \varepsilon^3\mathcal{J}^3_{i\mathrm{e}}(f_i, f_{\mathrm{e}})(\boldsymbol{C}_i) + \mathcal{O}(\varepsilon^4)}$$

- **The crossed collision operator $\mathcal{J}_{\mathrm{e}i}$, $i \in \mathrm{H}$, is defined as**

$$\mathcal{J}_{\mathrm{e}i}(f_{\mathrm{e}}, f_i) = \int \sigma_{ei}\Big(\frac{m_i|\boldsymbol{C}_{\mathrm{e}} - \varepsilon \boldsymbol{C}_i|^2}{m_i+\varepsilon^2}, \boldsymbol{\omega}\cdot\boldsymbol{e}\Big)|\boldsymbol{C}_{\mathrm{e}} - \varepsilon \boldsymbol{C}_i|\Big[f_{\mathrm{e}}(\boldsymbol{C}_{\mathrm{e}}')f_i(\boldsymbol{C}_i') - f_{\mathrm{e}}(\boldsymbol{C}_{\mathrm{e}})f_i(\boldsymbol{C}_i)\Big]\mathbf{d}\boldsymbol{\omega}\mathbf{d}\boldsymbol{C}_i$$

Theorem 2 (Degond, Lucquin 1996, Graille, M., Massot 2009)
$\mathcal{J}_{i\mathrm{e}}$, $i \in \mathrm{H}$, can be expanded in the form:

$$\boxed{\begin{gathered}\mathcal{J}_{\mathrm{e}i}(f_{\mathrm{e}}, f_i)(\boldsymbol{C}_{\mathrm{e}}) = \mathcal{J}^0_{\mathrm{e}i}(f_{\mathrm{e}}, f_i)(\boldsymbol{C}_{\mathrm{e}}) + \varepsilon\mathcal{J}^1_{\mathrm{e}i}(f_{\mathrm{e}}, f_i)(\boldsymbol{C}_{\mathrm{e}}) + \varepsilon^2\mathcal{J}^2_{\mathrm{e}i}(f_{\mathrm{e}}, f_i)(\boldsymbol{C}_{\mathrm{e}}) \\ +\varepsilon^3\mathcal{J}^3_{\mathrm{e}i}(f_{\mathrm{e}}, f_i)(\boldsymbol{C}_{\mathrm{e}}) + \mathcal{O}(\varepsilon^4)\end{gathered}}$$

Multiscale Chapman-Enskog method: summary

[Graille, M., Massot 2009]

Enskog expansion $\begin{cases} f_{\mathrm{e}} = f_{\mathrm{e}}^0(1 + \varepsilon\phi_{\mathrm{e}} + \varepsilon^2\phi_{\mathrm{e}}^2) + \mathcal{O}(\varepsilon^3) \\ f_i = f_i^0(1 + \varepsilon\phi_i) + \mathcal{O}(\varepsilon^2), \qquad i \in \mathrm{H} \end{cases}$

Order	Time	Heavy particles	Electrons
ε^{-2}	t_{e}	–	Eq. for f_{e}^0 Thermalization (T_{e})
ε^{-1}	t_h^0	Eq. for f_i^0, $i \in \mathrm{H}$ Thermalization (T_h)	Eq. for ϕ_{e} Electron momentum relation
ε^0	t^0	Eq. for ϕ_i, $i \in \mathrm{H}$ Euler eqs.	Eq. for $\phi_{\mathrm{e}}^{(2)}$ Zero-order drift-diffusion eqs.
ε	t^0/ε	Navier-Stokes eqs.	1^{st}-order drift-diffusion eqs.

- Sound scaling derived from dimensional analysis
- Rigorous multicomponent diffusion (Kolesnikov effect)
- Laws of thermodynamics are satisfied

Multifluid scaling of Boltzmann eq.

- Kinetic equation for species $i \in S$

$$\partial_t f_i + \boldsymbol{c}_i \cdot \boldsymbol{\partial_x} f_i + \frac{\boldsymbol{F}_i}{m_i} \cdot \boldsymbol{\partial}_{\boldsymbol{c}_i} f_i = \sum_{j \neq i} \mathcal{J}_{ij}(f_i, f_j) + \frac{1}{\varepsilon} \mathcal{J}_{ii}(f_i, f_i) + C_i^r$$

  - Fluid equations are decoupled for each species
  - Example: isothermal ion - electron mixture in neutral bath

$$\begin{aligned}
\partial_t n_e + \partial_x (n_e u_e) &= n_e \nu^{iz} \\
\partial_t n_i + \partial_x (n_i u_i) &= n_e \nu^{iz} \\
\partial_t (n_e u_e) + \partial_x \left(n_e u_e^2 + \frac{p_e}{m_e} \right) &= \frac{n_e e}{m_e} \partial_x \phi - n_e u_e \nu_{en} \\
\partial_t (n_i u_i) + \partial_x \left(n_i u_i^2 + \frac{p_i}{m_i} \right) &= -\frac{n_i e}{m_i} \partial_x \phi - n_i u_i \nu_{in}
\end{aligned}$$

- Coupling to Poisson's eq.

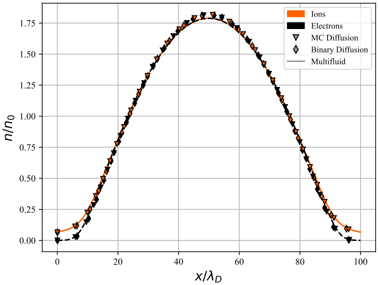
$$\partial_{xx}^2 \phi = \frac{e (n_e - n_i)}{\varepsilon_0}$$

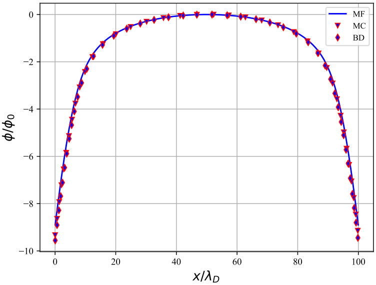
Comparison multifluid / multicomponent diffusion models

- Binary diffusion model

$$\begin{aligned}\partial_t n_e + \partial_x (n_e V_e) &= n_e \nu^{iz} \\ \partial_t n_i + \partial_x (n_i V_i) &= n_e \nu^{iz}\end{aligned}$$

  - Diffusion velocity: $V_k = -\frac{D_k}{n_k}\partial_x n_k - \mu_k \partial_x \phi$
  - Binary diffusion coefficient: $D_k = \frac{k_B T_k}{m_k \nu_{kn}}$
  - Species mobility: $\mu_k = \frac{q_k}{m_k \nu_{kn}}$

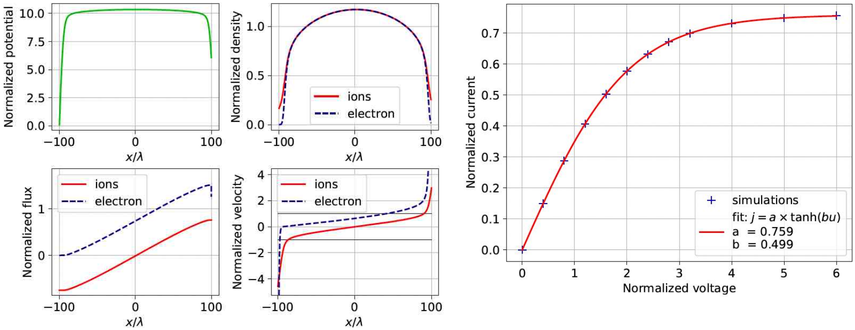




Simulation of 1D plasma sheath at 1000 Pa between 2 walls

[Gangemi, Alvarez Laguna, Hillewaert, M., 9th EUCASS 2022]

Multifluid simulation of electrostatic probe measurement in collisionless plasma



Simulation of 1D plasma sheath with difference of potential
[Berger, VKI RM report 2022]

Outline

Simulation of plasma sheath

Reactive collision operator

Calibration of models

Reactive collision operator

- Chemical reactions

$$\sum_{i\in\mathcal{F}^r}\mathfrak{X}_i \rightleftharpoons \sum_{k\in\mathcal{B}^r}\mathfrak{X}_k, \qquad r\in R$$

- Reactive collision operator $C_i = \sum_{r\in R} C_i^r(f_i)$
- Partial collision operator [Giovangigli 1998]

$$\begin{aligned}
C_i^r \;=\;& \nu_{ir}^{\mathrm{f}}\int\Big(\prod_{k\in\mathcal{B}^r} f_k\,\frac{\prod_{k\in\mathcal{B}^r}\beta_k}{\prod_{j\in\mathcal{F}^r}\beta_j}-\prod_{j\in\mathcal{F}^r} f_j\Big)\mathcal{W}_{\mathcal{F}^r}^{\mathcal{B}^r}\prod_{j\in\mathcal{F}_i^r}\mathrm{d}\boldsymbol{c}_j\prod_{k\in\mathcal{B}^r}\mathrm{d}\boldsymbol{c}_k\\
&-\nu_{ir}^{\mathrm{b}}\int\Big(\prod_{k\in\mathcal{B}^r} f_k\,\frac{\prod_{k\in\mathcal{B}^r}\beta_k}{\prod_{j\in\mathcal{F}^r}\beta_j}-\prod_{j\in\mathcal{F}^r} f_j\Big)\mathcal{W}_{\mathcal{F}^r}^{\mathcal{B}^r}\prod_{j\in\mathcal{F}^r}\mathrm{d}\boldsymbol{c}_j\prod_{k\in\mathcal{B}_i^r}\mathrm{d}\boldsymbol{c}_k,\\
& i\in \mathrm{S},\;\; r\in R
\end{aligned}$$

with statistical weight $\beta_i = \mathrm{h}_{\mathrm{P}}^3/(a_i m_i^3)$ of species i in phase space

Example: $\mathrm{N_2 + N \rightleftharpoons N + N + N}$

$$\mathcal{C}_{\mathrm{N}} = \int \left(f_{\mathrm{N}}(\boldsymbol{\zeta}) f_{\mathrm{N}}(\boldsymbol{\eta}) f_{\mathrm{N}}(\boldsymbol{\nu}) \frac{\beta_{\mathrm{N}}^2}{\beta_{\mathrm{N}_2}} - f_{\mathrm{N}}(\boldsymbol{c}_{\mathrm{N}}) f_{\mathrm{N}_2}(\boldsymbol{\xi}) \right) \mathcal{W}_{\mathrm{N}_2,\mathrm{N}}^{3\mathrm{N}}(\boldsymbol{c}_{\mathrm{N}}, \boldsymbol{\xi}, \boldsymbol{\zeta}, \boldsymbol{\eta}, \boldsymbol{\nu}) \mathrm{d}\boldsymbol{\zeta} \, \mathrm{d}\boldsymbol{\eta} \, \mathrm{d}\boldsymbol{\nu} \, \mathrm{d}\boldsymbol{\xi}$$

$$-3 \int \left(f_{\mathrm{N}}(\boldsymbol{c}_{\mathrm{N}}) f_{\mathrm{N}}(\boldsymbol{\zeta}) f_{\mathrm{N}}(\boldsymbol{\eta}) \frac{\beta_{\mathrm{N}}^2}{\beta_{\mathrm{N}_2}} - f_{\mathrm{N}}(\boldsymbol{\nu}) f_{\mathrm{N}_2}(\boldsymbol{\xi}) \right) \mathcal{W}_{\mathrm{N}_2,\mathrm{N}}^{3\mathrm{N}}(\boldsymbol{c}_{\mathrm{N}}, \boldsymbol{\xi}, \boldsymbol{\zeta}, \boldsymbol{\eta}, \boldsymbol{\nu}) \mathrm{d}\boldsymbol{\nu} \, \mathrm{d}\boldsymbol{\zeta} \, \mathrm{d}\boldsymbol{\eta} \, \mathrm{d}\boldsymbol{\xi}$$

$$\mathcal{C}_{\mathrm{N}_2} = \int \left(f_{\mathrm{N}}(\boldsymbol{\zeta}) \, f_{\mathrm{N}}(\boldsymbol{\eta}) \, f_{\mathrm{N}}(\boldsymbol{\nu}) \, \frac{\beta_{\mathrm{N}}^2}{\beta_{\mathrm{N}_2}} - f_{\mathrm{N}_2}(\boldsymbol{c}_{\mathrm{N}_2}) \, f_{\mathrm{N}}(\boldsymbol{\xi}) \right) \mathcal{W}_{\mathrm{N}_2,\mathrm{N}}^{3\mathrm{N}}(\boldsymbol{c}_{\mathrm{N}_2}, \boldsymbol{\xi}, \boldsymbol{\zeta}, \boldsymbol{\eta}, \boldsymbol{\nu}) \mathrm{d}\boldsymbol{\zeta} \, \mathrm{d}\boldsymbol{\eta} \, \mathrm{d}\boldsymbol{\nu} \, \mathrm{d}\boldsymbol{\xi}$$

How to write the reactive collision operator by means of differential cross-sections?

3-body collision

B. V. Alexeev, A. Chikhaoui, and I. T. Grushin, *Application of the generalized Chapman-Enskog method to the transport-coefficient calculation in a reacting gas mixture*, **Phys. Rev. E 49(4), 2809–2825 (1994)**

- Consider the 3-body collision

$$\mathrm{X}_1 + \mathrm{X}_2 \rightleftharpoons \mathrm{X}_3 + \mathrm{X}_4 + \mathrm{X}_5$$

- To reuse the binary collision formalism, the 3-body collision is decomposed into 2 steps:
  1. Activation

$$\mathrm{X}_1 + \mathrm{X}_2 \rightleftharpoons \mathrm{X}_\star + \mathrm{X}_3$$

     - Activated complex: $\mathrm{X}_\star$ with $m_\star = m_1$
     - Third-body: $\mathrm{X}_2 = \mathrm{X}_3$ with $m_2 = m_3$
  2. Dissociation (ionization)

$$\mathrm{X}_\star \rightleftharpoons \mathrm{X}_4 + \mathrm{X}_5$$

  with $m_4 + m_5 = m_\star$

Relative motion w.r.t. center of mass

- Activation: $\mathrm{X}_1 + \mathrm{X}_2 \rightleftharpoons \mathrm{X}_\star + \mathrm{X}_3$

  Jacobi variables: $\begin{cases} \boldsymbol{c}_1 &= \boldsymbol{G}_0 + \frac{m_2}{M}\boldsymbol{g}_{12} \\ \boldsymbol{c}_2 &= \boldsymbol{G}_0 - \frac{m_1}{M}\boldsymbol{g}_{12} \end{cases}$ and $\begin{cases} \boldsymbol{c}_\star &= \boldsymbol{G}_0 + \frac{m_3}{M}\boldsymbol{g}_{\star 3} \\ \boldsymbol{c}_3 &= \boldsymbol{G}_0 - \frac{m_\star}{M}\boldsymbol{g}_{\star 3} \end{cases}$

  - Mass $M = m_1 + m_2$
  - Center of mass velocity $\boldsymbol{G}_0 = (m_1\boldsymbol{c}_1 + m_2\boldsymbol{c}_2)/M$
  - Relative velocity $\boldsymbol{g}_{12} = \boldsymbol{c}_1 - \boldsymbol{c}_2$
  - Relative velocity $\boldsymbol{g}_{\star 3} = \boldsymbol{c}_\star - \boldsymbol{c}_3$

- Dissociation: $\mathrm{X}_\star \rightleftharpoons \mathrm{X}_4 + \mathrm{X}_5$

  Jacobi variables: $\begin{cases} \boldsymbol{c}_4 &= \boldsymbol{c}_\star + \frac{m_5}{m_\star}\boldsymbol{g}_{45} = \boldsymbol{G}_0 + \frac{m_3}{M}\boldsymbol{g}_{\star 3} + \frac{m_5}{m_\star}\boldsymbol{g}_{45} \\ \boldsymbol{c}_5 &= \boldsymbol{c}_\star - \frac{m_4}{m_\star}\boldsymbol{g}_{45} = \boldsymbol{G}_0 + \frac{m_3}{M}\boldsymbol{g}_{\star 3} - \frac{m_4}{m_\star}\boldsymbol{g}_{45} \end{cases}$

  - Mass $m_\star = m_4 + m_5$
  - Center of mass velocity $\boldsymbol{c}_\star = (m_4\boldsymbol{c}_4 + m_5\boldsymbol{c}_5)/m_\star$
  - Relative velocity $\boldsymbol{g}_{45} = \boldsymbol{c}_4 - \boldsymbol{c}_5$
  - Relative velocity $\boldsymbol{g}_{\star 3} = \frac{m_4}{m_\star}\boldsymbol{c}_4 + \frac{m_5}{m_\star}\boldsymbol{c}_5 - \boldsymbol{c}_3$

Energy conservation

- Activation:

$$\tfrac{1}{2}m_1|\mathbf{c}_1|^2+E_1+\tfrac{1}{2}m_2|\mathbf{c}_2|^2+E_2=\tfrac{1}{2}m_\star|\mathbf{c}_\star|^2+E_\star+\tfrac{1}{2}m_3|\mathbf{c}_3|^2+E_3$$

- Dissociation:

$$\tfrac{1}{2}m_\star|\mathbf{c}'_\star|^2+E_\star=\tfrac{1}{2}m_4|\mathbf{c}_4|^2+E_4+\tfrac{1}{2}m_5|\mathbf{c}_5|^2+E_5$$

- 3-body collision:

$$\tfrac{1}{2}m_1|\mathbf{c}_1|^2+\tfrac{1}{2}m_2|\mathbf{c}_2|^2=\tfrac{1}{2}m_3|\mathbf{c}_3|^2+\tfrac{1}{2}m_4|\mathbf{c}_4|^2+\tfrac{1}{2}m_5|\mathbf{c}_5|^2+\Delta E$$

with $\Delta E = E_3 + E_4 + E_5 - E_1 - E_2$

$\Rightarrow$ After some algebra

$$\mu_{12}g_{12}^2=\mu_{\star 3}g_{\star 3}^2+\mu_{45}g_{45}^2+2\Delta E$$

- $\mu_{12}=\frac{m_1 m_2}{M}$
- $\mu_{\star 3}=\frac{m_\star m_3}{M}$
- $\mu_{45}=\frac{m_4 m_5}{m_\star}$

Differential cross-section for 3-body collision

- Change of variables

$$\mathcal{W}_{12}^{345} \mathrm{d}\boldsymbol{c}_3 \mathrm{d}\boldsymbol{c}_4 \mathrm{d}\boldsymbol{c}_5 \ \mathrm{d}\boldsymbol{c}_1 \mathrm{d}\boldsymbol{c}_2 = g_{12} \ \mathrm{d}\sigma_{12}^{345} \ \mathrm{d}\boldsymbol{c}_1 \mathrm{d}\boldsymbol{c}_2$$

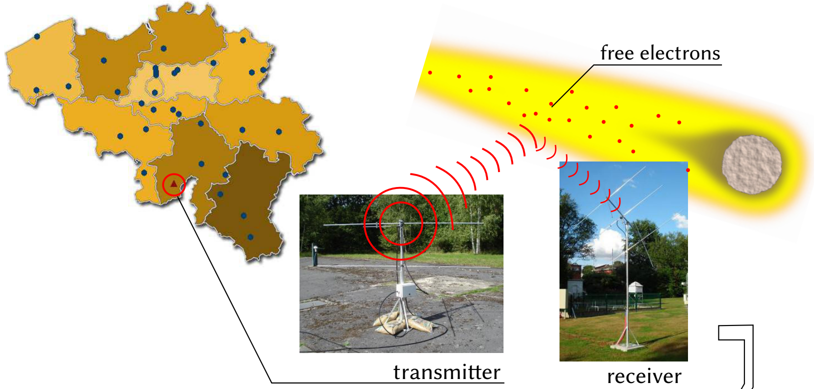
with differential cross-section expressed alternatively as

$$\mathrm{d}\sigma_{12}^{345} = \frac{\sigma_{12}^{345} \ g_{\star 3}^2 \mathrm{d}g_{\star 3} \ \mathrm{d}\boldsymbol{m}\mathrm{d}\boldsymbol{n}}{\frac{16}{3}\pi^2 \left(\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}}\right)^{3/2}}$$

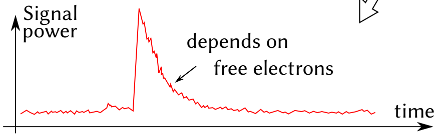
- Parametrization: $\sigma_{12}^{345} = \sigma_{12}^{345}(g_{12}, g_{\star 3}, \boldsymbol{m}, \boldsymbol{n})$
  - Relative velocity before collision: $g_{12} = |\boldsymbol{g}_{12}|$
  - Relative velocity after collision: $g_{\star 3} = |\boldsymbol{g}_{\star 3}|$
  - Solid angle of relative velocity $\boldsymbol{g}_{\star 3}$: $\boldsymbol{m} = \boldsymbol{g}_{\star 3}/|\boldsymbol{g}_{\star 3}|$
  - Solid angle of relative velocity $\boldsymbol{g}_{45}$: $\boldsymbol{n} = \boldsymbol{g}_{45}/|\boldsymbol{g}_{45}|$
- Domain
  - $\boldsymbol{m}, \ \boldsymbol{n} \in \mathbb{S}^2$
  - $g_{12} \in]0, \infty[$
  - $g_{\star 3} \in \left]0, \sqrt{\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}}}\right[$

  since $g_{45}^2 = \mu_{45}^{-1/2} \left(\mu_{12} g_{12}^2 - 2\Delta E - \mu_{\star 3} g_{\star 3}^2\right)^{1/2}$

Belgian RAdio Meteor Stations (BRAMS) network

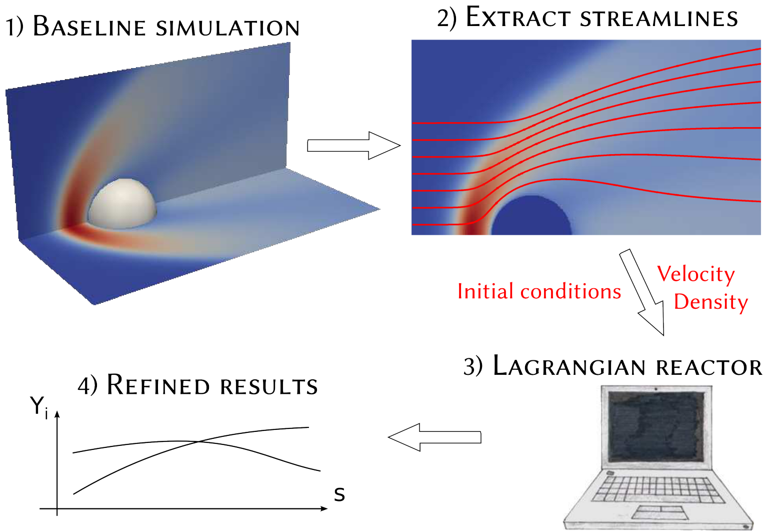


GOAL:
correlate radio signal
to meteoroid size



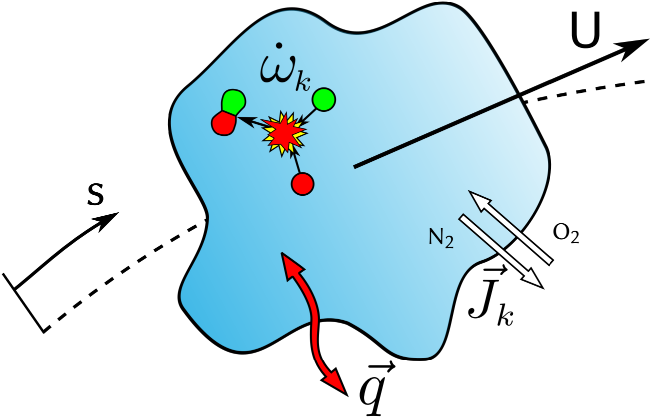
[Lamy *et al.*, *Meteoroids Conference Proceedings*, **NASA/CP-2011-216469** (2011) 351]

Thermo-chemical reactor following the streamlines

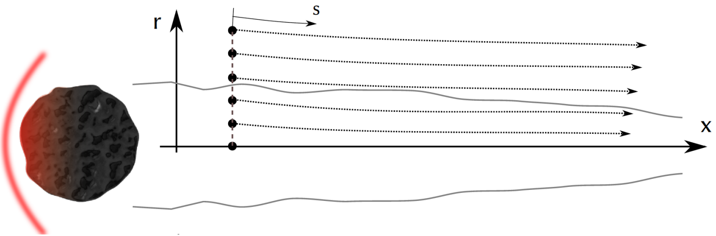


[Boccelli, Bariselli, Dias, Magin, *Plasma Sources Science and Technology* 28 (2019) 065002]

Lagrangian reactor: models for mass and energy conservation



Lagrangian reactor with diffusion (Maxwell's transfer eqs.)



- Baseline simulation provides: velocity $\boldsymbol{v}^*$, density ρ^*, and enthalpy variation ΔH^*
- Lagrangian formulation: steady problem, ambipolar diffusion

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}(y_i) &= \frac{\omega_i - \boldsymbol{\partial}_{\boldsymbol{x}} \cdot (\rho_i \boldsymbol{V}_i)}{\rho^* |\boldsymbol{v}^*|}, \qquad i \in \mathrm{S} \\ \frac{\mathrm{d}}{\mathrm{d}s}(H) &= \frac{\Delta H^*}{\Delta s}\end{aligned}$$

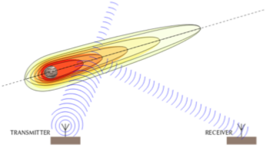
Conditions for the baseline SPARTA DSMC simulation

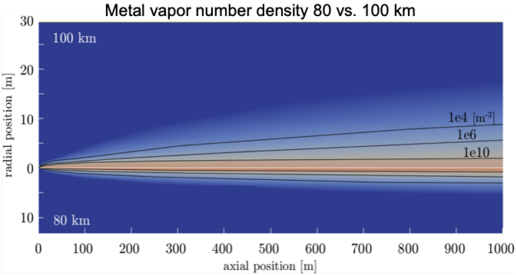
- Velocity: 32 km/s
- Altitude: 80 and 100 km
- Size: 1 mm diameter
- Surface temperature: 2000 K
- Ablated vapor mixture used in DSMC: Si, Si^+, SiO, SiO_2, Mg, Mg^+, MgO Fe, Fe^+, FeO Na, Na^+, NaO

Oxide	Mass %	Oxide	Mass %
SiO_2	34.0	CaO	1.89
MgO	24.2	Na_2O	1.1
FeO	36.3	K_2O	0.1
Al_2O_3	2.5	TiO_2	0.01

Evolution of the electrons in the trail (Lagrangian solver)

Faster diffusion at 100 km



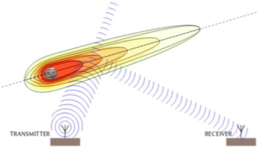


$$\omega_p = \sqrt{\frac{n_e e^2}{\epsilon_0 m_e}} > 49 \text{ MHz}$$

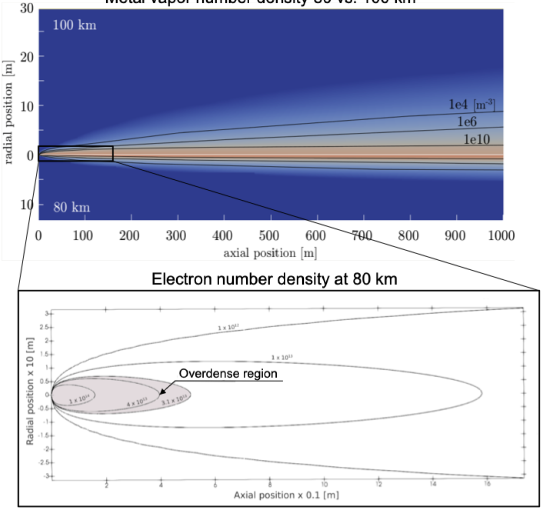
At 80 km the ***overdense region*** reaches 50 m in length

Evolution of the electrons in the trail (Lagrangian solver)

Faster diffusion at 100 km



Metal vapor number density 80 vs. 100 km



$$\omega_p = \sqrt{\frac{n_e e^2}{\epsilon_0 m_e}} > 49 \text{ MHz}$$

At 80 km the ***overdense region*** reaches 50 m in length

Outline

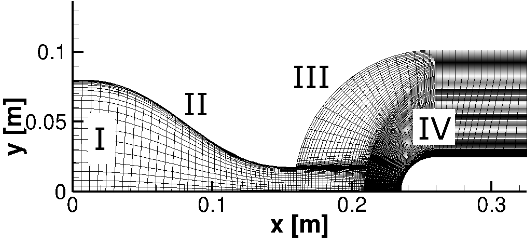
Simulation of plasma sheath

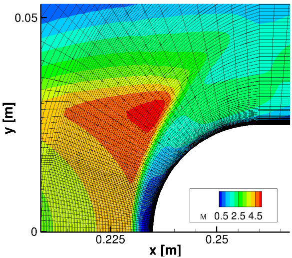
Reactive collision operator

Calibration of models

US3D CFD solver for hypersonic flows (U Minnessota)

- 3D Finite-Volume discretization
- Modified Steger-Warming numerical scheme with MUSCL reconstruction
- Data Parallel Line Relaxation (DPLR) to obtain rapid convergence to steady-state

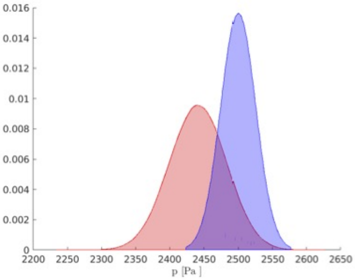


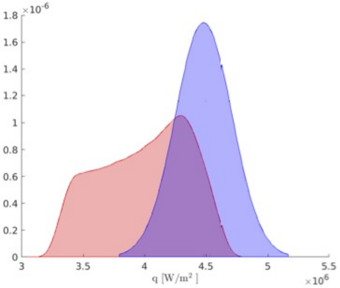


Left: computational domain I) exit of plasma torch, II) sonic nozzle surface, III) expansion chamber and IV) probe. **Right**: zoom on numerical grid adapted with the shock to avoid carbuncle
[Capriati, Turchi, Congedo, M., 9th EUCASS 2022]

Multifidelity surrogate model based on hierarchical Kriging

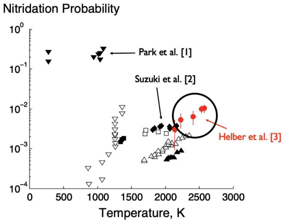
Tag	cells	Δx [m]	h_i	t_{CPU} [min]
I	172224	5E-7	1	$\approx$ 1600
II	43056	1E-6	2	$\approx$ 200
III	10764	2E-6	4	$\approx$ 30
IV	2691	4E-6	8	$\approx$ 4



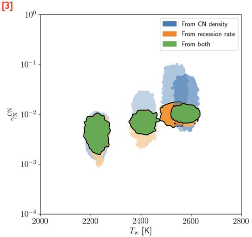


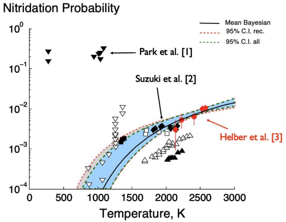
Probabilistic density functions for stagnation pressure and heat flux
[Capriati, Turchi, Congedo, M., 9th EUCASS 2022]

Stochastic calibration of carbon nitridation model from plasma wind tunnel experiments



Bayesian inference methodology





Integration of all available measurements from Helber *et al.*

$$\gamma_N^{CN} = A\exp\left(\frac{-T_a}{T_w}\right)$$

[del Val, Lemaitre, Congedo, M., under review 2022]

Conclusion

- Hypersonics is a multiscale and multiphysics problem
- Kinetic theory is a powerful tool to derive sound fluid models for plasmas
- Well identified mathematical structure of the conservation eqs. allows for development of numerical schemes
- Don't forget to calibrate and validate your computational models!

Total cross-section for isotropic 3-body collision

- Assume isotropic deflection angles for arising particles

$$
\begin{aligned}
\int \mathrm{d}\sigma_{12}^{345} &= \int_0^{\sqrt{\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}}}} \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \frac{\sigma_{12}^{345} \; g_{\star 3}^2 \mathrm{d}g_{\star 3} \; \mathrm{d}\boldsymbol{m} \mathrm{d}\boldsymbol{n}}{\frac{16}{3}\pi^2 \left(\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}} \right)^{3/2}} \\
&= \frac{\sigma_{12}^{345}}{\frac{16}{3}\pi^2} \int_{\mathbb{S}^2} \mathrm{d}\boldsymbol{m} \int_{\mathbb{S}^2} \mathrm{d}\boldsymbol{n} \int_0^{\sqrt{\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}}}} \frac{g_{\star 3}^2 \mathrm{d}g_{\star 3}}{\left(\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}} \right)^{3/2}} \\
&= \frac{\sigma_{12}^{345}}{\frac{16}{3}\pi^2} 4\pi 4\pi \frac{1}{\left(\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}} \right)^{3/2}} \left[\frac{1}{3} g_{\star 3}^3 \right]_0^{\sqrt{\frac{\mu_{12} g_{12}^2 - 2\Delta E}{\mu_{\star 3}}}} \\
&= \sigma_{12}^{345}
\end{aligned}
$$

- The total cross-section is σ_{12}^{345}