



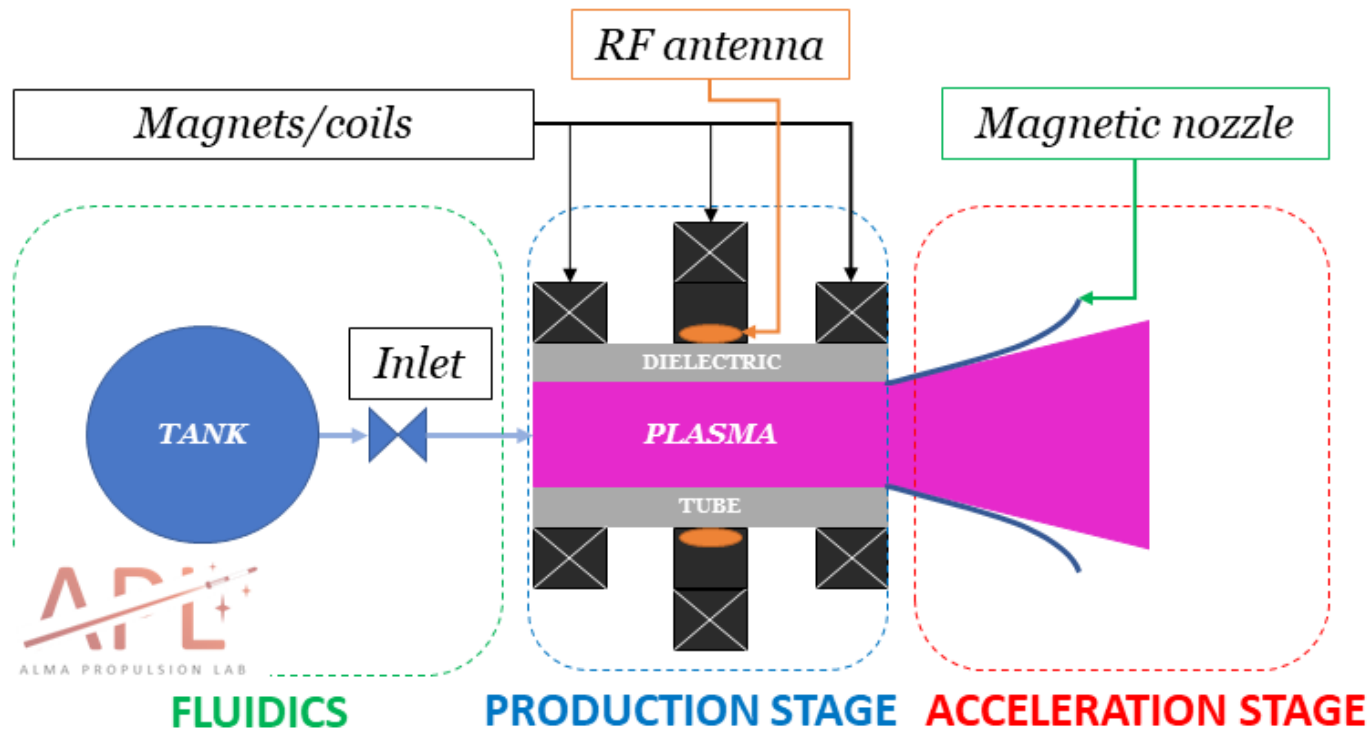
ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA



NUMERICAL SUITE FOR THE SIMULATION, DESIGN AND OPTIMIZATION OF CATHODE-LESS PLASMA THRUSTERS

Nabil Souhair, Raoul Andriulli, Mirko Magarotto, Fabrizio Ponti

Cathode-less Plasma Thrusters Layout



Simple design that does not involve electrodes or a neutralizer.



- Low cost
- Versatile: it can be operated with multi propellants
- Suitability for the CubeSat market (e.g., REGULUS-i2 50W)

Magnetically Enhanced Plasma Thruster



Numerical suite for cathode-less plasma thrusters



PREDICTION OF HPT PERFORMANCE

PLASMA CHEMISTRY

Effects of chemistry set on plasma parameters in the production stage

- Detailed Collisional Radiative Models (CRM)
- Analysis of EP traditional propellants such as Xe, Kr, Ar
- Analysis of alternative propellants such as Iodine and Air
- Acceleration stage through analytical model or Particle-In-Cell

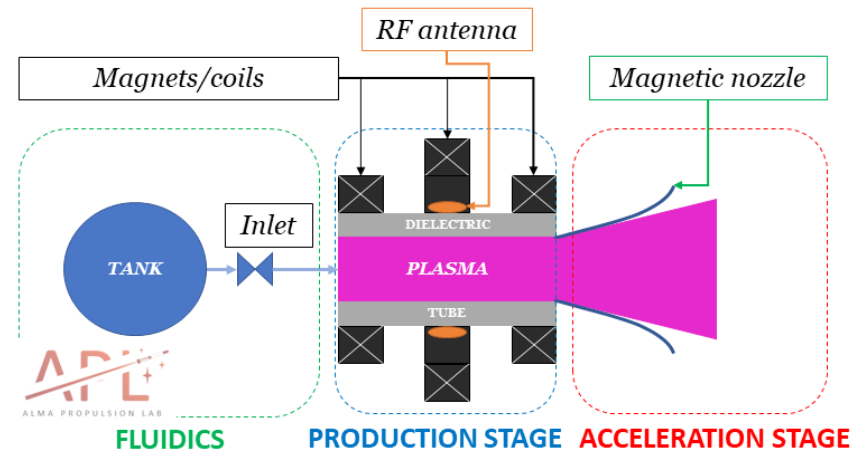
0D GLOBAL MODELS

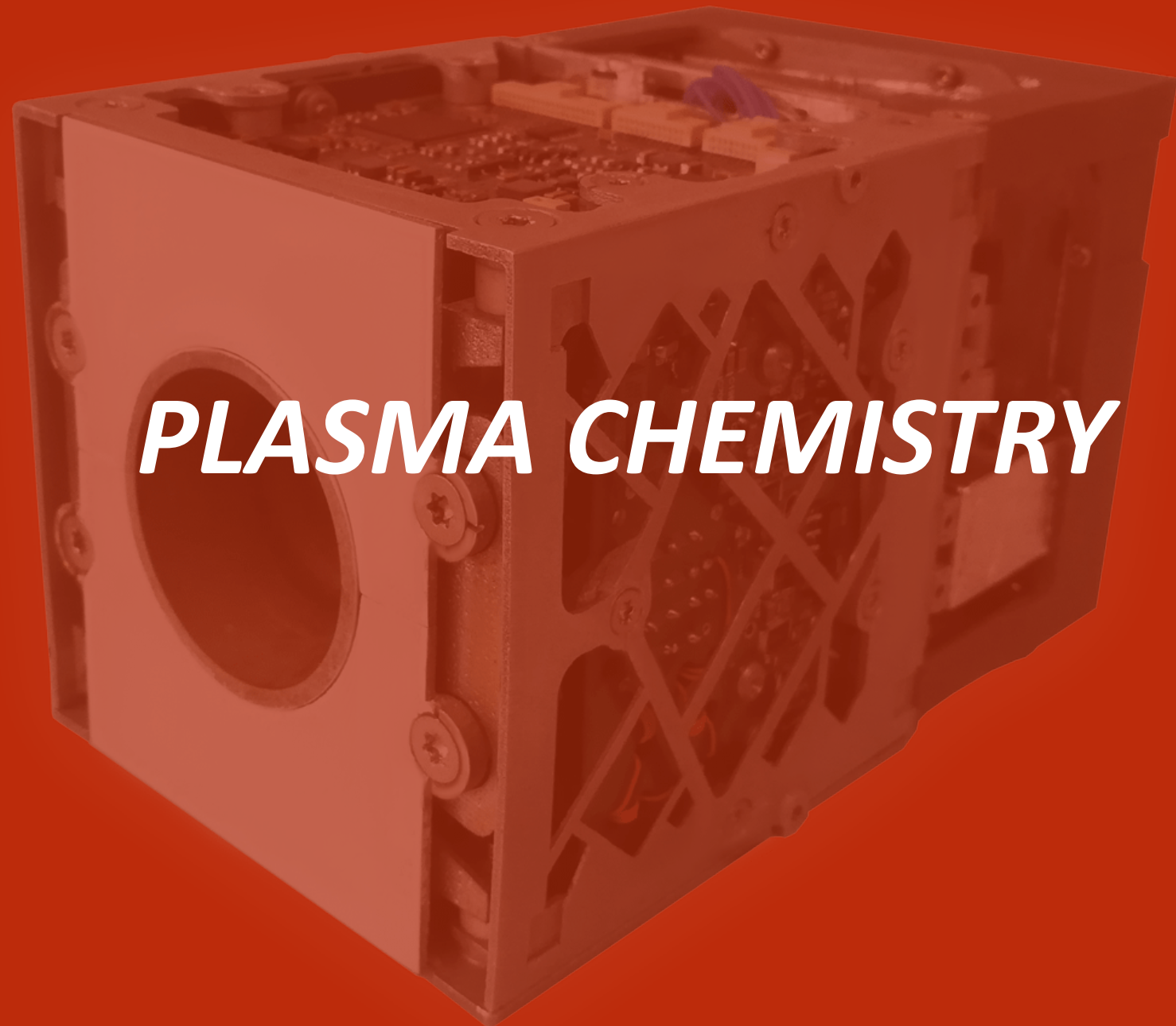
PLASMA GENERATION + TRANSPORT

Accurate prediction of plasma profiles

- Deposited plasma power by means of a EM module
- Plasma profiles through the Fluid Approach
- Acceleration stage through Fluid or Particle-In-Cell

3D PLASMA SIMULATION STRATEGY



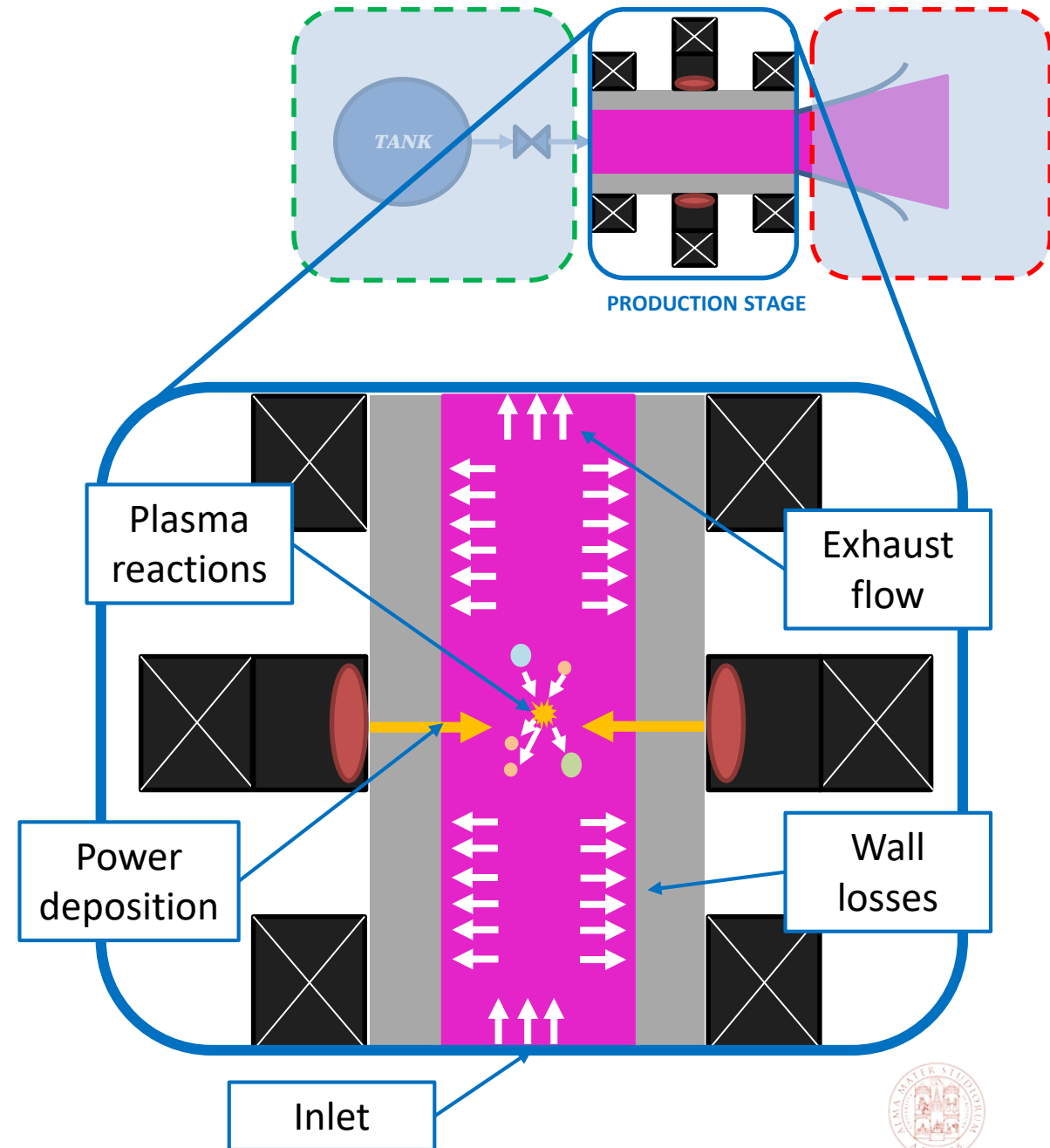


PLASMA CHEMISTRY



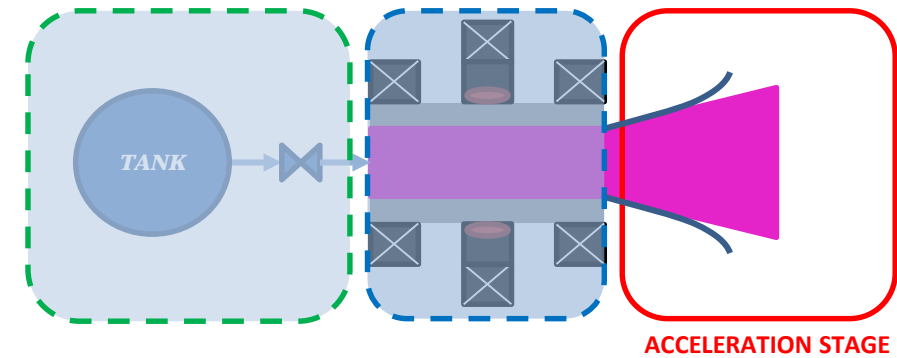
PLASMA CHEMISTRY: Global Models

- Balance of species population
- Balance of electron energy
- Source/sink term due to reactions
- Electron impact collisions with Maxwellian EEDF
- Wall losses and outlet according to Bohm sheath theory
- Acceleration stage handled by means of an analytic or Particle-In-Cell simulations



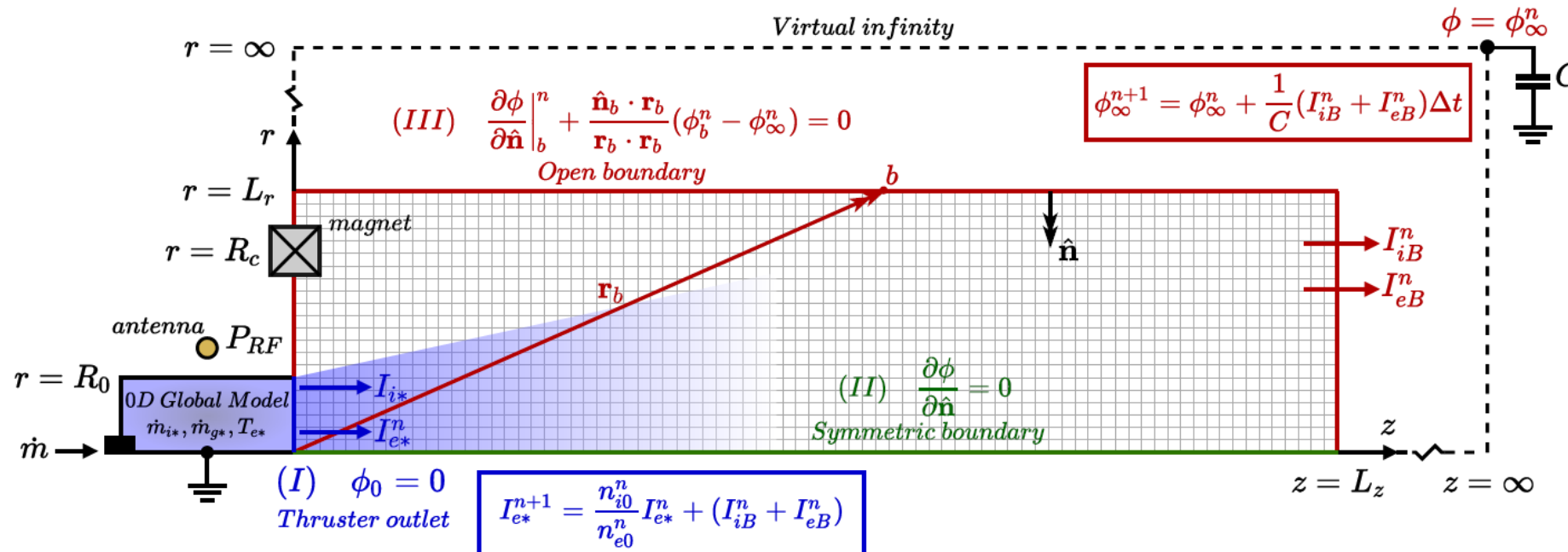
ACCELERATION STAGE: PiC

- Particle In Cell 2D3V
- Ions and electrons modelled as macroparticles
- Dynamics solved by means of Boris algorithm
- Plasma potential and electric field solved through a Poisson solver via an explicit SOR scheme
- Collisions through Monte Carlo Collision (MCC)
- Anomalous diffusion is accounted according to Boeuf

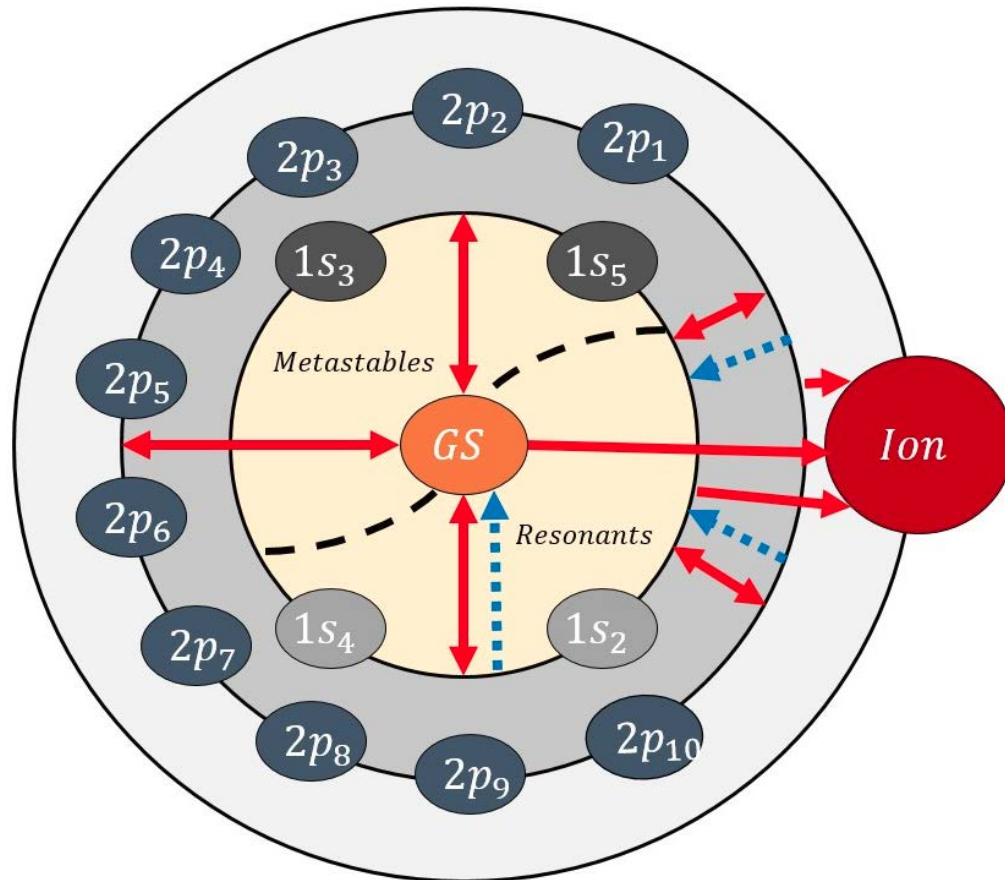


Total thrust is calculated through:

$$F = F_0 + \int_0^{L_r} \int_0^{L_z} -j_{e\theta} B_r \cdot 2\pi r \, dr dz$$



NOBLE GASES: Collisional-Radiative model [Souhair, Physics of Plasma, 2021]



- Argon, neon, krypton and xenon gas
- Excited levels $1S$, $2P$ (*Paschen* notation) since in low pressure regime
- Collisional and radiative transitions considered:
 - Electron impact excitation
 - Electron impact species exchange
 - Electron impact scattering
 - Electron impact ionization
 - Radiative decay toward lower states
- Novel lumping methodology for the energy levels developed



CRM LUMPING METHODOLOGY [Souhair, Physics of Plasma, 2021]

Assumptions:

- Effective species lumped in **1S** and **2P** groups
- **Maxwellian** electron energy distribution function
- Local Thermodynamic Equilibrium (**LTE**) between excited species according to McWirther formula:

$$n_e > 10^{19} T_e^{0.5} (\Delta U)^3$$

- ❖ Lumped rate coefficients for electron collision transitions:

$$K_{IJ} = \sum_i^{N_i} \left[\frac{\sum_j^{N_j} K_{ij}}{\sum_k^{N_i} \frac{g_k}{g_i} \exp\left(-\frac{U_k - U_i}{k_B T_0}\right)} \right]$$

- ❖ Rate coefficients for inverse transitions computed according to the *Principle of Detailed Balancing*
- ❖ Energy levels averaged over their degenerancies

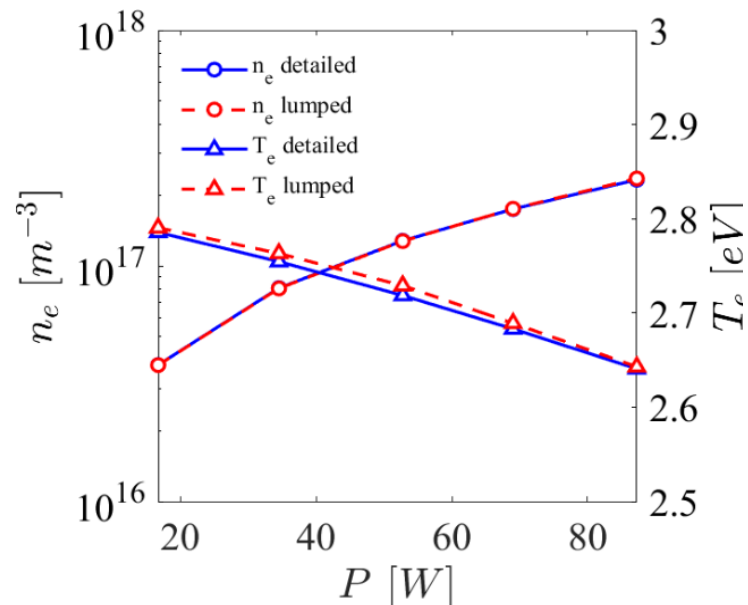
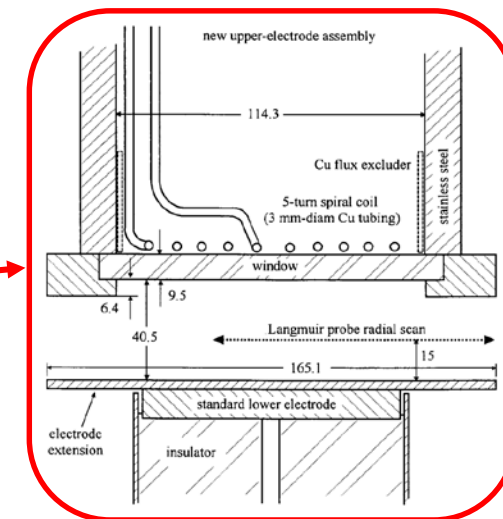
$$U_I = \frac{\sum_i^{N_i} g_i U_i}{\sum_i^{N_i} g_i}$$

- ❖ Lumped degenerancies given by

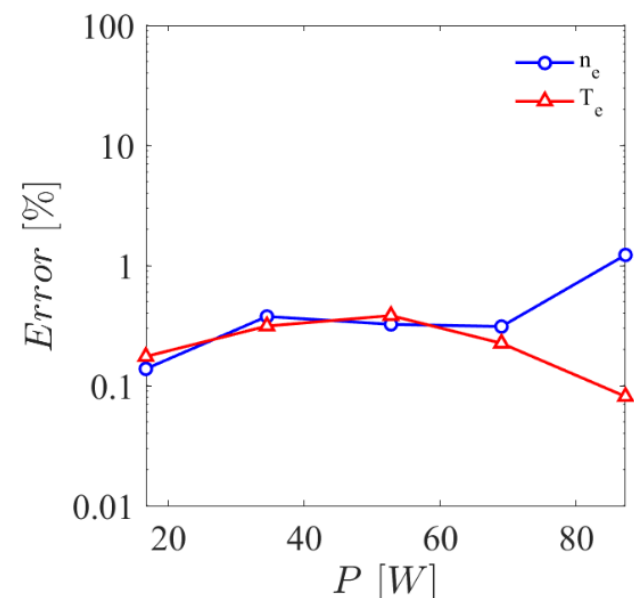
$$g_I = \sum_i^{N_i} g_i$$

Validation:

- GEC ICP reactor test case considered [Schwabedissen 1996]
- Lumped vs detailed reaction
- Global model (0D) was developed



a) Electron density (n_e) and electron temperature (T_e) in function of the deposited power (P), data are obtained with the lumping strategy or the detailed simulation of the excited states



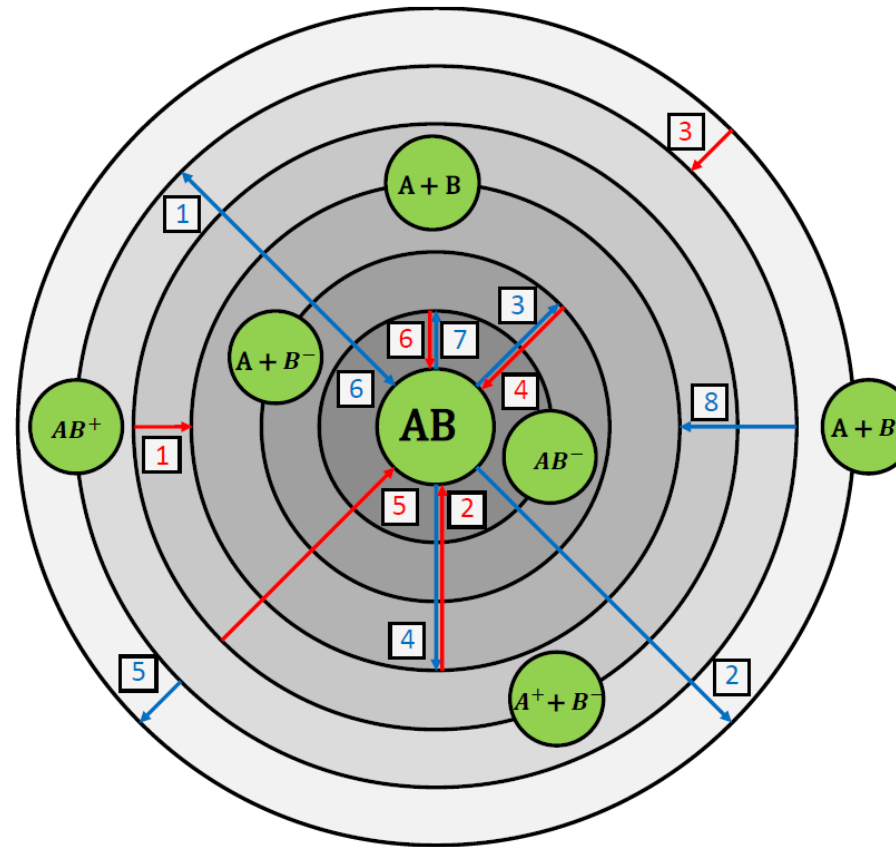
b) Percent error between n_e and T_e calculated with the detailed and the lumping methodologies.



ALTERNATIVE PROPELLANTS: Iodine & Air

- Species considered: $N_2, N, O_2, O, NO, N_2O, NO_2, I_2, I, I_2^+, I^+, I^-, e$
- Reactions:

#	Reaction	Name
1	$e + A \rightarrow A + e$	Atomic Elastic Scattering
2	$e + A \rightarrow A^* + e$	Atomic Excitation
3	$e + A \rightarrow A^+ + e + e$	Atomic Ionization
4	$e + A^- \rightarrow A + e + e$	Atomic Detachment
5	$e + A^+ \rightarrow A$	Atomic Neutralization
6	$e + A \rightarrow A^-$	Atomic Attachment
7	$e + AB \rightarrow AB + e$	Molecular Elastic Scattering
8	$e + AB \rightarrow AB^* + e$	Molecular Excitation
9	$e + AB \rightarrow AB^+ + e + e$	Molecular Ionization
10	$e + AB \rightarrow A + B^+ + e + e$	Molecular Dissociative Ionization
11	$e + AB \rightarrow A + B^-$	Molecular Dissociative Attachment
12	$e + AB \rightarrow A + B + e$	Molecular Dissociation
13	$e + AB^+ \rightarrow A + B^+ + e$	Molecular Ion Dissociation
14	$e + AB^+ \rightarrow AB$	Molecular Neutralization
15	$e + AB \rightarrow AB^-$	Molecular Attachment
16	$e + AB^+ \rightarrow A + B$	Molecular Dissociative Neutralization
17	$e + AB^- \rightarrow AB + e + e$	Molecular Detachment
18	$A^+ + B \rightarrow A + B^+$	Charge Exchange
19	$A^+ + B^- \rightarrow A + B$	Mutual Neutralization
20	$A + B \rightarrow AB$	Recombination
21	$A + B^+ \rightarrow AB^+$	Ion recombination
22	$A + B^- \rightarrow AB + e$	Associative Detachment
23	$A^+ + B^- \rightarrow AB$	Associative Neutralization



→ Heavy particle collision
→ Electronic collision

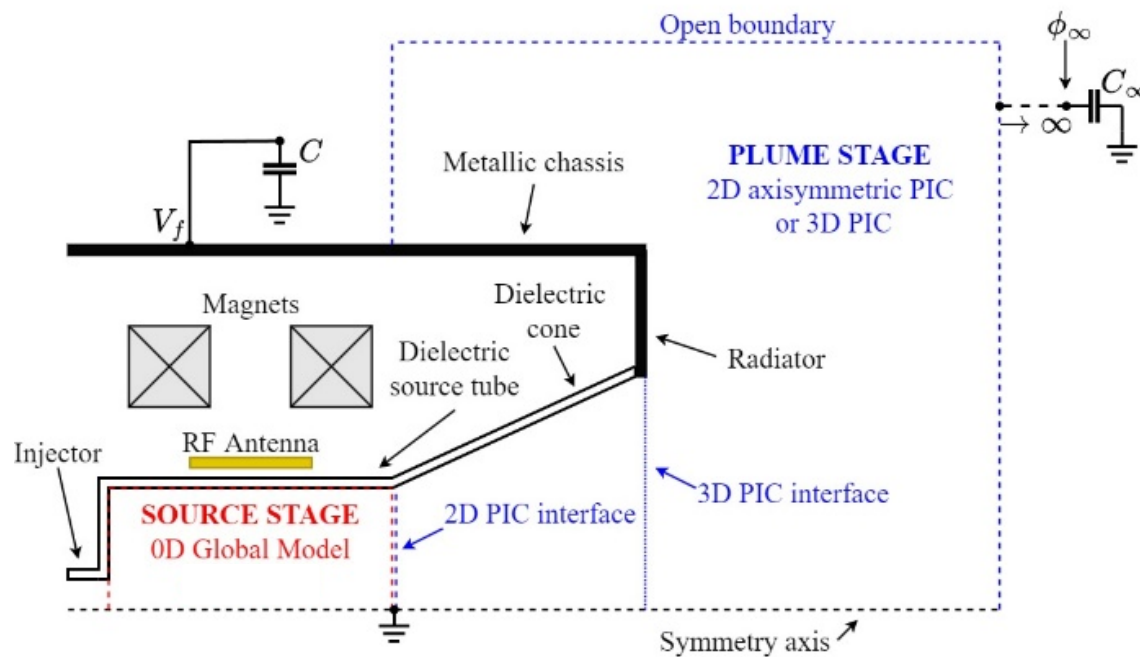
A&B Generic species (N, O, N_2, O_2, NO, I)

- 1) Molecular ionization
 - 2) Molecular dissociative ionization
 - 3) Molecular dissociative attachment
 - 4) Molecular dissociation
 - 5) Molecular ion dissociation
 - 6) Molecular neutralization
 - 7) Molecular attachment
 - 8) Molecular ion dissociative attachment
- 1) Mutual neutralization
 - 2) Recombination
 - 3) Ionic recombination
 - 4) Associative detachment
 - 5) Associative neutralization
 - 6) Detachment



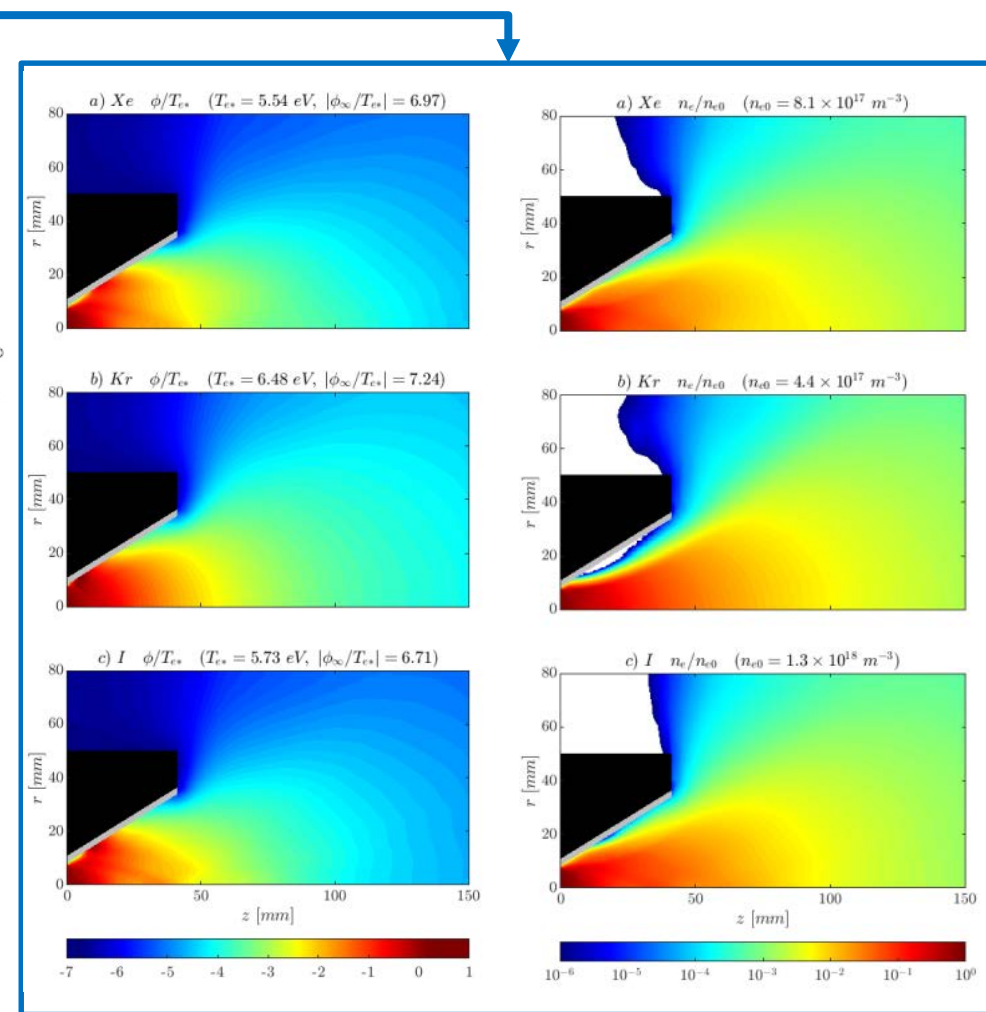
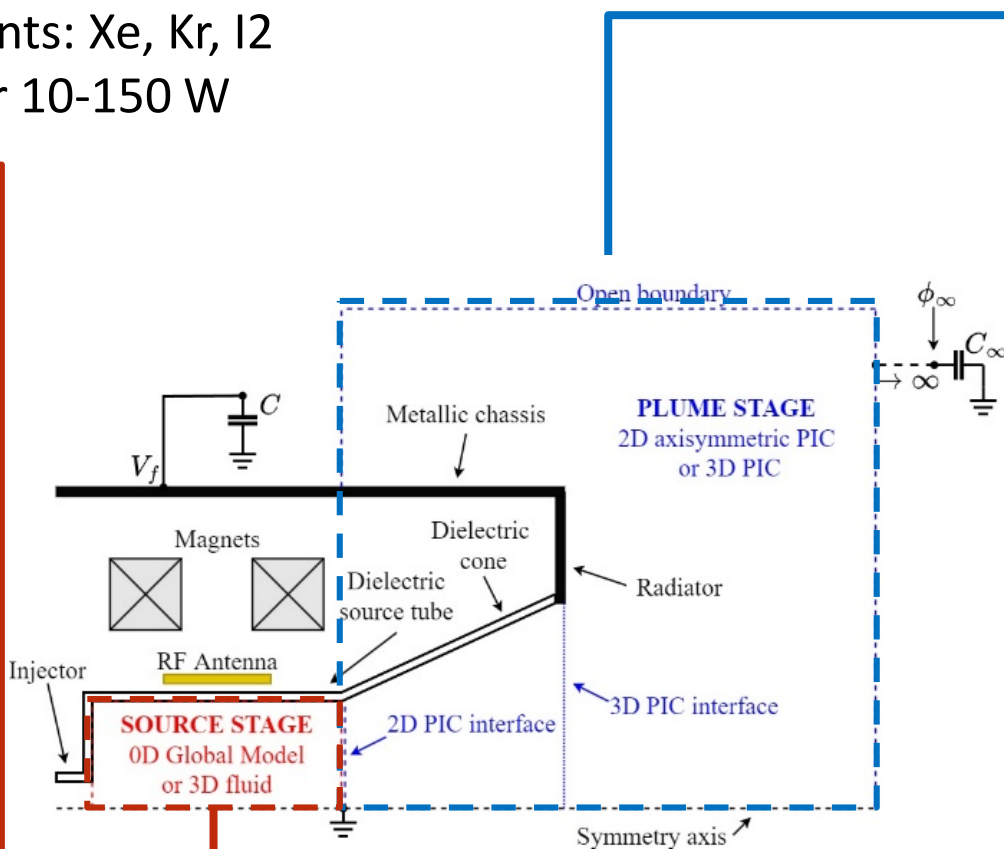
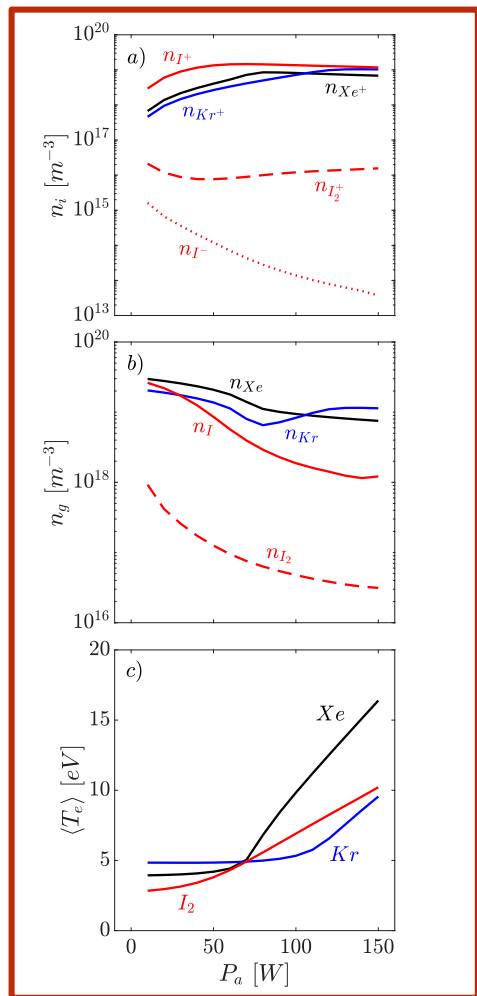
REGULUS Simulation Setup

- GM + PIC: particles injected from the thruster outlet
- Self-consistent open boundary conditions
- Simulations performed on CINECA supercomputer [ISCRA grant]



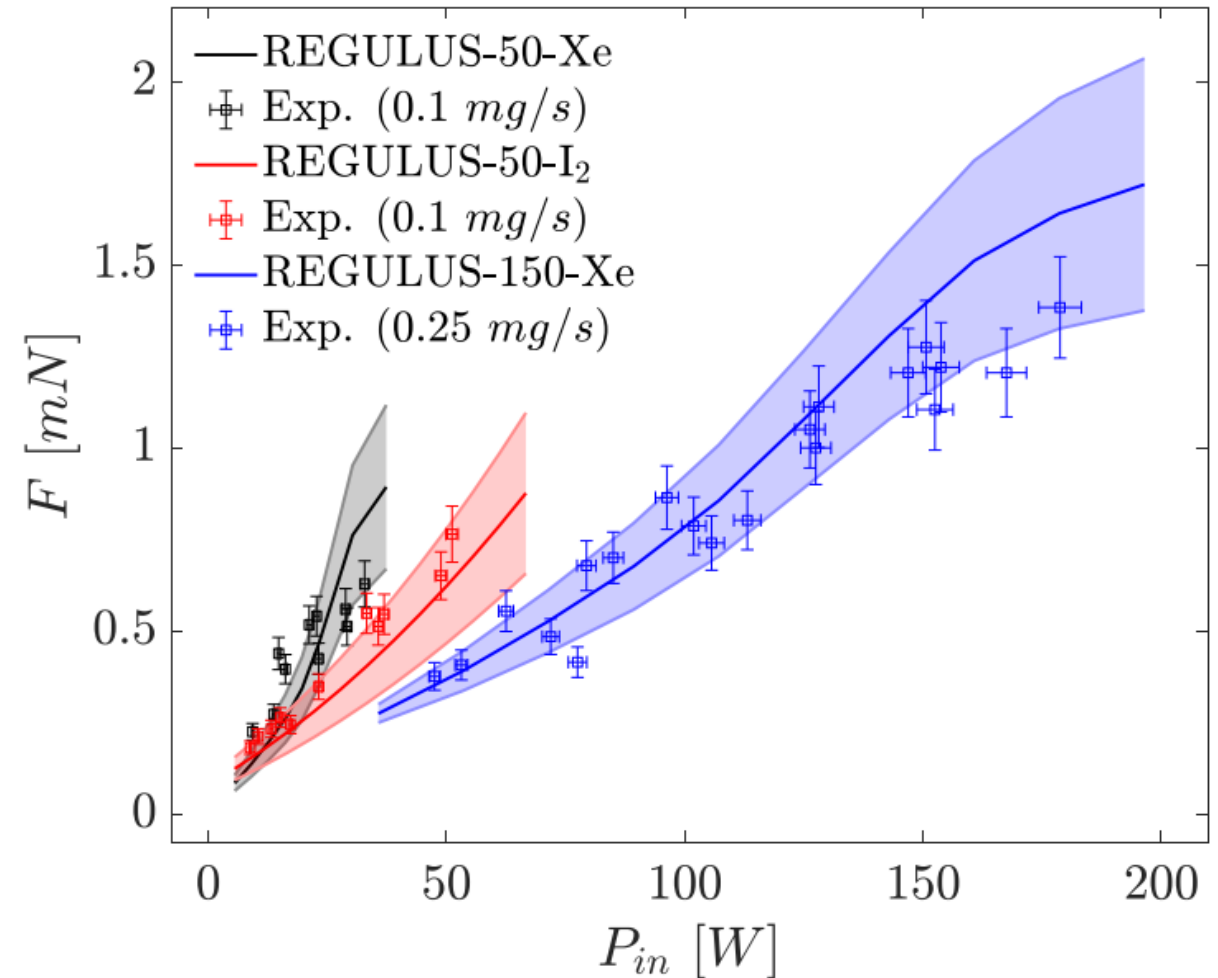
REGULUS Simulation Setup

- Several propellants: Xe, Kr, I₂
- Absorbed power 10-150 W



REGULUS Results

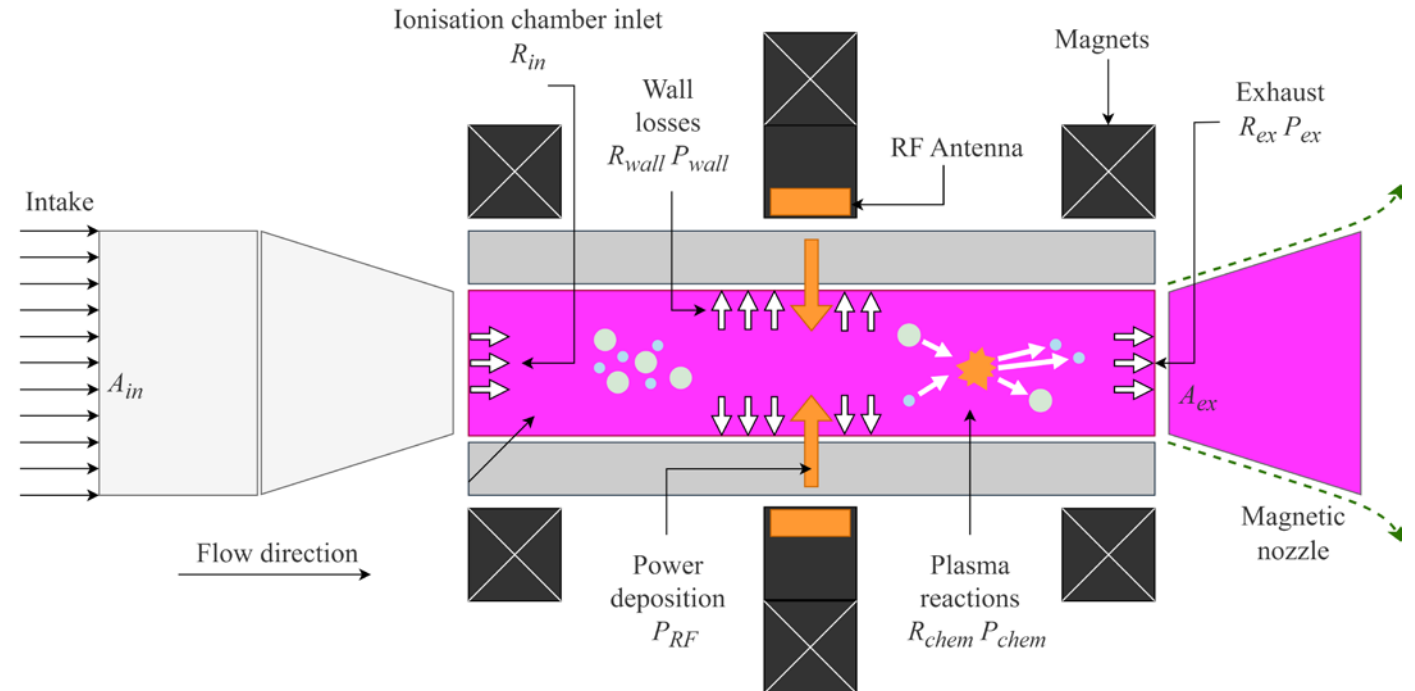
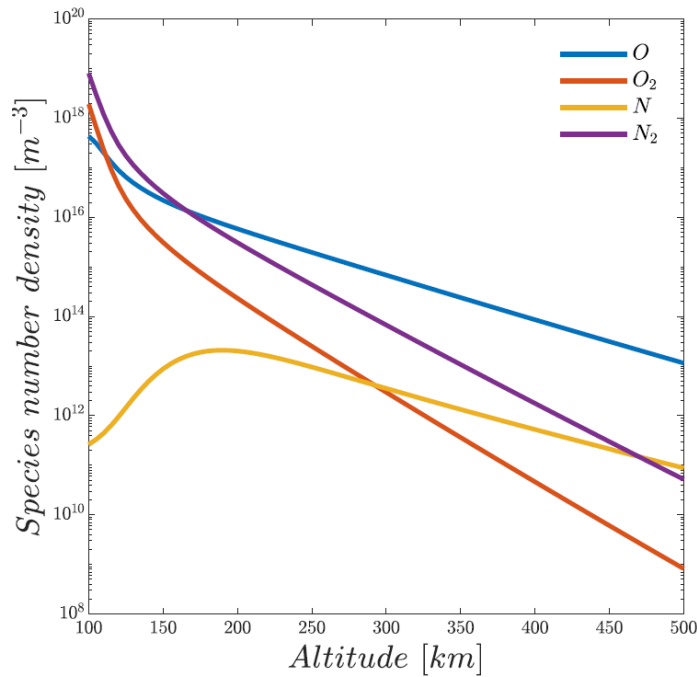
- Excellent agreement for REGULUS-150-Xe between 50-150 W
 - 33 % overestimation at higher power
- Good agreement for REGULUS-50-Xe
- 20 % underestimation for REGULUS-50-I₂



ATMOSPHERE-BREATHING EP with HPT

[Souhair & Dalle Fabbriche, Aerospace, 2023]

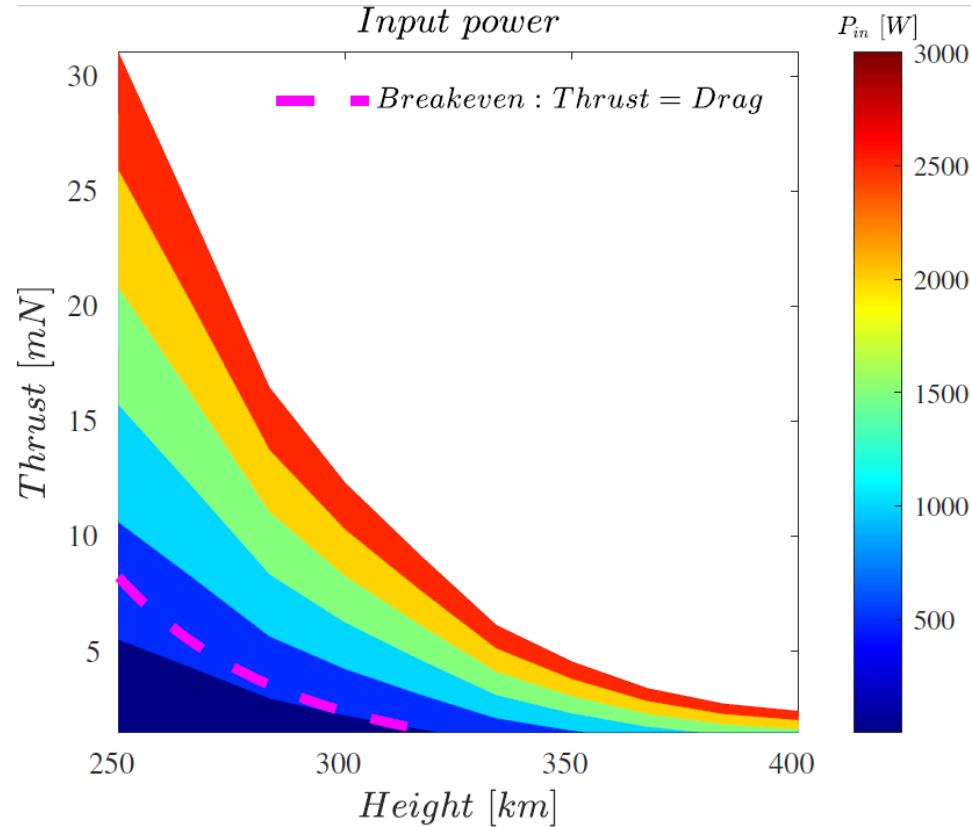
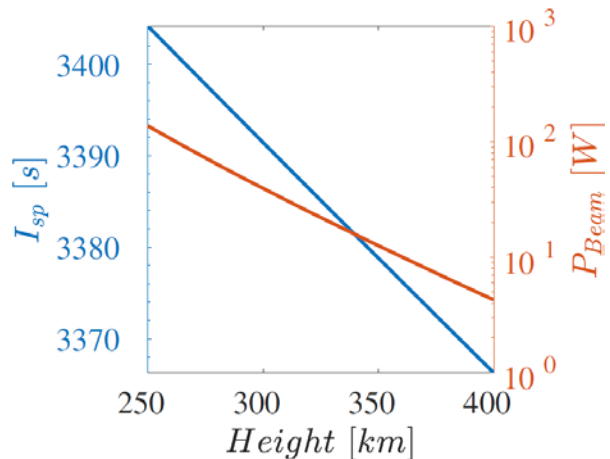
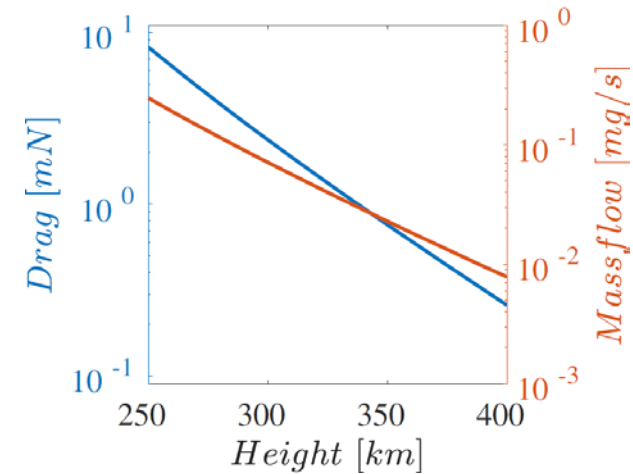
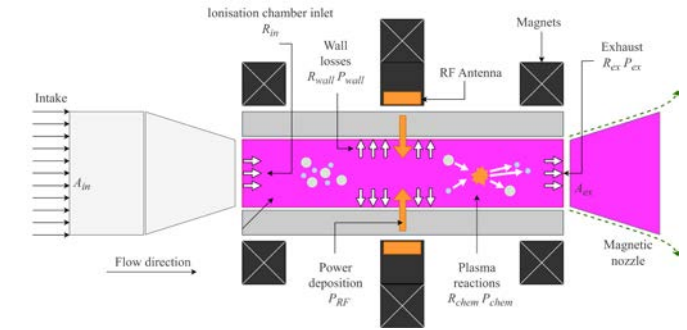
- ABEP unlocks VLEO with unprecedented market opportunities
- Air Global Model needed for assessment of innovative missions such as ABEP
- Different air composition depending on s/c position

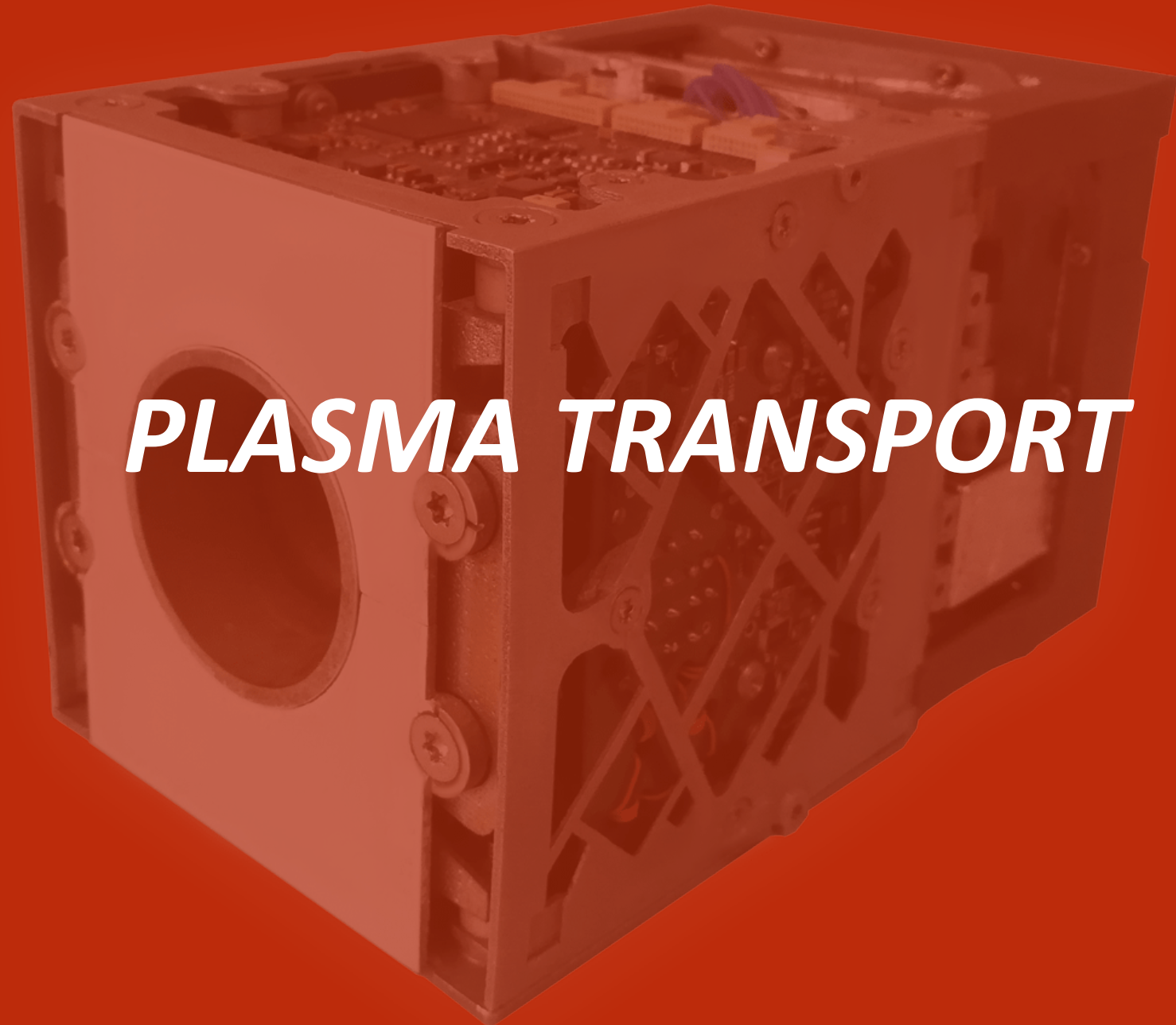


ATMOSPHERE-BREATHING EP with HPT

[Souhair & Dalle Fabbriche, Aerospace, 2023]

- Air chemistry model needed for innovative missions such as ABEP
- Assessment of mission requirement for VLEO missions
- Feasibility analysis and preliminary design with air GM
- Example, GOCE like s/c





PLASMA TRANSPORT



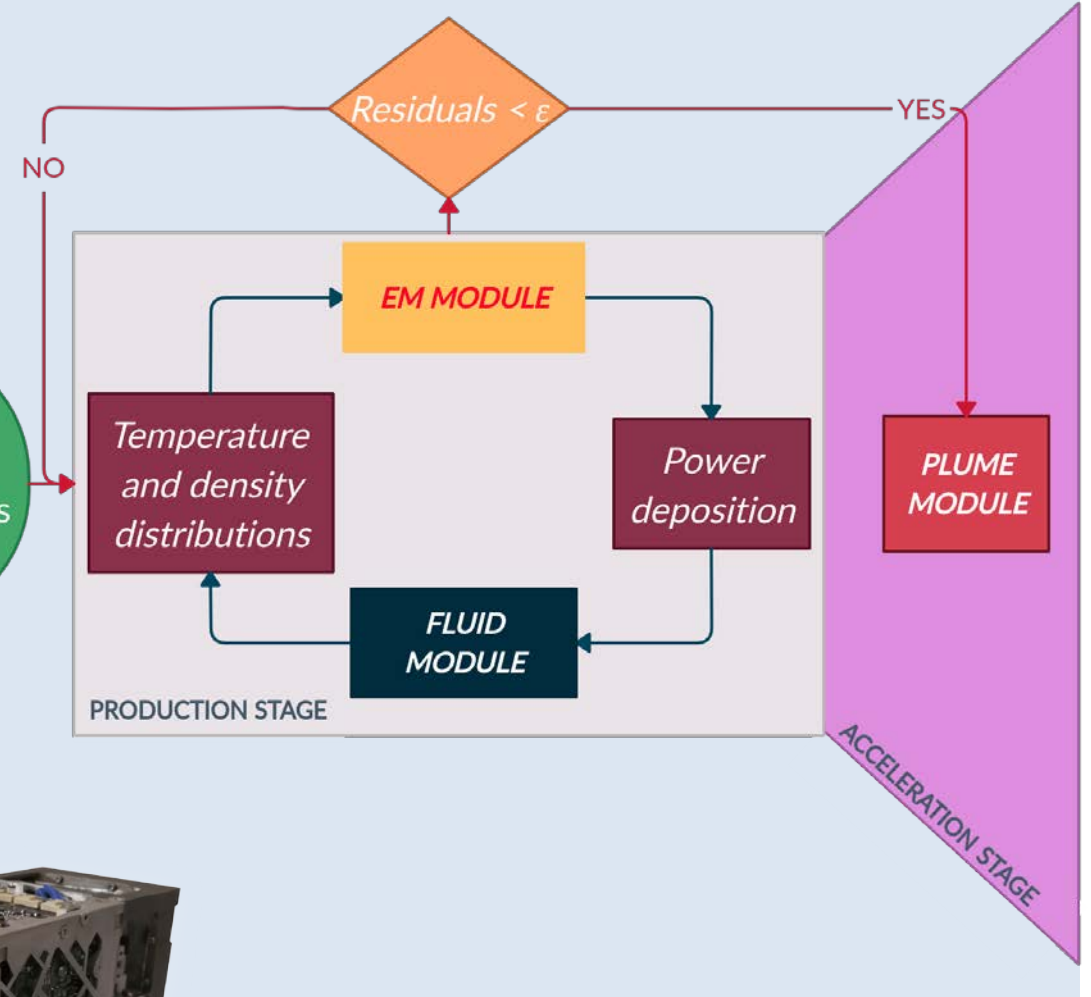
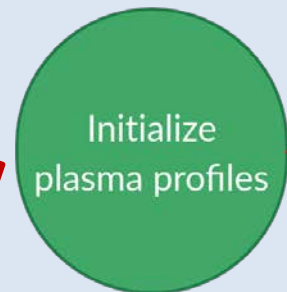
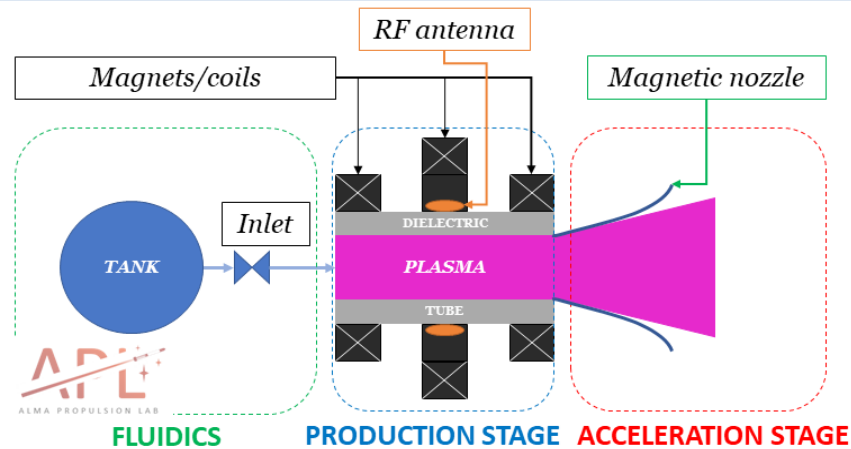
3D Simulation strategy for Cathode-less Plasma Thrusters

PRODUCTION STAGE:

- EM module ADAMANT (FEM)
- FLUID module (Finite Volumes Method)
- Iterative convergence

ACCELERATION STAGE:

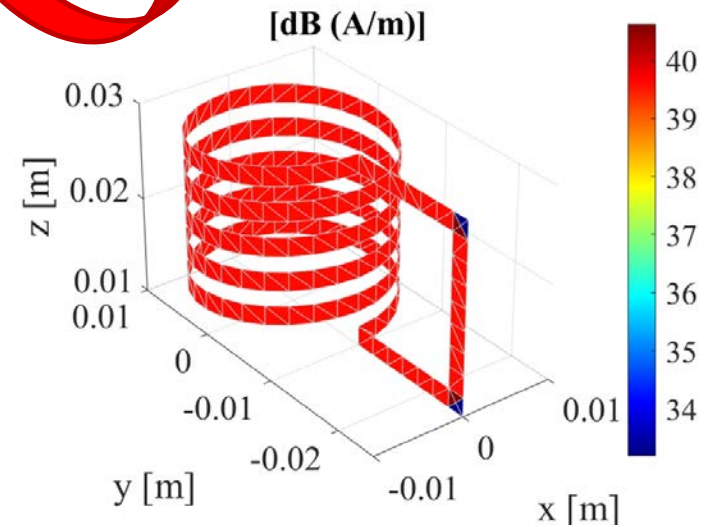
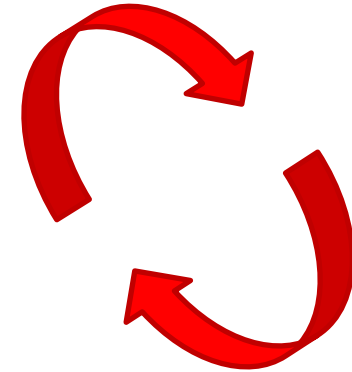
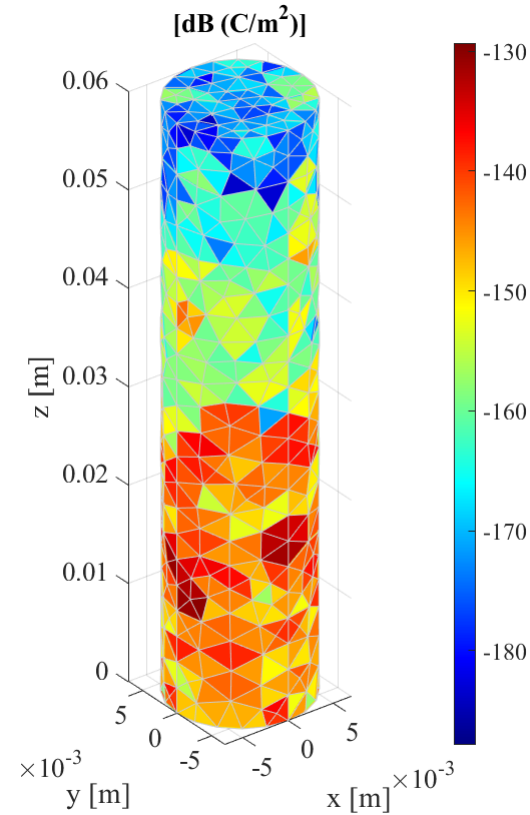
- Analytical PLUME model [Lafleur 2011]
- PIC 2D (STARFISH)



EM MODULE: plasma - antenna coupling

EM module (ADAMANT) provides:

- Plasma power deposition profile for the Fluid module
- Current pattern on the antenna.
- Antenna impedance \rightarrow matching network design



FLUID MODULE: governing equations

Electrons:

- Drift-diffusion (*collision frequency* \gg *velocity gradient*)
- Electron energy equation fully solved

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = R_e$$

CHEMISTRY
EM module

$$\frac{\partial}{\partial t} \left(\frac{3}{2} q n_e T_e \right) + \nabla \cdot \left(\frac{5}{2} q T_e \Gamma_e + \overline{k_e} \nabla T_e \right) + q E \cdot \Gamma_e = R_\varepsilon + \frac{1}{2} Re \{ J_P^* \cdot E_P \}$$

$$\varepsilon_0 \nabla^2 \phi = -q(n_i - n_e)$$

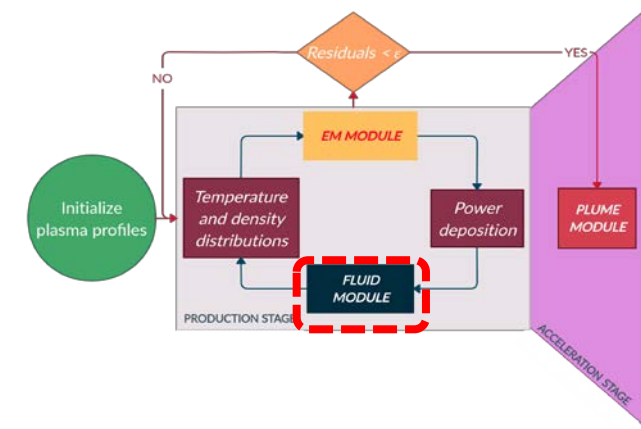
$$\Gamma_e = \overline{\mu}_e n_e E - \overline{D}_e n_e \frac{\nabla p_e}{p_e}$$

$$\overline{\mu}_k = \mu_k \overline{T}_r, \quad \overline{D}_k = D_k \overline{T}_r$$

$$\overline{T}_r = \frac{1}{1 + \chi_c^2} \begin{pmatrix} 1 + \chi_x^2 & \chi_x \chi_y - \chi_z & \chi_x \chi_z + \chi_y \\ \chi_x \chi_y + \chi_z & 1 + \chi_y^2 & \chi_y \chi_z - \chi_x \\ \chi_x \chi_z - \chi_y & \chi_y \chi_z + \chi_x & 1 + \chi_z^2 \end{pmatrix}$$

MAGNETIZATION

- Secondary electron emission accounted with Vaughan
- Anomalous diffusion according to Boeuf: $v_{Bohm} = v + \alpha \omega_C$



Ions:

- Energy eqt. resolved instead of isotherm hyp.
- Ions non-magnetized ($R_{LARMOR} \approx L_{char}$)

$$\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \mathbf{u}_i = R_i$$

$$\frac{\partial}{\partial t} (n_i \mathbf{u}_i) + \nabla \cdot (n_i \mathbf{u}_i) = -\nabla p_i + q n_i \mathbf{E} - m_i n_i \nu_i \mathbf{u}_i$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_i \right) + \nabla \cdot \left(\frac{5}{2} p_i \mathbf{u}_i + k_i \nabla T_i \right) - \mathbf{u}_i \cdot \nabla p_i = R_{\varepsilon_i}$$

Neutrals and excited species:

$$\frac{\partial n_0}{\partial t} + \nabla \cdot n_0 \mathbf{u}_0 = R_0$$

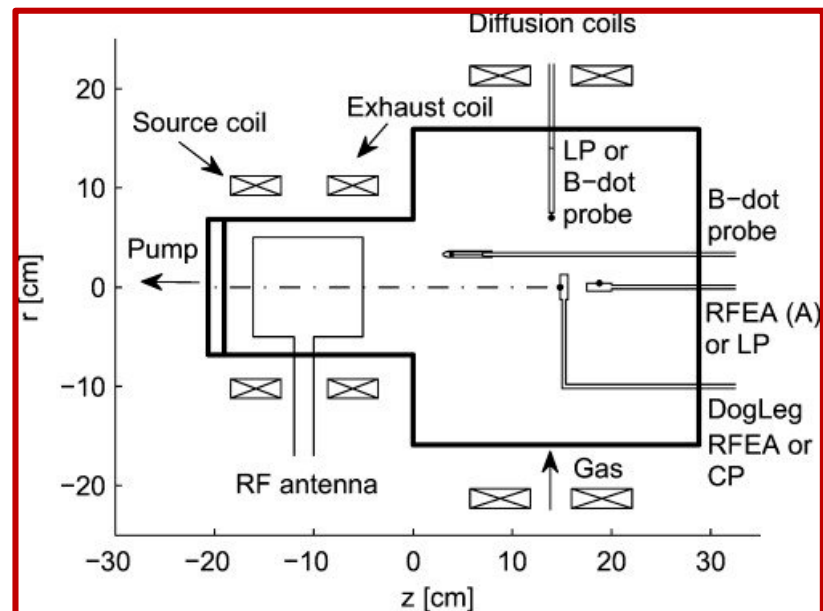
$$\frac{\partial}{\partial t} (n_0 \mathbf{u}_0) + \nabla \cdot (n_0 \mathbf{u}_0) = -\nabla p_0 - m_0 n_0 \nu_0 \mathbf{u}_0$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_i \right) + \nabla \cdot \left(\frac{5}{2} p_0 \mathbf{u}_0 + k_0 \nabla T_0 \right) - |\mathbf{u}_0 \cdot \nabla p_0 = R_{\varepsilon_0}$$

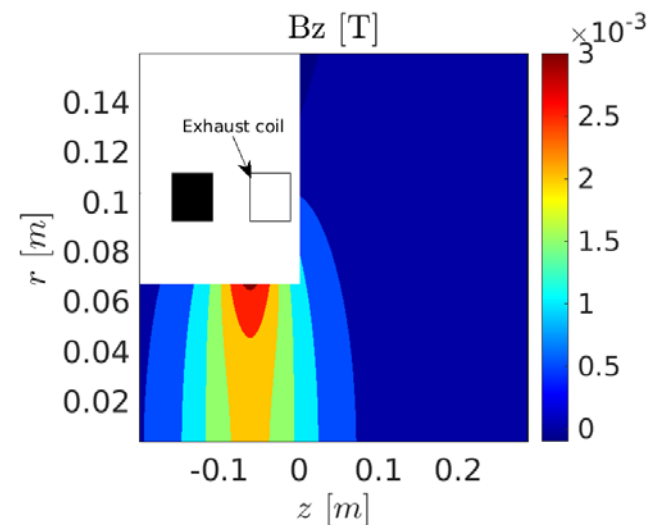
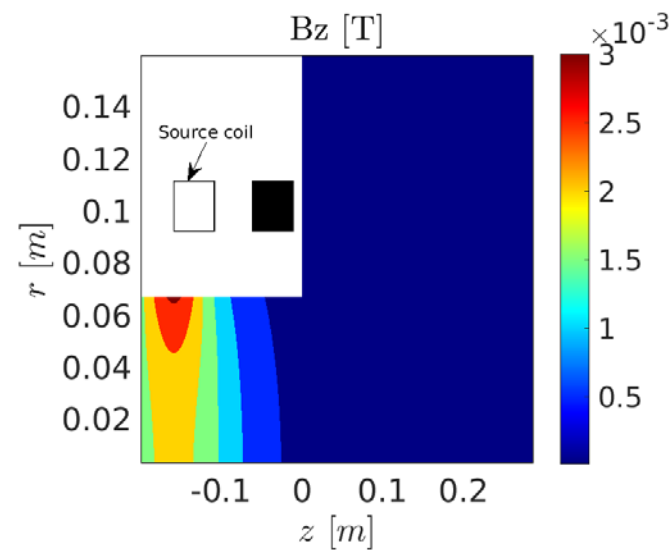


Validation

- Validation against experiments on Argon fed Helicon reactor “piglet” [Lafleur, 2011]
- Two coil configurations: SOURCE, EXHAUST
- LP measurement of plasma density at the centerline

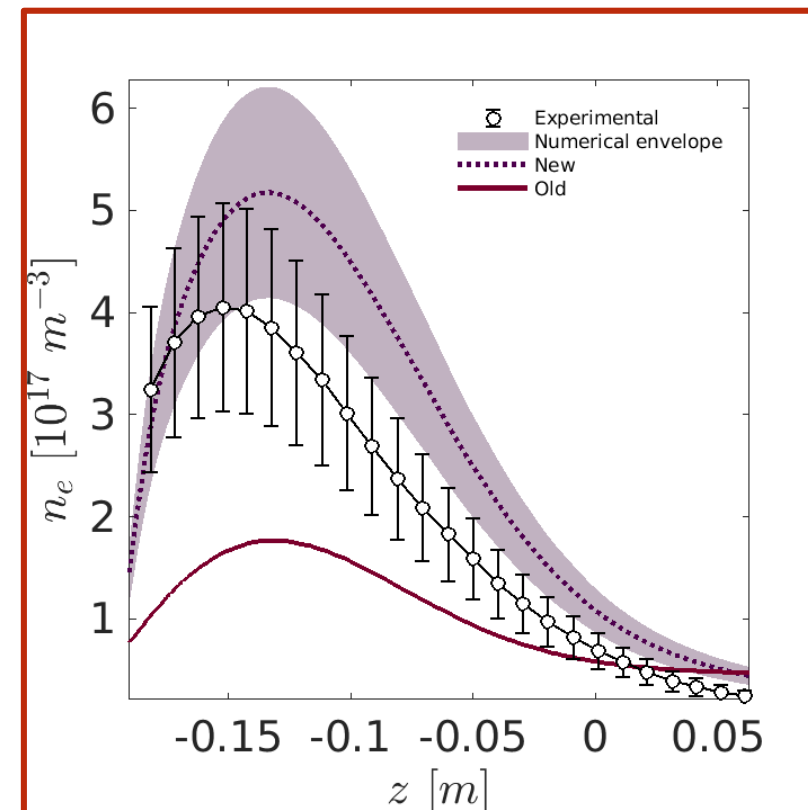
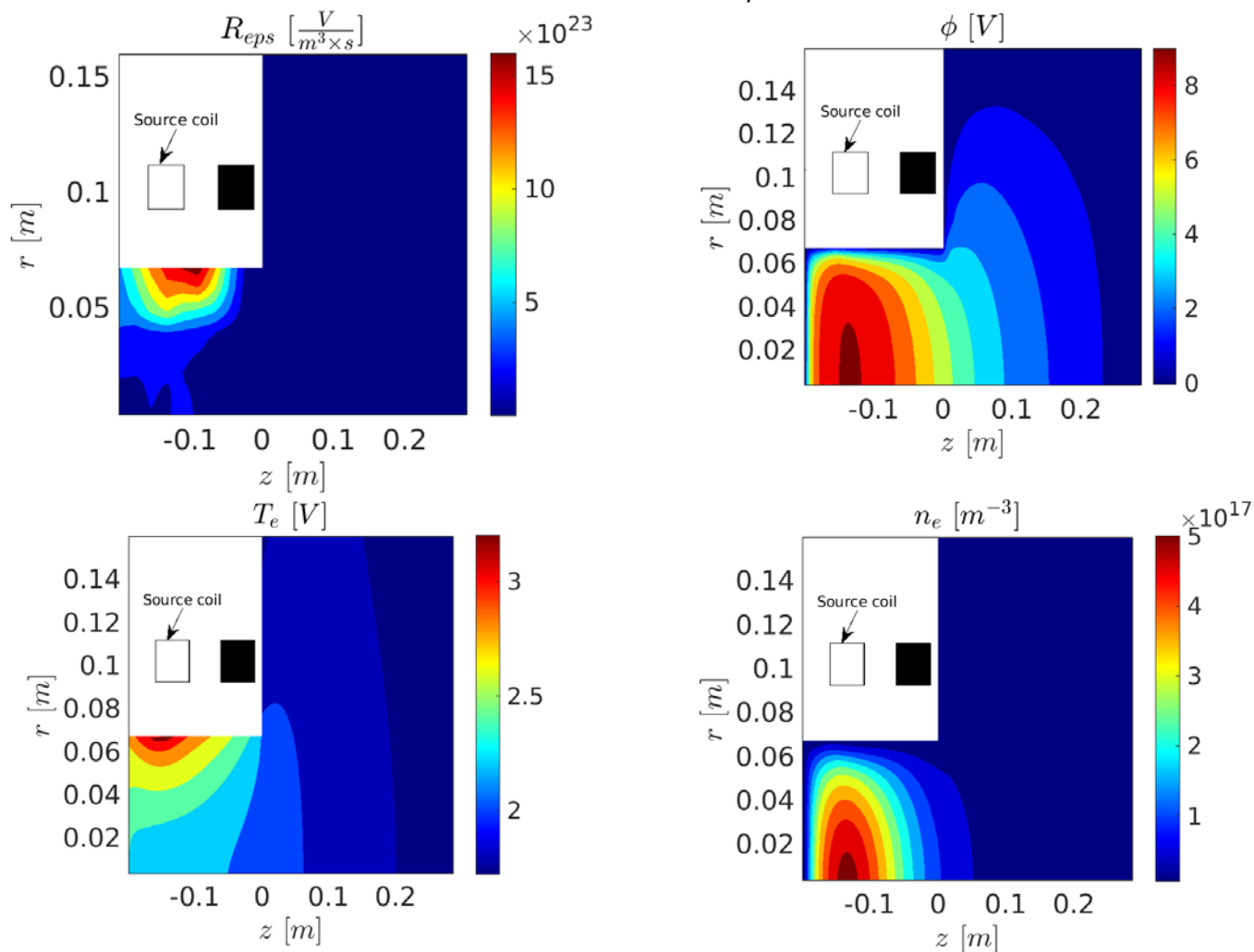
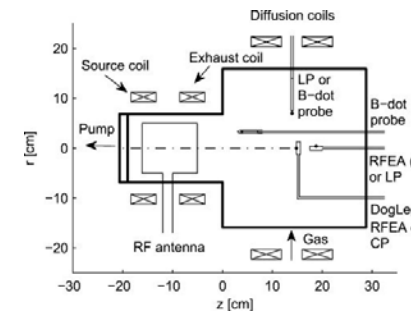


Parameter	Value
Source diameter	0.136 m
Source length	0.2 m
Expansion chamber diameter	0.320 m
Expansion chamber length	0.288 m
RF input power	250 W
Antenna frequency	13.56 MHz
Magneto-static field (axis peak)	2.1 mT
Gas pressure	2.7 mTorr



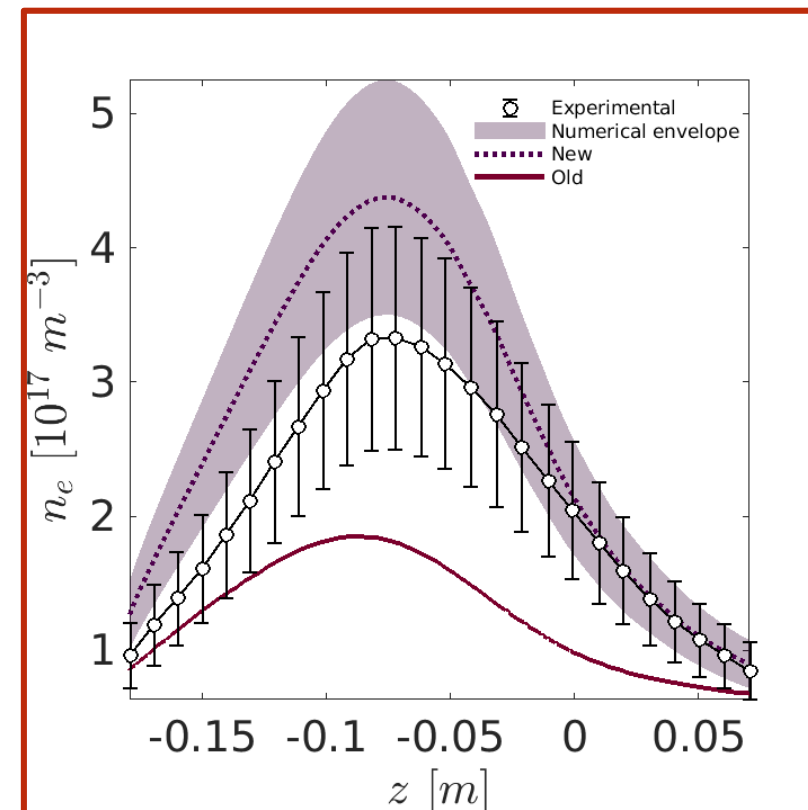
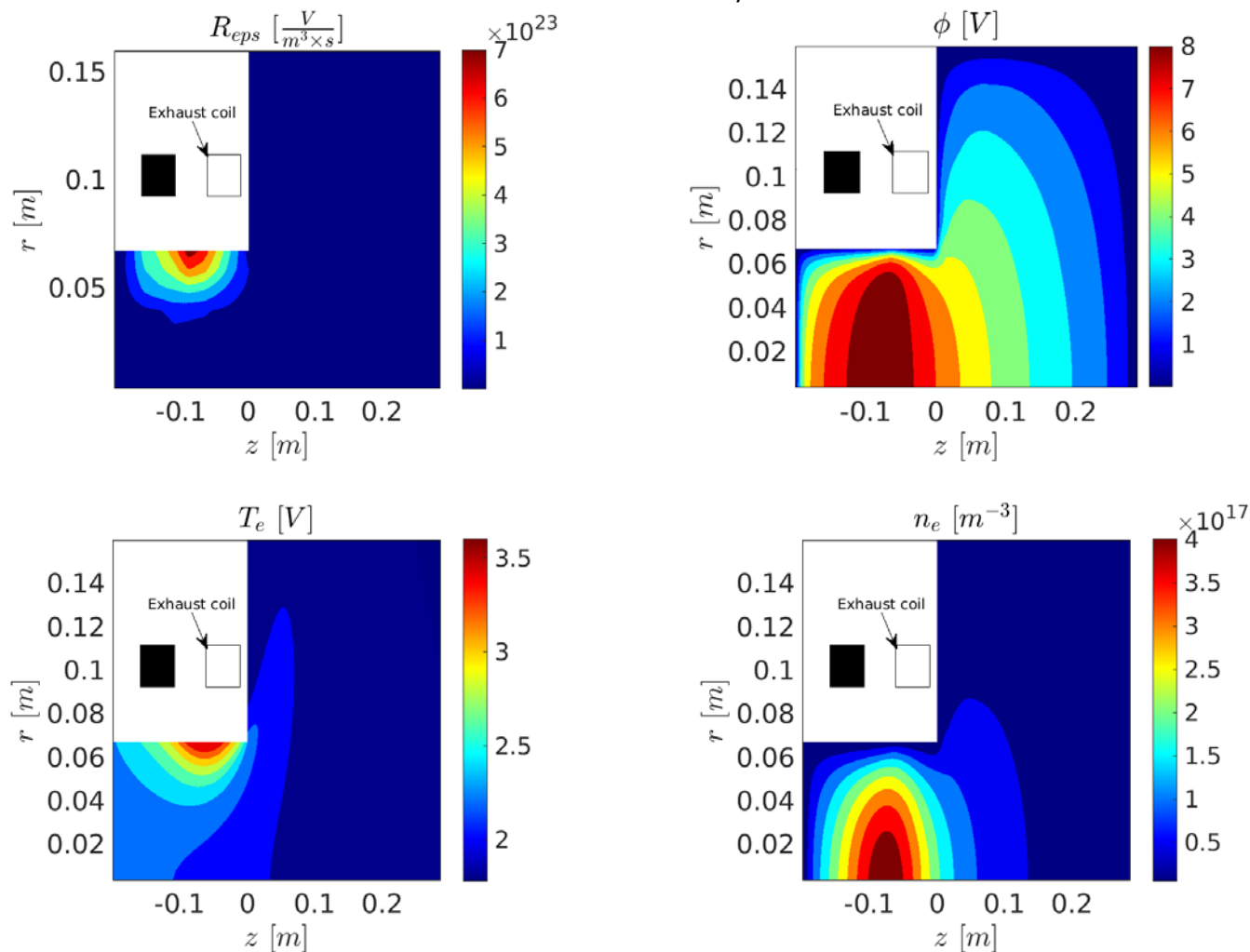
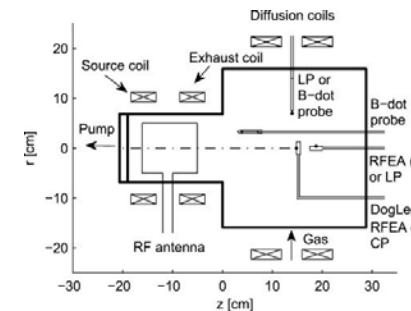
Validation: SOURCE case

- Plasma peaked at the centerline.
- Electron density and temperature profiles are affected by magnetic topology.
- Deposited power density not significantly influenced by magnetic topology.
- New model deviates of only 24% w.r.t. measurements, and 78% w.r.t. old model [Magarotto, 2020].
- Measurement error band of 25% and numerical uncertainty of 20%.



Validation: EXHAUST case

- Plasma peaked at the centerline.
- Electron density and temperature profiles are affected by magnetic topology.
- Deposited power density not significantly influenced by magnetic topology.
- New model deviates of only 25% w.r.t. measurements, and 55% w.r.t. old model [Magarotto, 2020].
- Measurement error band of 25% and numerical uncertainty of 20%.

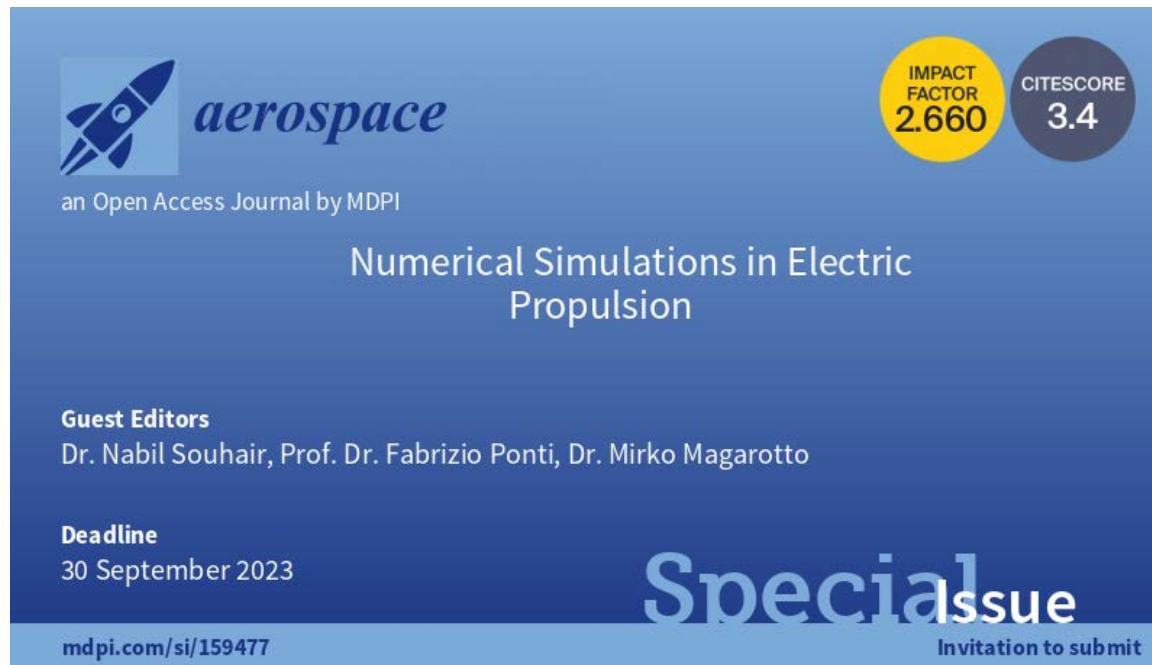


CONCLUSIONS

- Development of a Global Model (GM) for analyzing Plasma Thrusters working with noble gases and alternative propellants.
- Propulsive performance of REGULUS (iodine-fed HPT) addressed by coupling GM and PIC methodology, with the GM adapted with iodine chemistry model.
- 3D numerical tool developed for analyzing HPT in terms of plasma transport and physical models employed, validated successfully against experiments in literature.

Currently on progress & future developments:

- Validate air chemistry model against experimental data, ongoing campaign in co-op with University of Stuttgart.
- Find accurate cross-section for reactions in air and iodine plasma and fine tuning chemistry models.
- Implement iodine and air chemistry model on 3D numerical strategy, improve physical models and boundary conditions.
- Improving FLUID + PIC coupling.
- Compare models with experimental measurements of plasma thrusters fed with xenon, iodine, and air for validation.



The image shows the cover of the journal 'Aerospace', an Open Access Journal by MDPI. The cover features the journal's logo (a rocket) and the title 'Numerical Simulations in Electric Propulsion'. It also displays the Impact Factor (2.660) and Citescore (3.4). The guest editors are Dr. Nabil Souhair, Prof. Dr. Fabrizio Ponti, and Dr. Mirko Magarotto. The deadline is 30 September 2023. The cover includes the MDPI logo, the journal's website (mdpi.com/si/159477), and the text 'Special Issue' and 'Invitation to submit'.

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Numerical Simulations in Electric Propulsion

Guest Editors
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Deadline
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BACKUP SLIDES

CONCLUSIONS

- Development of a Global Model (GM) for analyzing Plasma Thrusters working with noble gases and alternative propellants.
- A novel lumping strategy has been proposed to account for dynamics of excited states in low pressure discharges fed with noble gases.
- Propulsive performance of REGULUS (iodine-fed HPT) addressed by coupling GM and PIC methodology, with the GM adapted with iodine chemistry model.
- Air-breathing HPT being characterized experimentally (on-going) to validate GM air chemistry.
- 3D numerical tool developed for analyzing HPT in terms of plasma transport and physical models employed, validated successfully against experimental measurements.

Currently on progress & future developments:

- Validate air chemistry model against experimental data, ongoing campaign at University of Stuttgart.
- Find accurate cross-section for reactions in air and iodine chemistry models through spectroscopic experiments or quantum methodologies.
- Implement iodine and air chemistry model on 3D numerical strategy, improve physical models and boundary conditions.
- Use FLUID + PIC strategy to obtain accurate propulsive performance data with reasonable computing time, optimize thruster design.
- Compare models with experimental measurements of HPT fed with xenon, iodine, and air for validation.

Novelty:

- Development of a GM with several chemistry models to analyze the performance of HPT fed with noble gases such as argon, neon, krypton, and xenon, as well as innovative propellants such as iodine and air
- Development of a novel lumping methodology for reducing computational cost without affecting accuracy when modeling excited species in plasma chemistry for both GM and multidimensional codes
- Development of a GM with an iodine chemistry set and collection of cross-sections and reaction rates from literature, allowing for design of novel thrusters using iodine propellant and performing preliminary optimizations
- Development of a chemistry model for air-breathing technology and a GM capable of simulating a HPT for preliminary estimation of an air-breathing thruster performance and assessment of both propulsion and system analysis of the thruster operating at various altitudes
- Development of a 3D numerical code capable of simulating HPT in terms of plasma generation and transport, resolving both EM wave propagation and plasma transport, handling Helicon sources, treating discharges with a generic 3D geometry, and modeling the actual RF antenna by solving the current distribution thereof, and resolving generic plasma sources driven by RF antennas if all the plasma species can be considered Maxwellian, with the FLUID module stand-alone also simulating DC discharges if the Maxwellian hypothesis is respected.



NUMERICAL DISCRETIZATION

Finite Volume Methodology (FVM)

- Integration over a mesh cell

$$\iiint_V \left(\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{u}) - R \right) dV = 0$$

- After discretization we obtain a linear algebraic equation

$$a_P n_P = \sum_N a_N n_N + b_P$$

- Extending to all the cells, we obtain a linear system

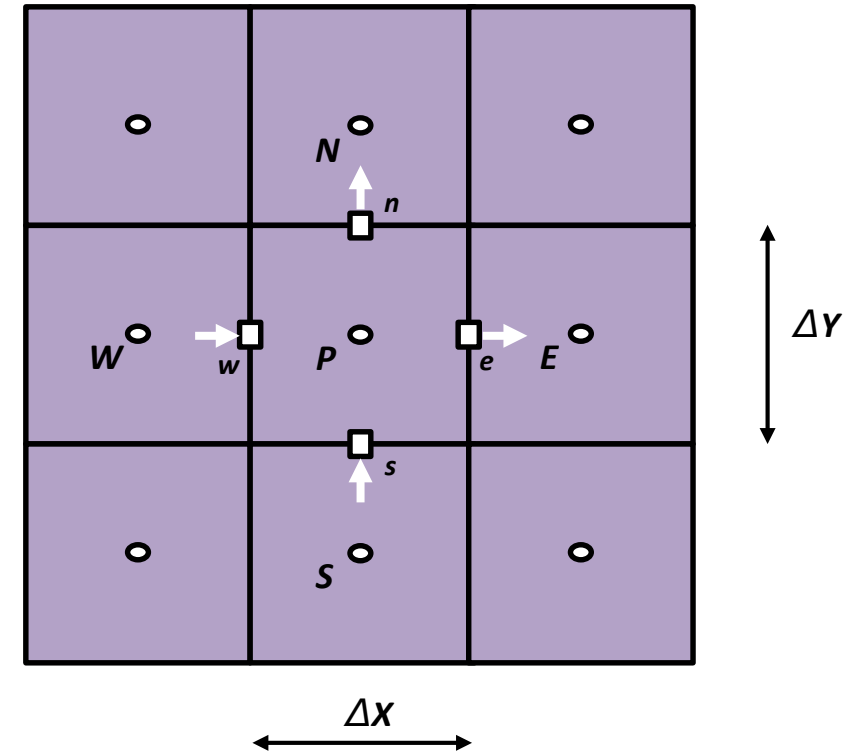
$$[\mathbf{A}][\mathbf{n}] = [\mathbf{b}]$$

$$\begin{bmatrix} * & * & * \\ * & * & * \\ & * & * \\ * & * & * \end{bmatrix} \begin{bmatrix} n_1 \\ \vdots \\ \vdots \\ n_N \end{bmatrix} = \begin{bmatrix} * \\ * \\ * \\ * \end{bmatrix}$$

- A is a sparse matrix (* represents non-zero elements) to be solved with an iterative algorithm (e.g., Gauss-Seidel)

Staggered mesh grid:

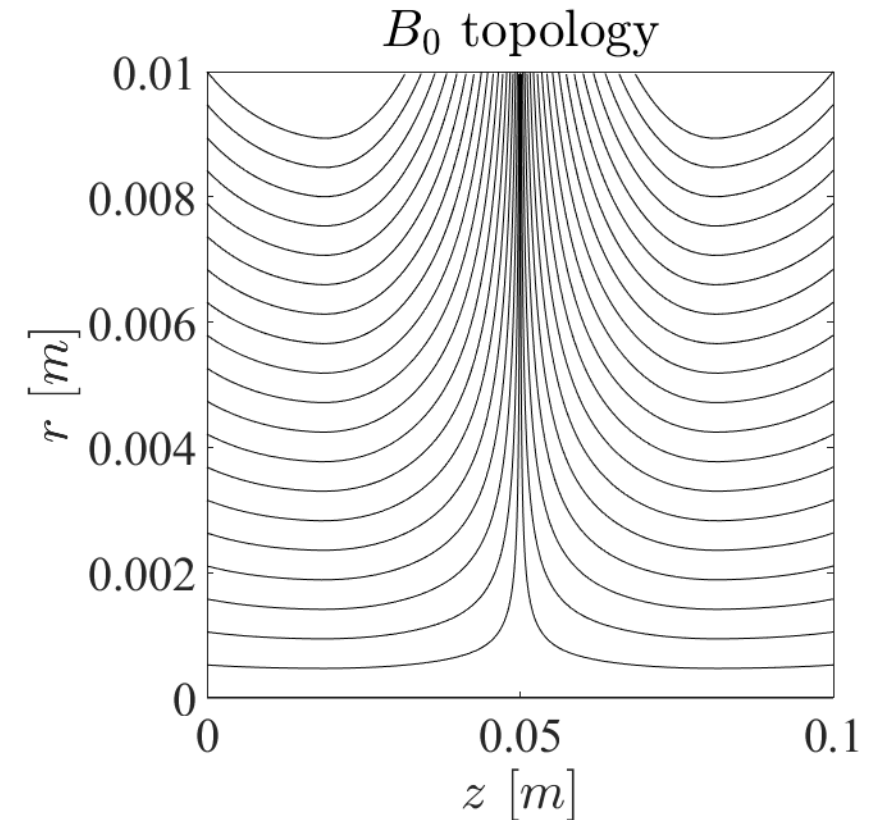
- Computation over cell centers
- Flux interpolated at face centers



RESULTS: set-up of the simulations

- A Helicon plasma test case has been considered
- Magnetic topology B_0 with cusp to test the solvers (induce strong spatial gradients)
- Assumed deposited power density $1.6 \times 10^7 \text{ W/m}^3$

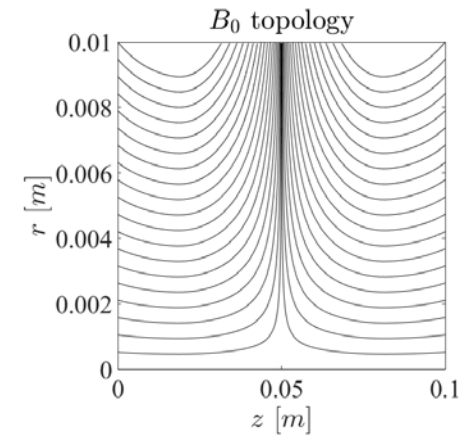
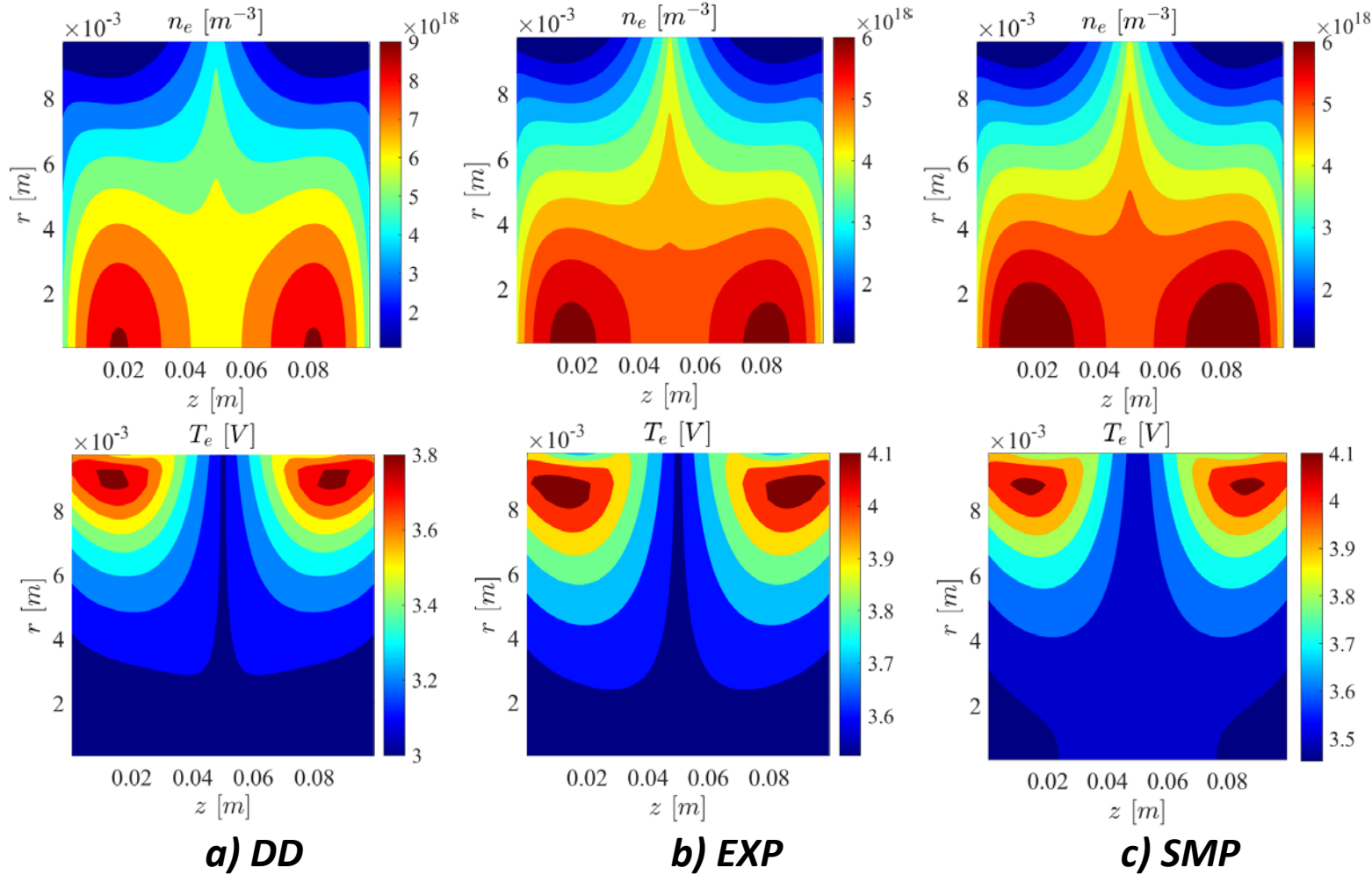
Parameters of the simulations	
Radius	0.01 m
Length	0.10 m
B_0 (peak)	0.05 T
T_0	300 K
p_0	30 mTorr



RESULTS

Comparison in terms of discharge electron density and temperature, between:

- Drift Diffusion (**DD**)
- Explicit solution of momentum/mass balance (**EXP**)
- SIMPLE coupling of momentum/mass balance (**SMP**)



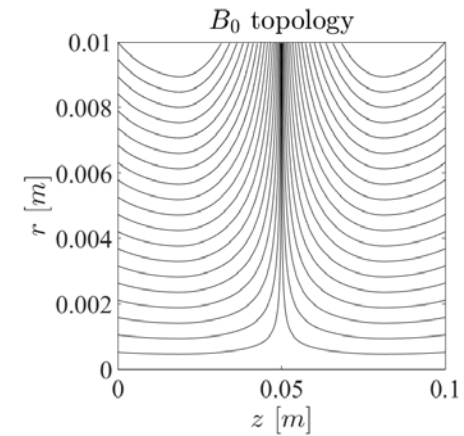
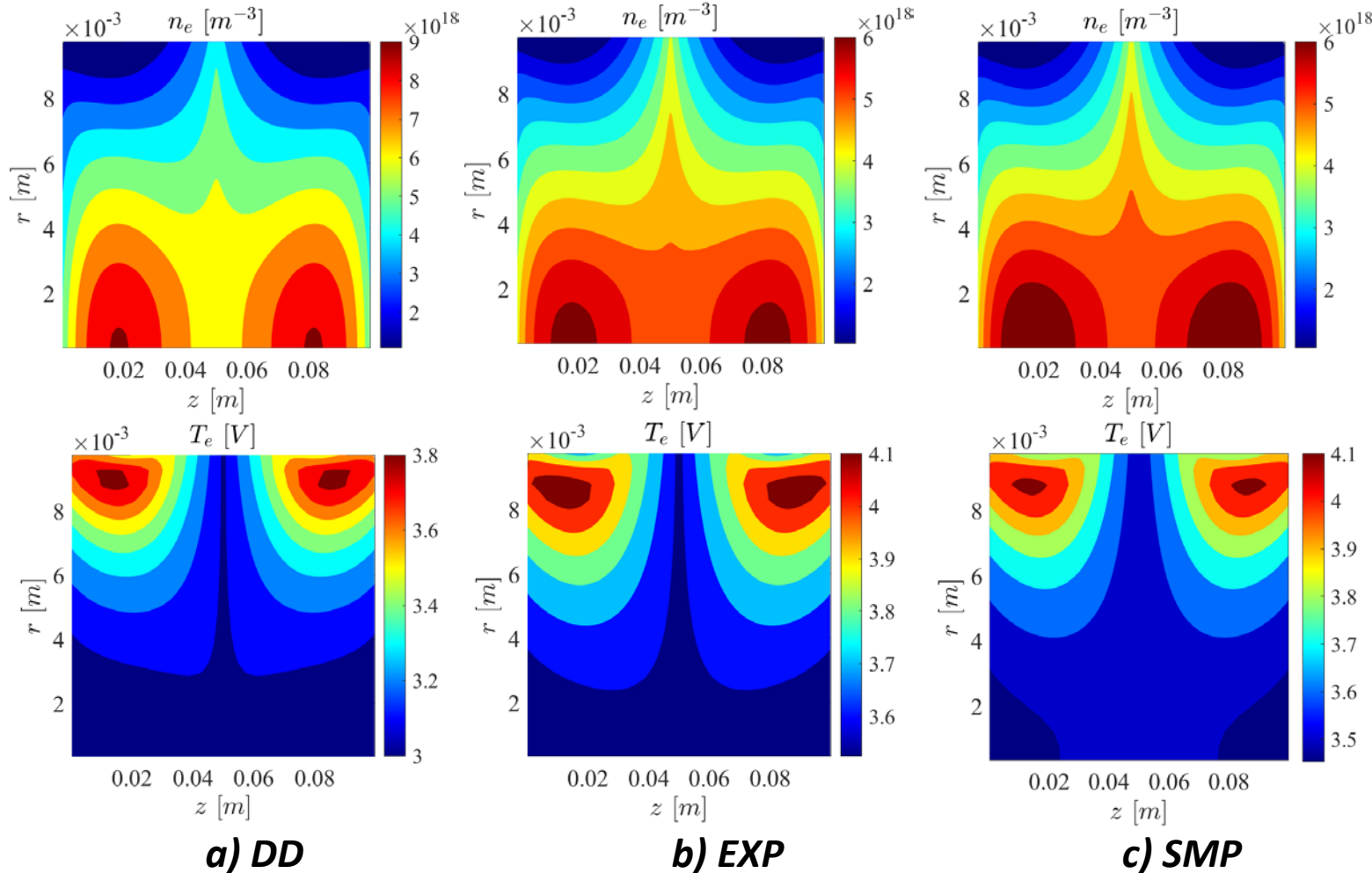
- Overall agreement of the trends
- DD overestimates n_e w.r.t. full momentum (EXP, SMP)
- Deviation up to 38%



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Propulsive performance:

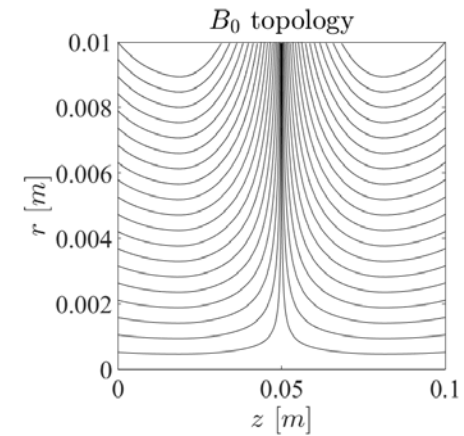
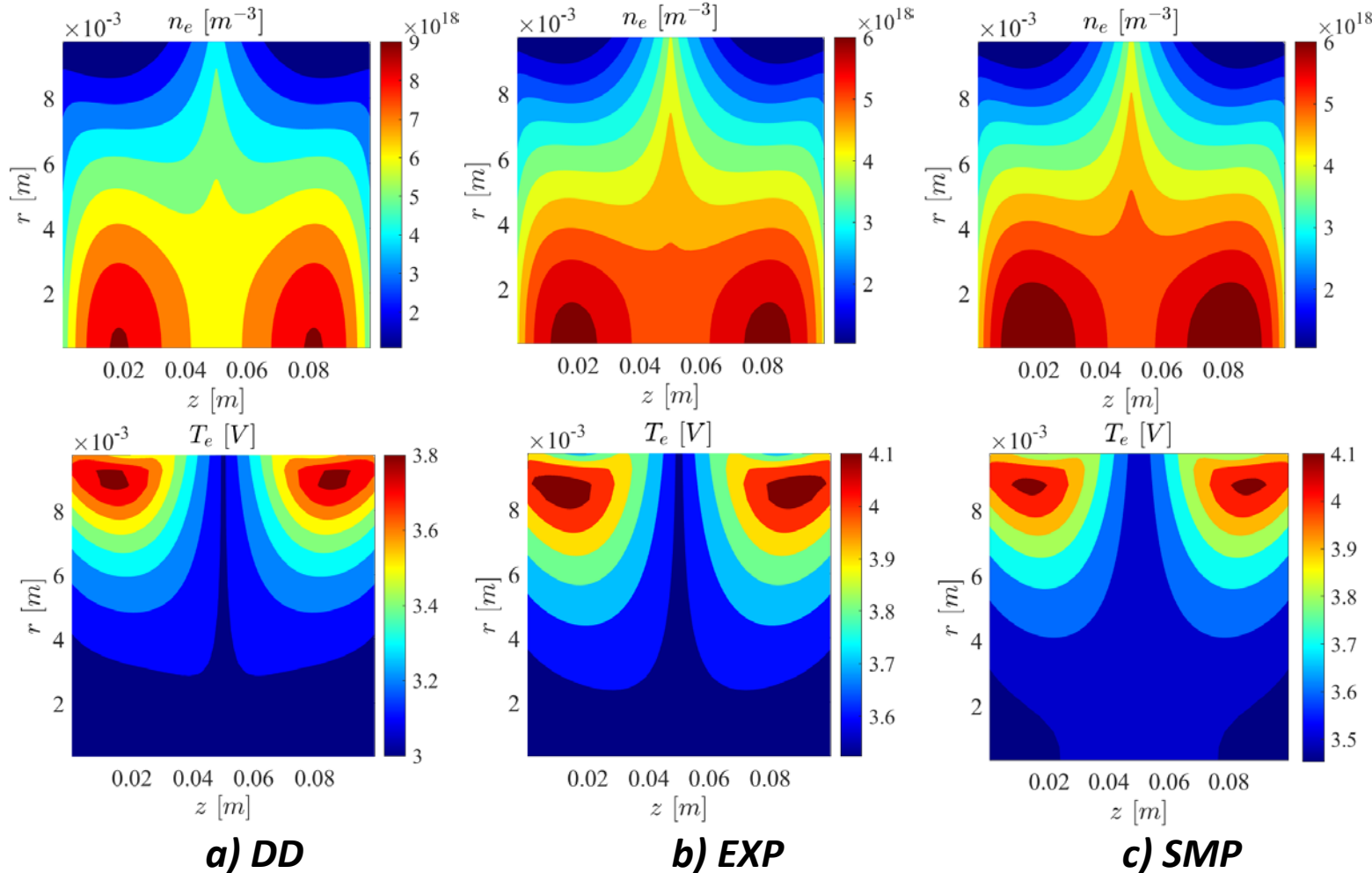
Model	Thrust [mN]
DD	6.32
EXP	4.50
SMP	4.69



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Computational effort on a 4k hex mesh:

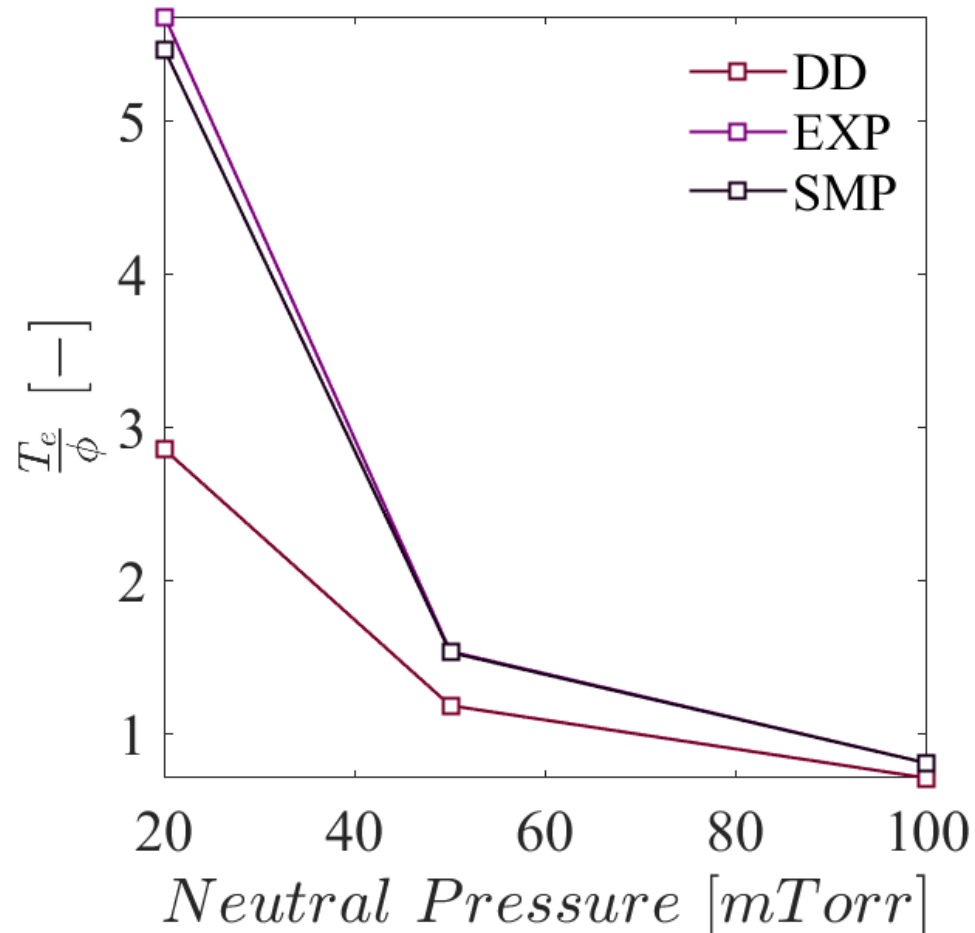
Model	Time [s]
DD	200
EXP	700
SMP	70



RESULTS: sensitivity analysis

A sensitivity analysis was done over the neutral pressure p_0 (20 ÷ 100 mTorr)

- At higher pressure (highly collisional regime) convergence of the approaches
- At low pressure (weak collisional regime) convective gradients cannot be neglected



Toward lower pressure regimes it is important to solve the full momentum equation to accurately predict performance!

