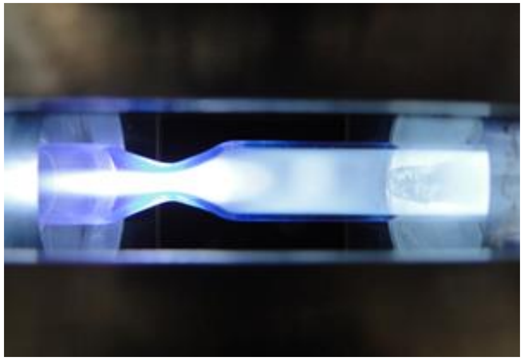
DIFFERENT PRESSURE REGIMES OF A SURFACE-WAVE DISCHARGE IN ARGON: A MODELING INVESTIGATION



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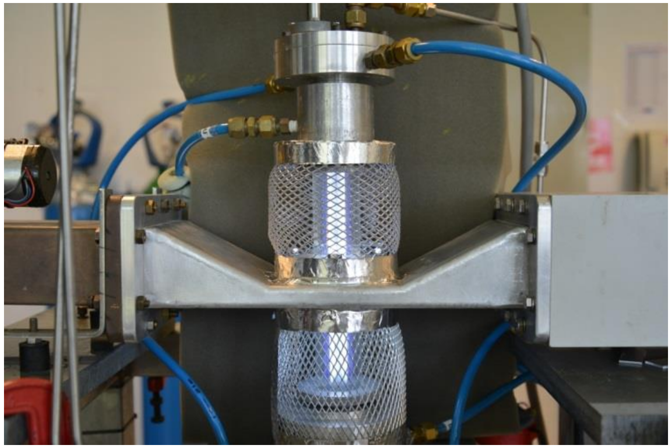
Microwave plasmas



- Simple configuration
- Low running costs
- Broad range of pressures
- Strong power coupling
- Low-temperature plasma ($T_g \ll T_e$)

Applications

- Gas treatment, surface deposition, sterilization, …
- Recently: CO_2 conversion

Aim of this study

- Modeling of microwave CO_2 plasmas in different pressure regimes
- Argon: first step
- Limited computational resources: necessity to reduce the CO_2 chemistry set

Outline of the presentation

I. Description of the model in Ar
II. Comparison of the results at different pressures
III. Benchmarking
IV. Reduction of the chemistry set of CO_2

The 2D-fluid model

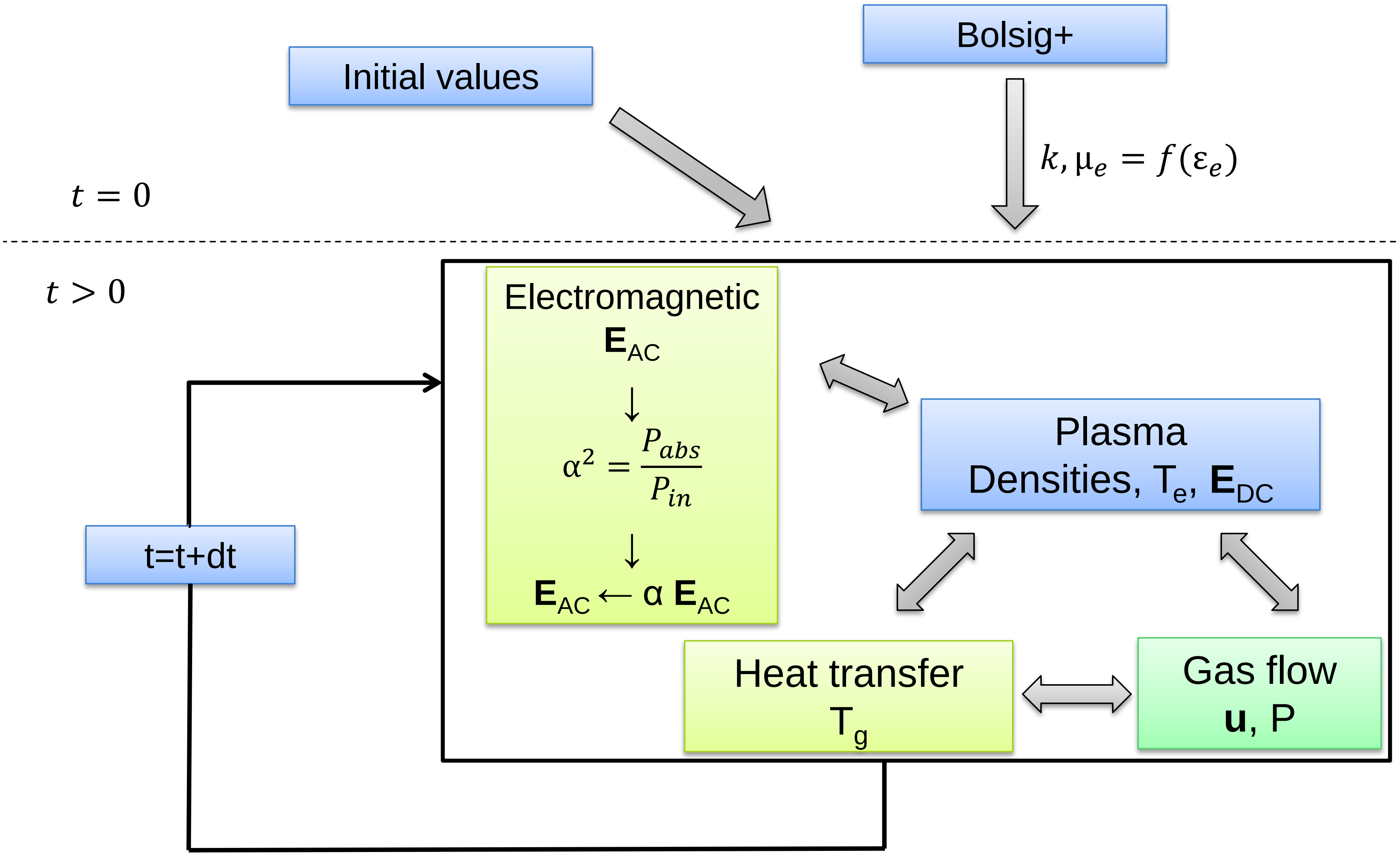
I. Plasma module
   - Electron, ion and metastable densities (continuity equations)
   - Electron temperature (energy balance equation)
   - Plasma potential (Poisson equation)

II. Microwave module
   - MW- Electric field (wave equation)

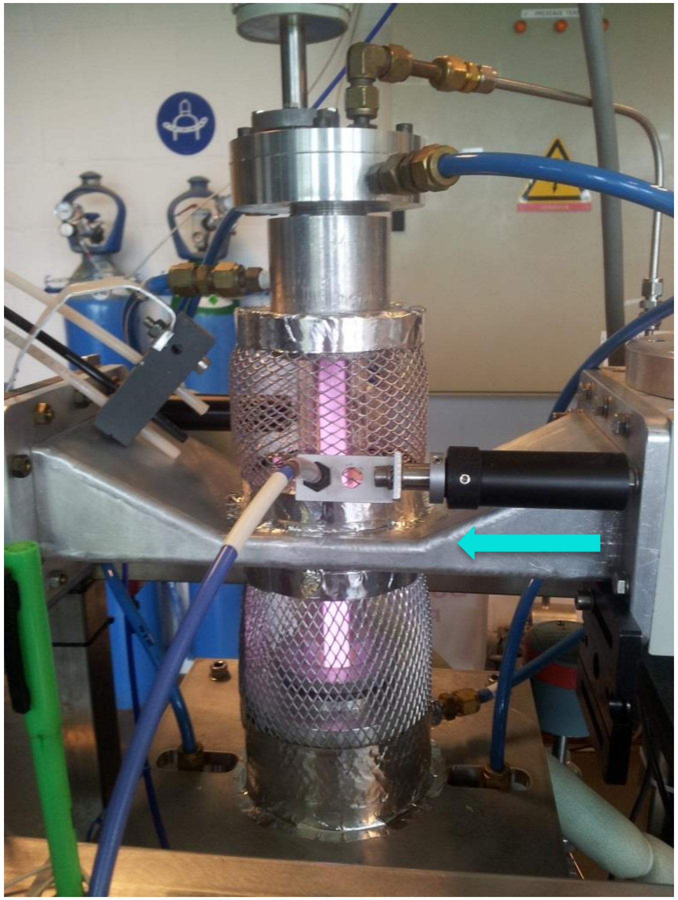
III. Gas flow module
   - Pressure, gas velocity (Navier-Stokes equations)

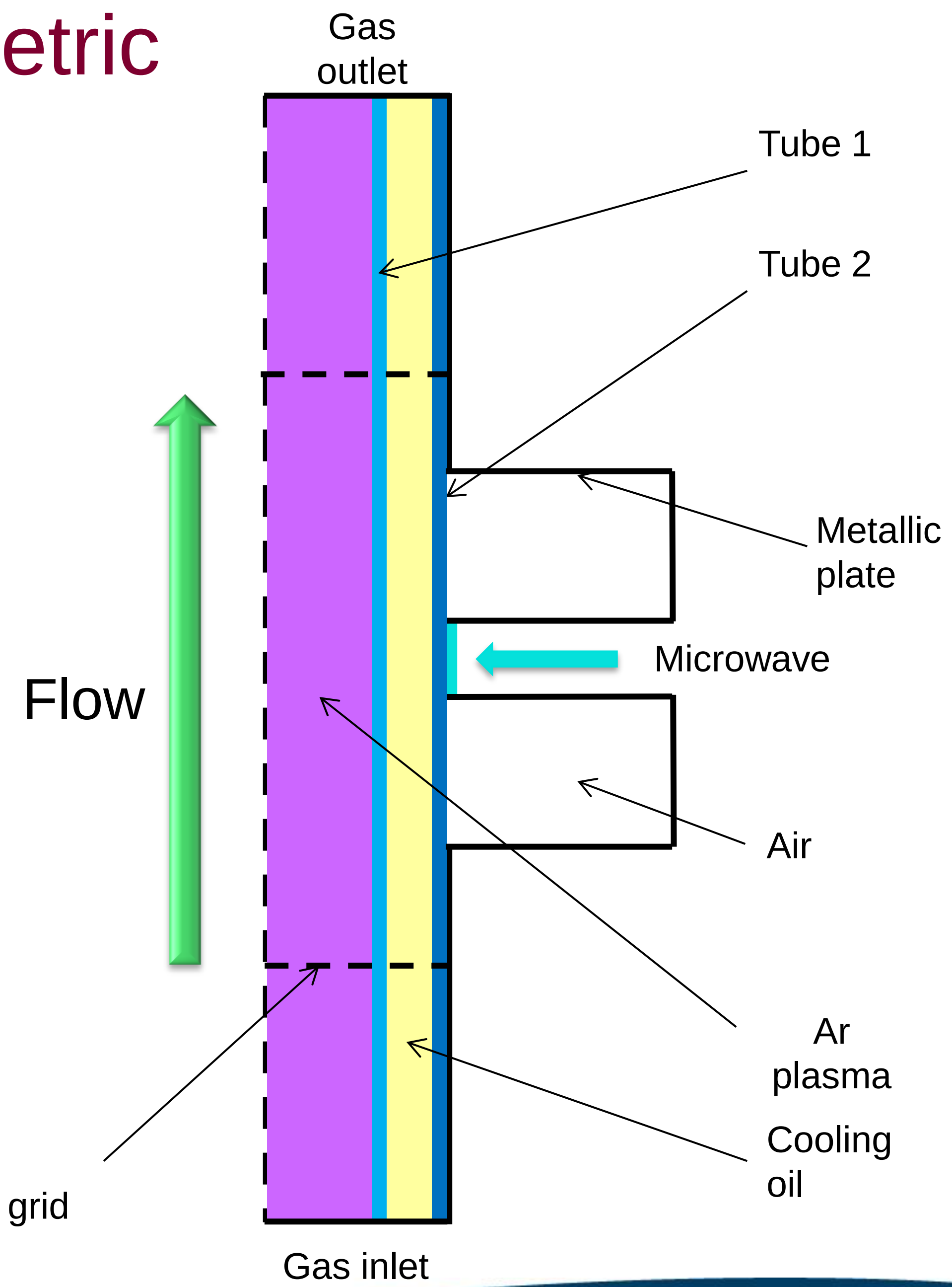
IV. Heat transfer module
   - Gas temperature (Heat equation)

Fluid time-dependent model



Geometry: 2D axisymmetric



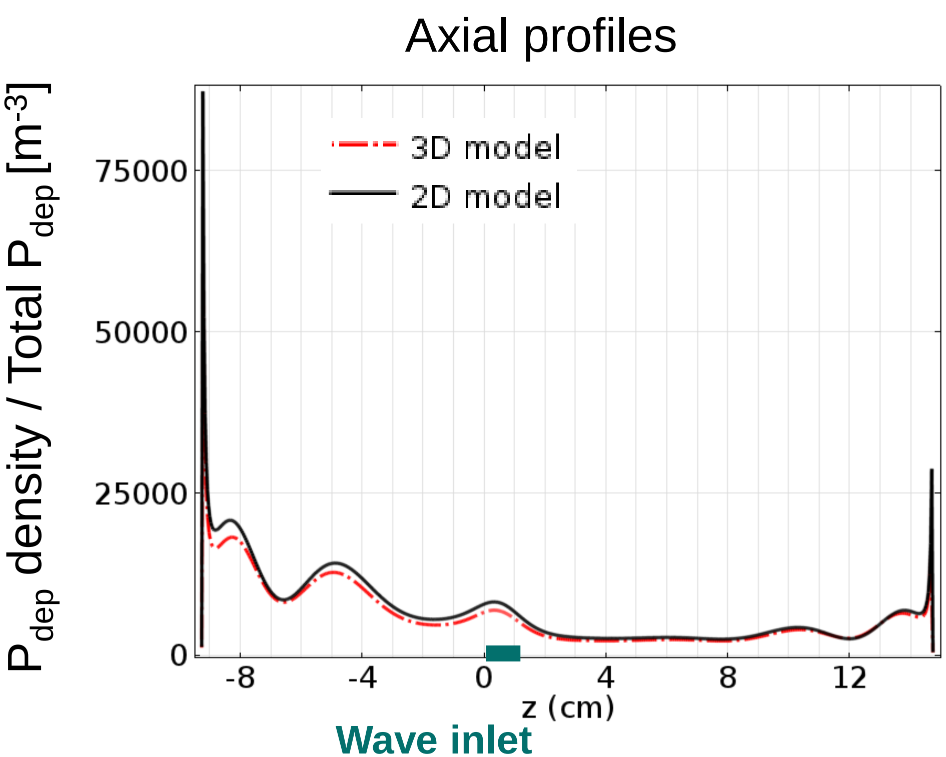


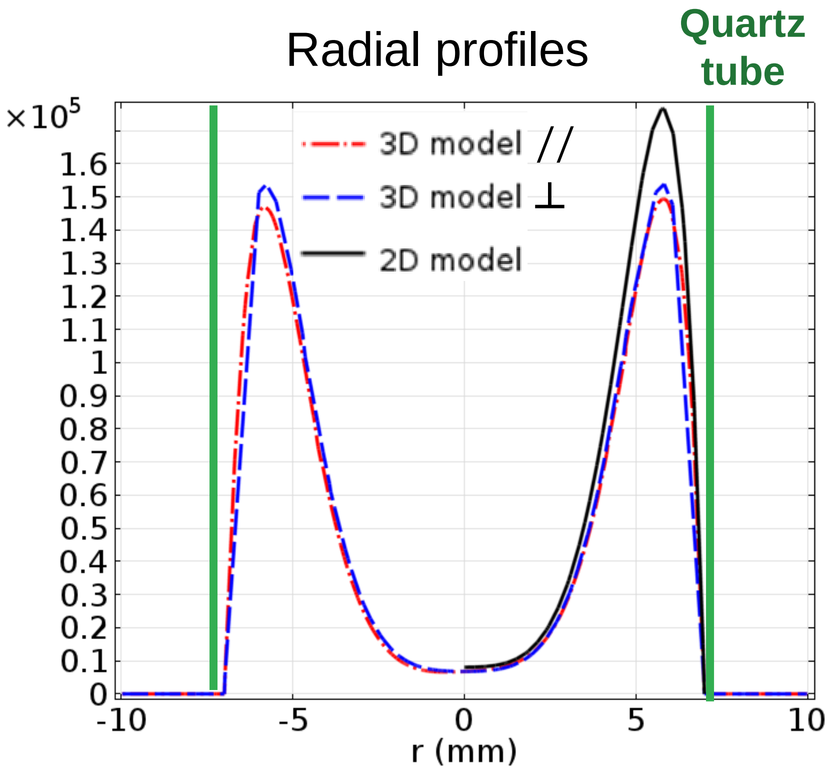
UMONS
Université de Mons

2D axisymmetric approximation?

Analytical profile of electron density → EM model

Comparison of the absorbed power density





Argon chemistry

7 species

- ✓ Ar, Ar(4s), Ar(4p), Ar^+, Ar_2^+, Ar_2^*,e

17 electron impact reactions

- ✓ E.g.: e + Ar → e + Ar(4s)
- ✓ From Bolsig+ & literature

11 Heavy species collisions reactions

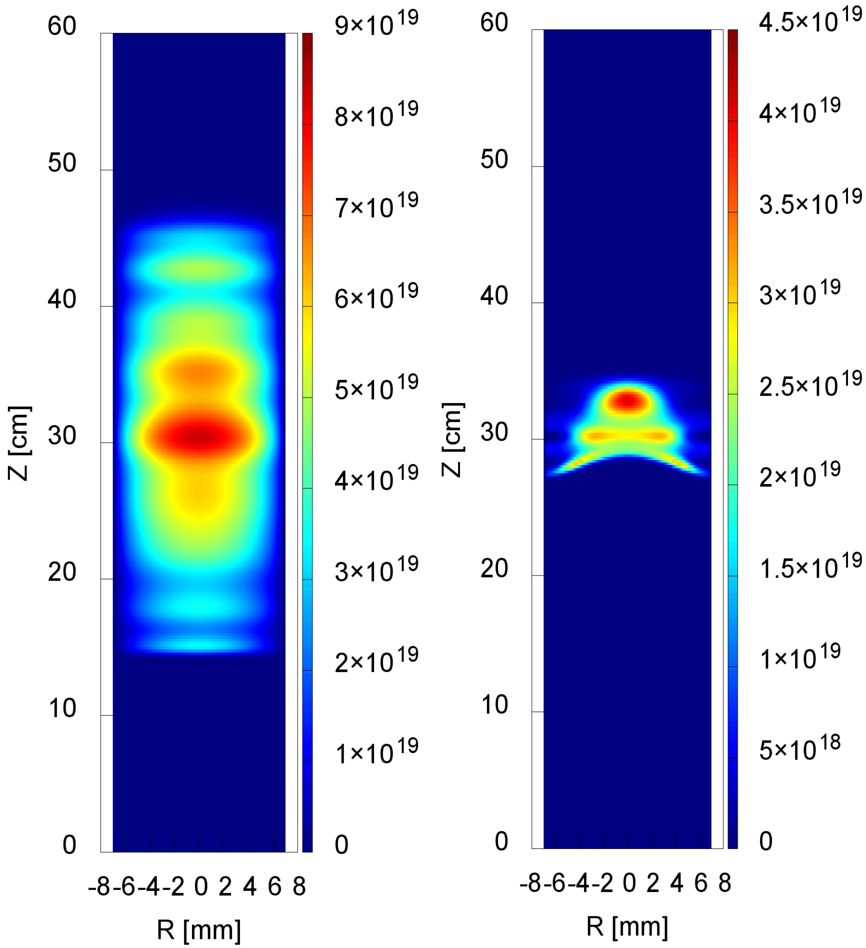
- ✓ E.g.: Ar(4p) + 2Ar → Ar_2^* + Ar
- ✓ Rates from the literature

3 radiative transitions

- ✓ E.g.: Ar(4s) → Ar + $h\nu$
- ✓ Probabilities & escape factors from literature

Electron density (m^{-3})

Conditions: 500 sccm – 100 W deposited power – 2.45 GHz



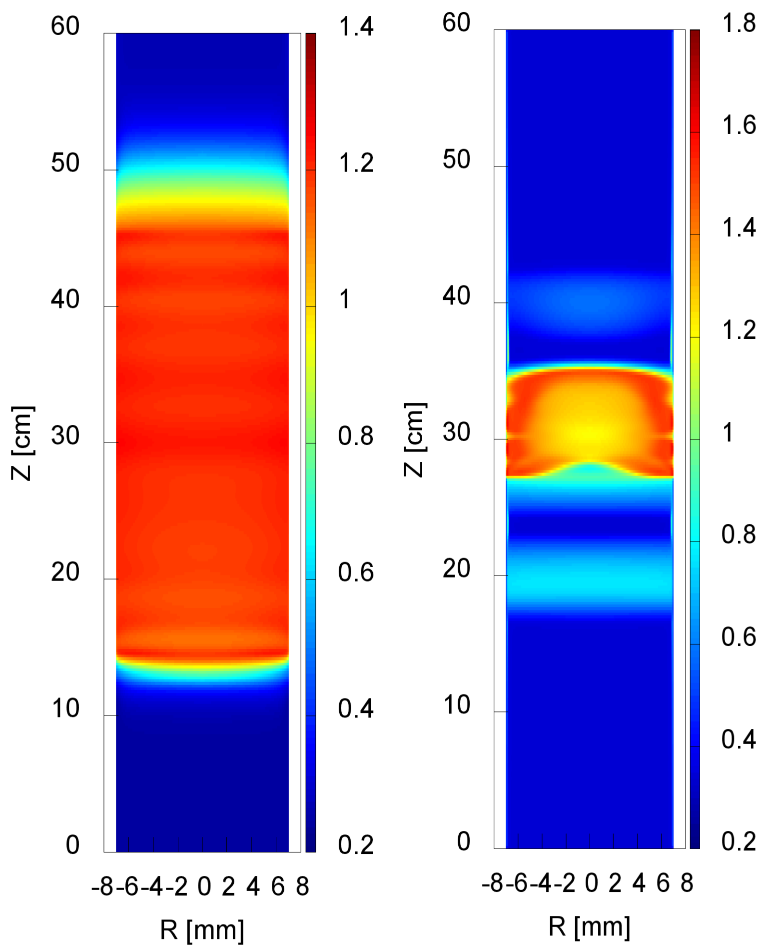
10 mbar

1 bar

- Strong axial contraction
- Different radial profiles
- Lower electron density at higher pressure
- Atmospheric pressure:
  ring-shaped plasma?

Electron temperature (eV)

Conditions: 500 sccm – 100 W deposited power – 2.45 GHz



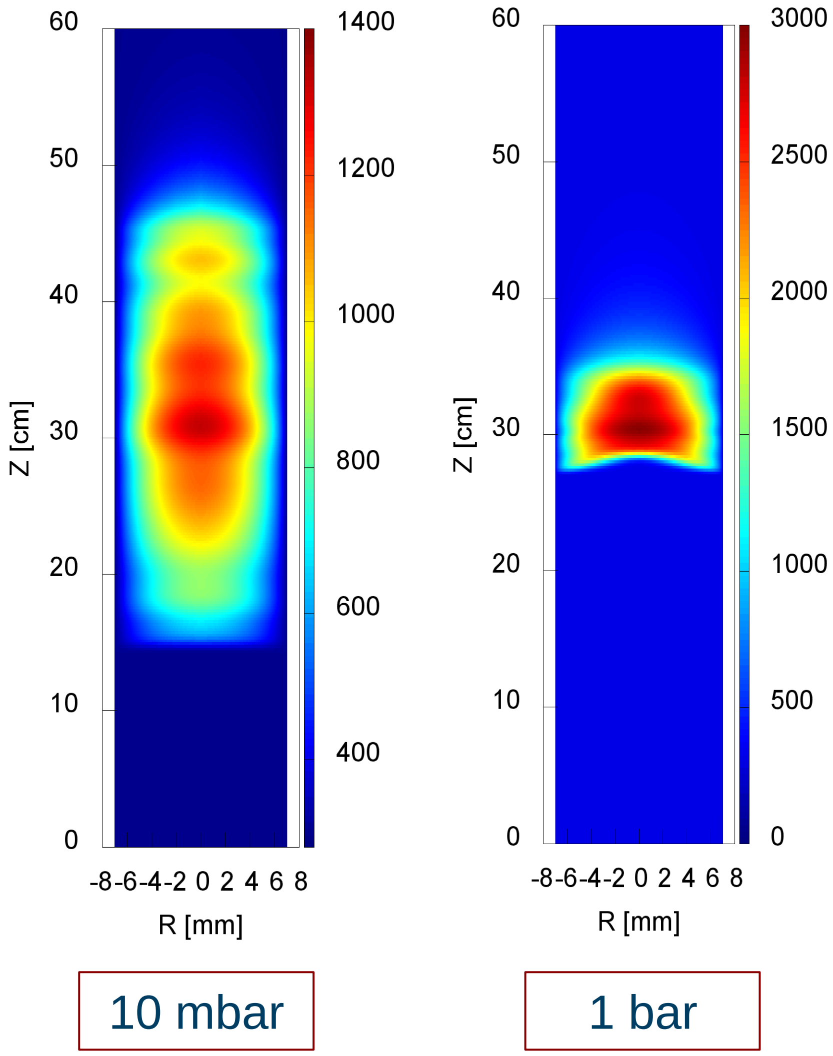
10 mbar

1 bar

- Intermediate pressure: Homogeneous
- Atmospheric pressure: Higher near the sides

Gas temperature (K)

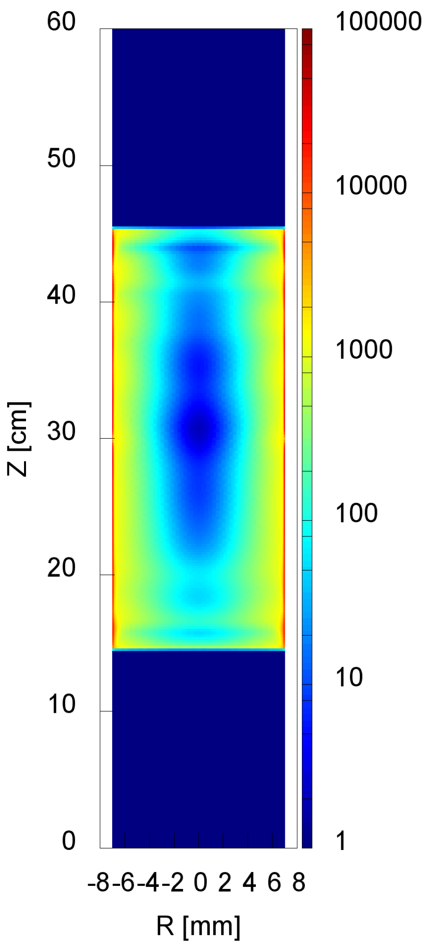
Conditions: 500 sccm – 100 W deposited power – 2.45 GHz



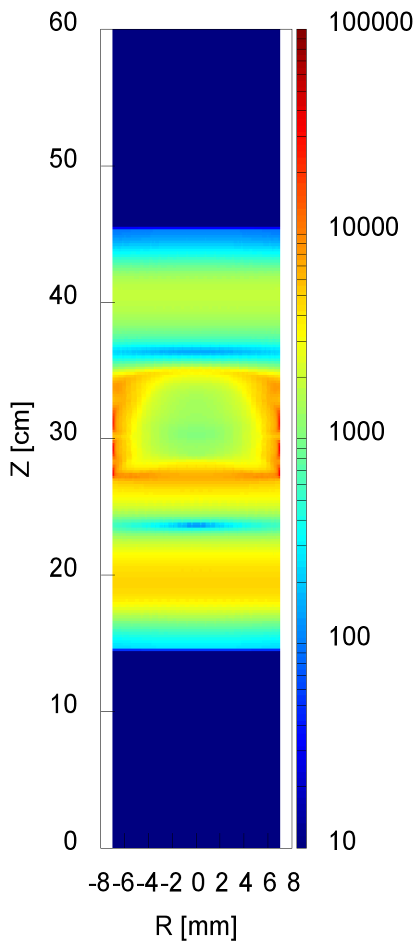
- Higher gas temperature at atmospheric pressure
- Same power applied over a smaller volume

Microwave electric field ($V.m^{-1}$)

Conditions: 500 sccm – 100 W deposited power – 2.45 GHz



10 mbar

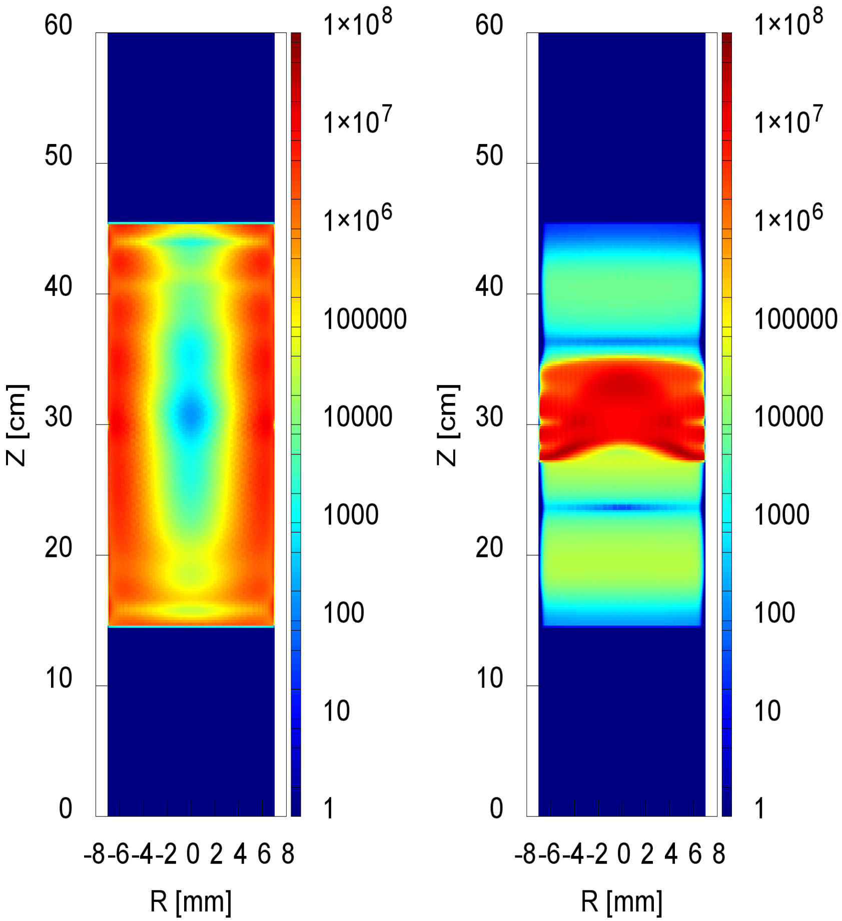


1 bar

- Confinement of the MW
- Skin effect
- The MW penetrates further into the plasma at 1 bar

Microwave Power deposition ($W.m^{-3}$)

Conditions: 500 sccm – 100 W deposited power – 2.45 GHz



10 mbar

1 bar

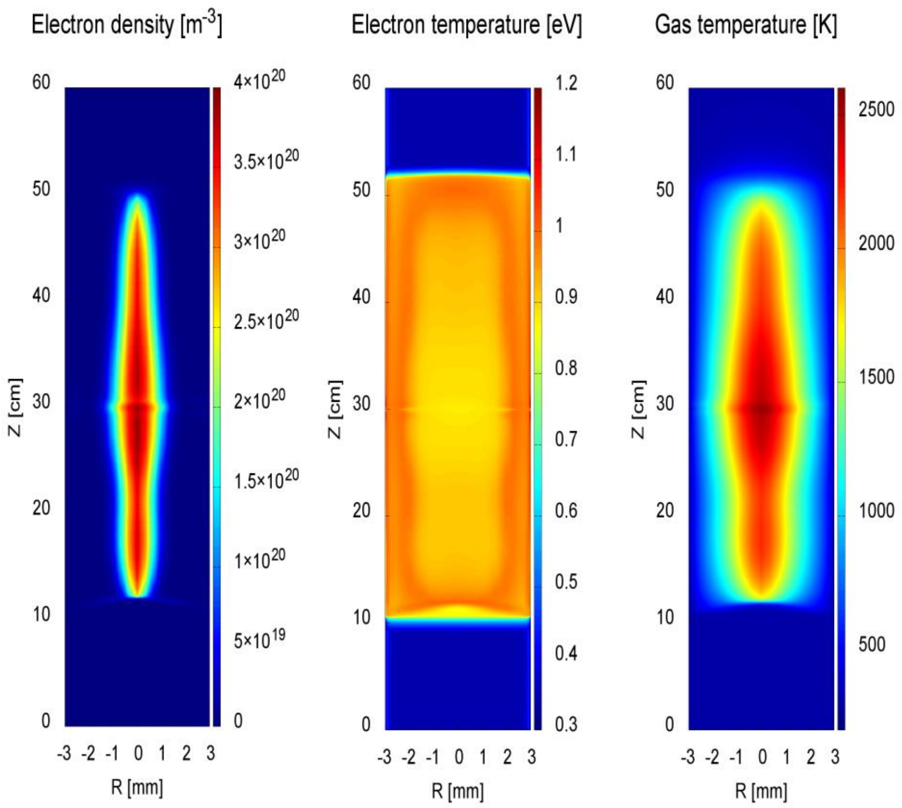
- Intermediate pressure: Power deposition on the edge of the plasma
- Atmospheric pressure: Stronger on the edge of the plasma but penetrates further

Benchmarking

Intermediate pressure

- Trends in good agreement with literature
- Collaboration with ULB and UMons

See:
Violeta Georgieva
TL-22 Thursday afternoon

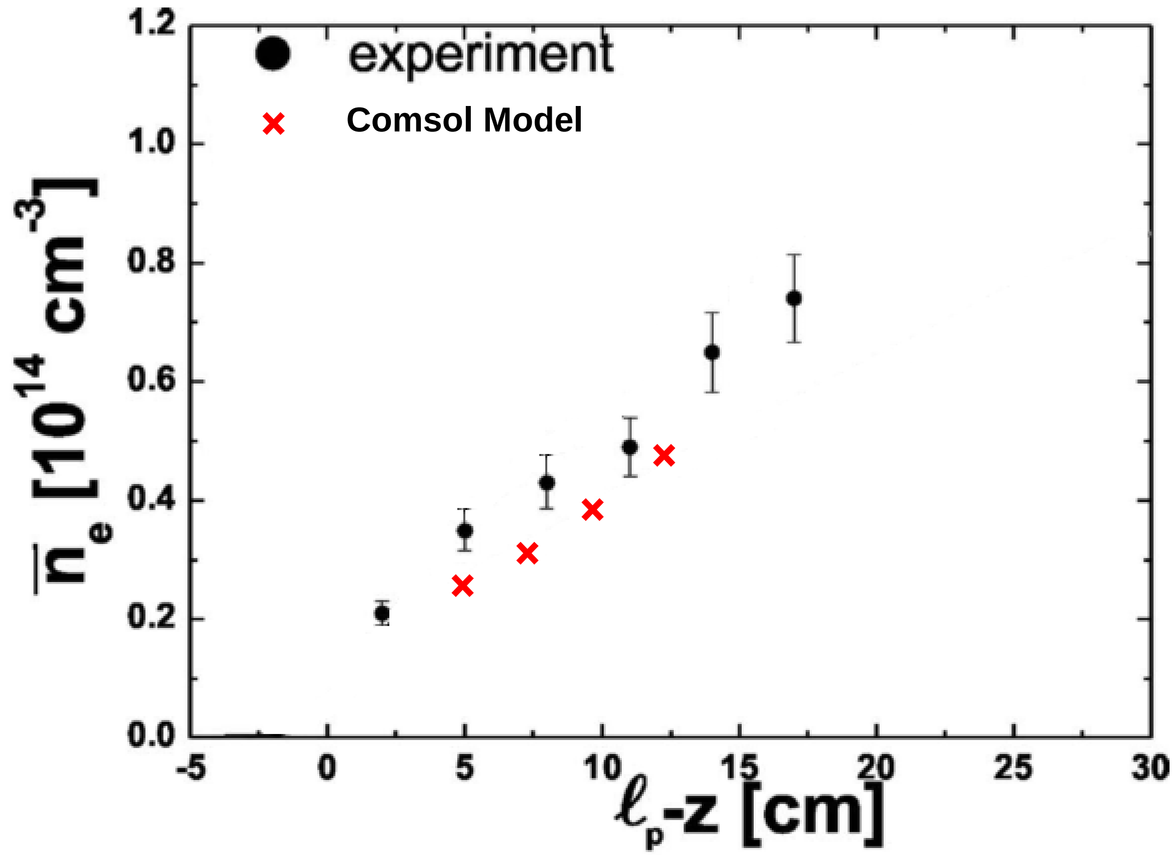


Atmospheric pressure

Conditions: 250 sccm,150W, 915 MHz, 1bar
Different geometry (*Kabouzi et al., Phys Rev. E* ***75****, 2007*)
Inner radius: 3mm

Benchmarking with Kabouzi *et al.*

Conditions : Atmospheric pressure – 250 sccm gas flow
150W deposited power – 915 MHz
Different geometry (Kabouzi *et al.*)



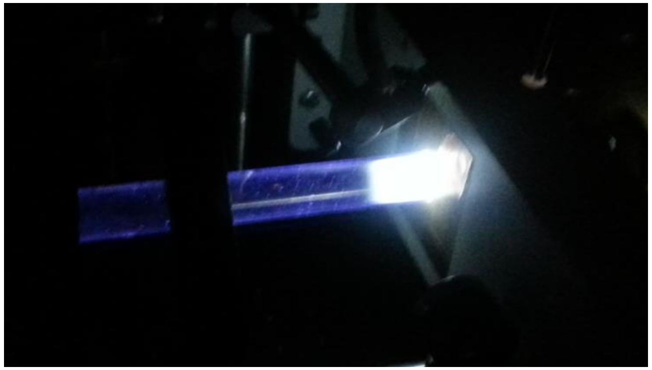
- Radially integrated electron density

CO_2 chemistry reduction

CO_2 conversion → **Good energy efficiency with MW plasmas**

Vibrational excitation: key to efficient dissociation

Modelling: importance of the vibrational distribution function



More information:
Annemie Bogaerts
GL-9 Thursday afternoon

CO_2 chemistry reduction

Argon set

- 7 species
- 31 reactions

➡ **Calculation time: >1day**

Original CO_2 set

- 127 species
- ~10.000 reactions

➡ **Not suitable for 2D-modelling**

➡ **Drastic reduction of the chemistry set required**

0D Model (ZD Plaskin): 4 coupled modules

Boltzmann solver

Species kinetics

$$\frac{dn_i}{dt} = \sum_j \left(a_{ij}^{Right} - a_{ij}^{Left}\right) k_j \prod_m n_m^{Left}$$

Gas heating

$$N\frac{\gamma k}{\gamma - 1}\frac{dT_g}{dt} = P_{e,el} + \sum_j R_j \Delta H_j - P_{ext}$$

$$\frac{d}{dt}\left(\frac{3}{2} n_e k_B T_e\right) = \vec{j}\cdot\vec{E} - \sum_i \frac{3}{2} n_e \nu_{mi}\left(\frac{2m_e}{M_i}\right) k_B \left(T_e - T_i\right) + \sum_l n_e k_l N_l \Delta\varepsilon_l$$

Electron energy

- Remove minor species
- Keep the vibrational distribution of CO_2 unchanged

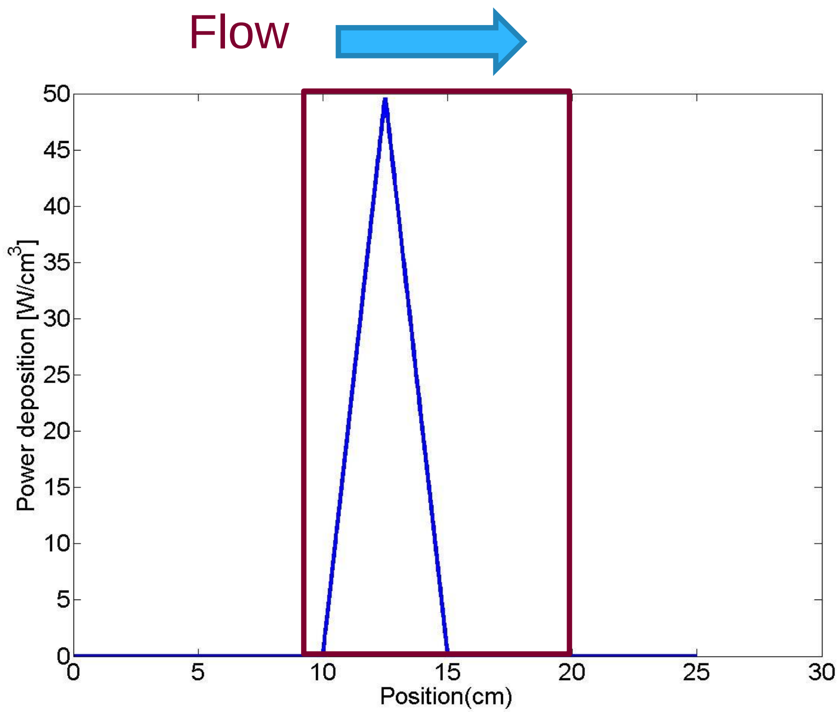
Reduced set

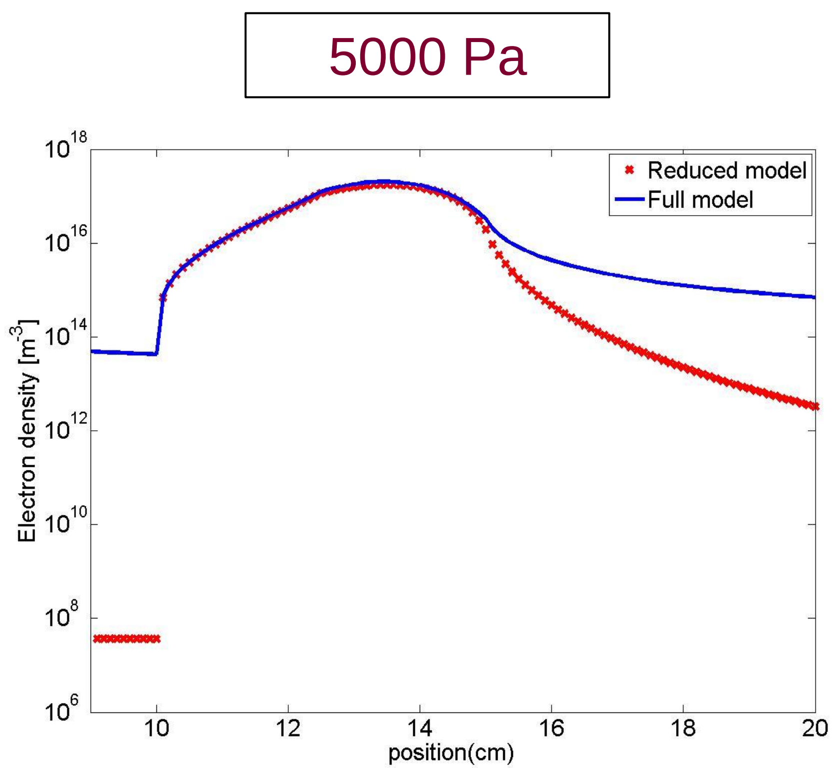
- 35 species
- ~1.000 reactions

Comparison full and reduced models

Test scenarios:

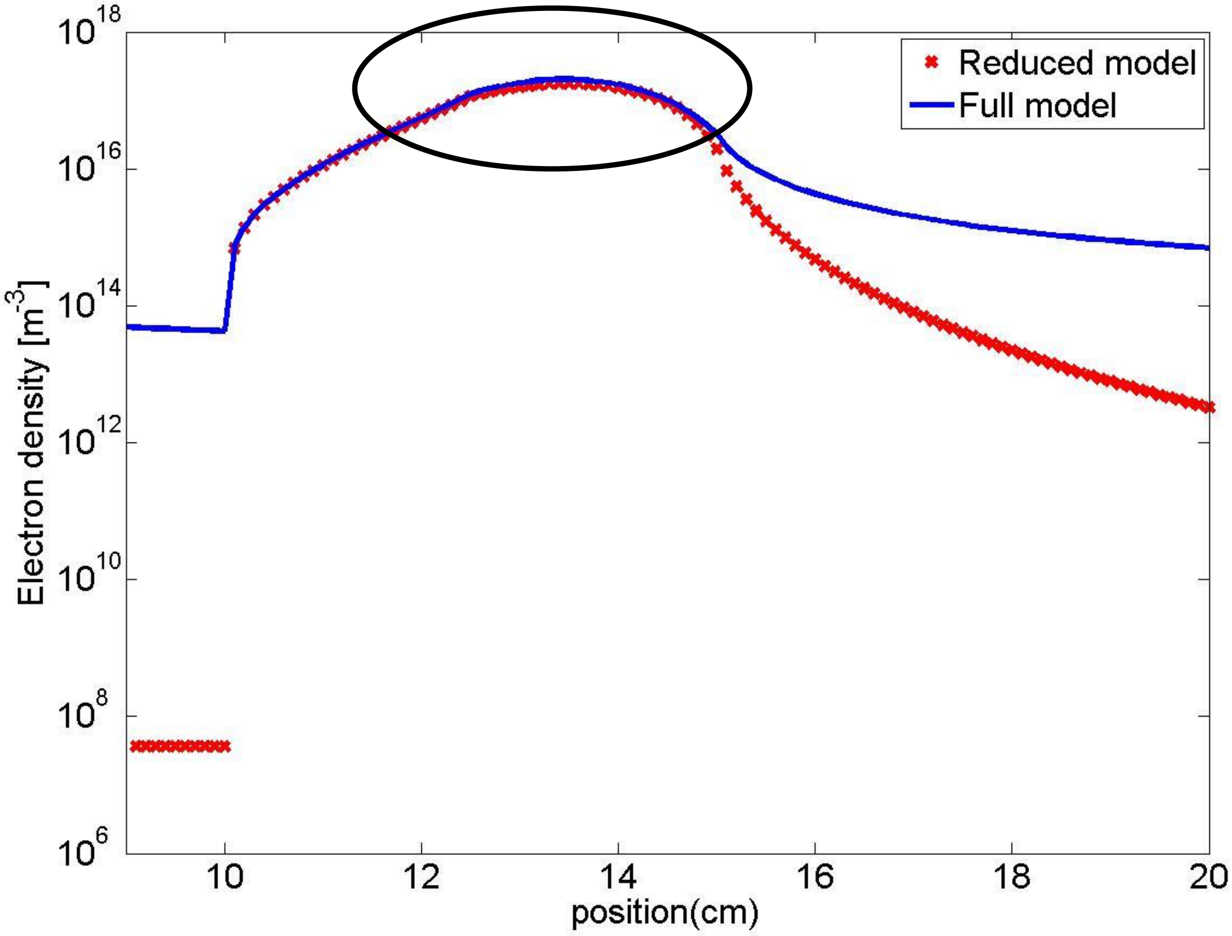
- MW plasma (250 W)
- Power deposition: triangular shape
- 5000 Pa / 50 000 Pa
- Pure CO_2





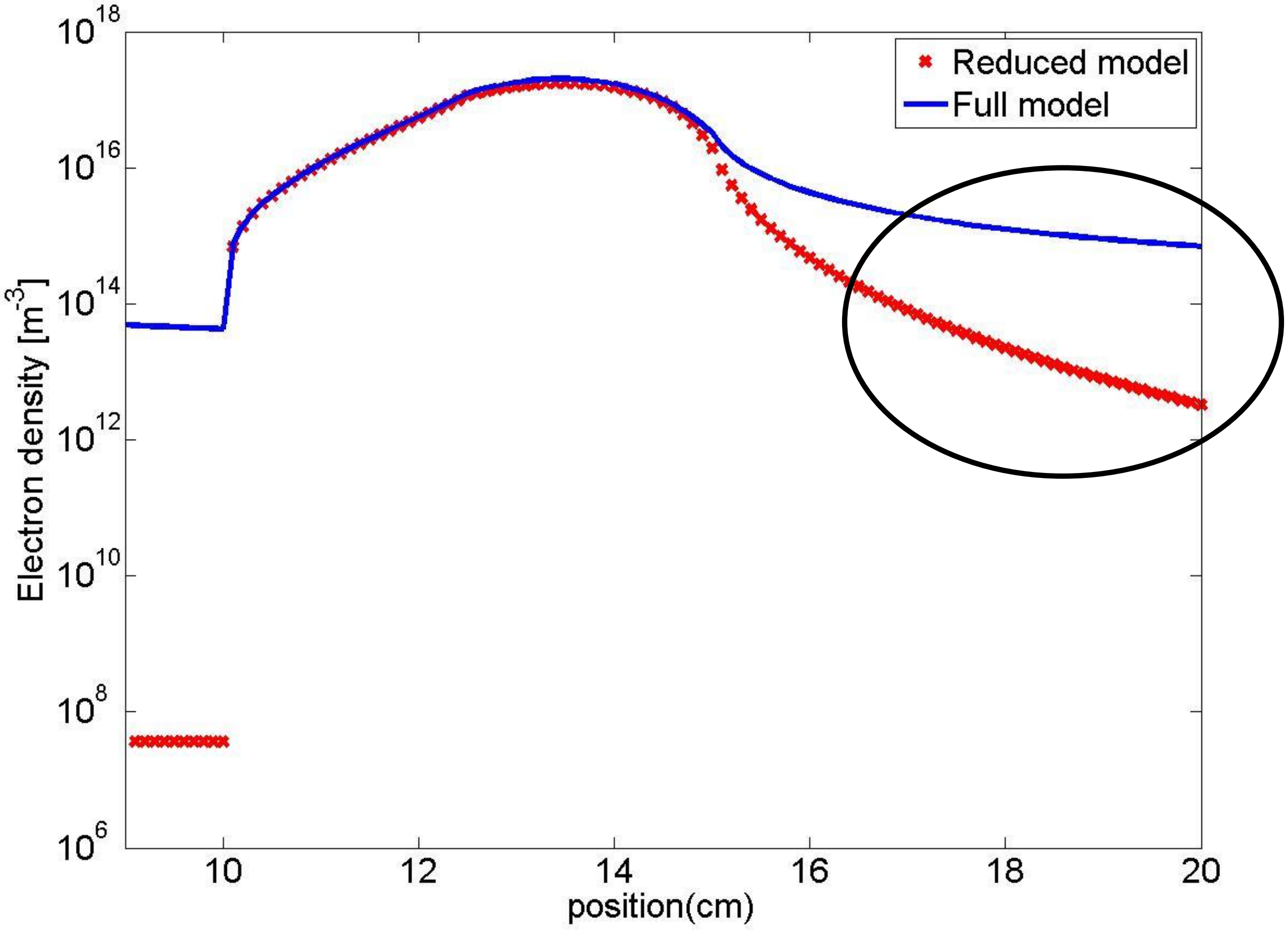
Comparison full and reduced models

Electron density inside the plasma: small deviation (<10%), good agreement



Comparison full and reduced models

Electron density in the post-discharge:
larger deviation, not affecting the results



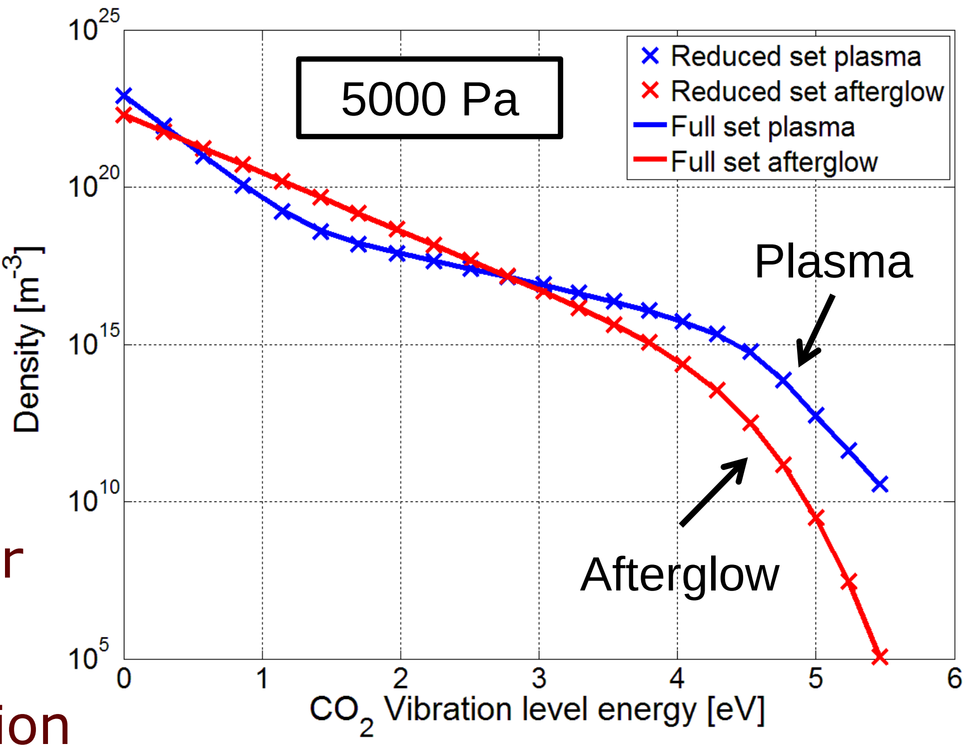
Comparison full and reduced models

Test scenarios:

- MW plasma (250 W)
- 5000 Pa / 50 000 Pa
- Pure CO_2

Reduction:

- Excellent agreement
- Reduced set still too large for 2D-model
- Use of more complex reduction techniques needed



CO produced [10^{21} m^{-3}]	Full set	Reduced set	Difference
5000 Pa	6,73	6,53	3 %
50 000 Pa	0,184	0,182	0,6 %

Comparison full and reduced models

Test scenarios:

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Reduction:

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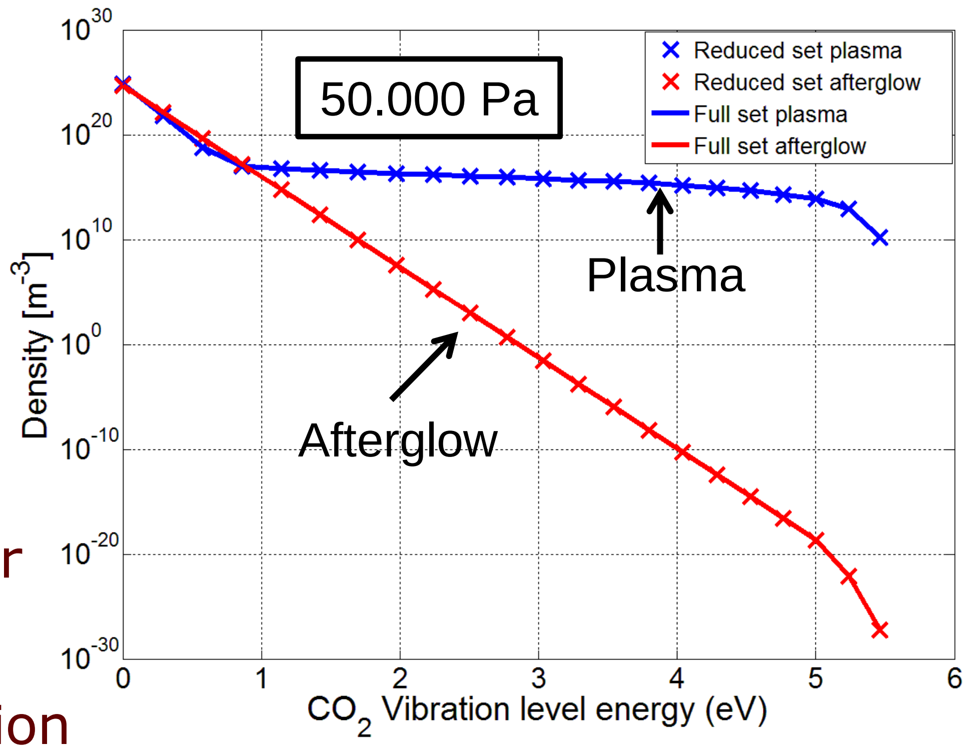

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Conclusions

Argon model

- Results at 1000 Pa and atmospheric pressure
- Contraction of the plasma when increasing the pressure

CO_2 chemistry

- Very good agreement between the full and reduced models
- Small deviation in electron density with little consequence on the vibrational distribution function
- More complex reduction techniques to be used

Thank you for your attention !