Numerical and experimental analysis of microwave micro-plasmas in air

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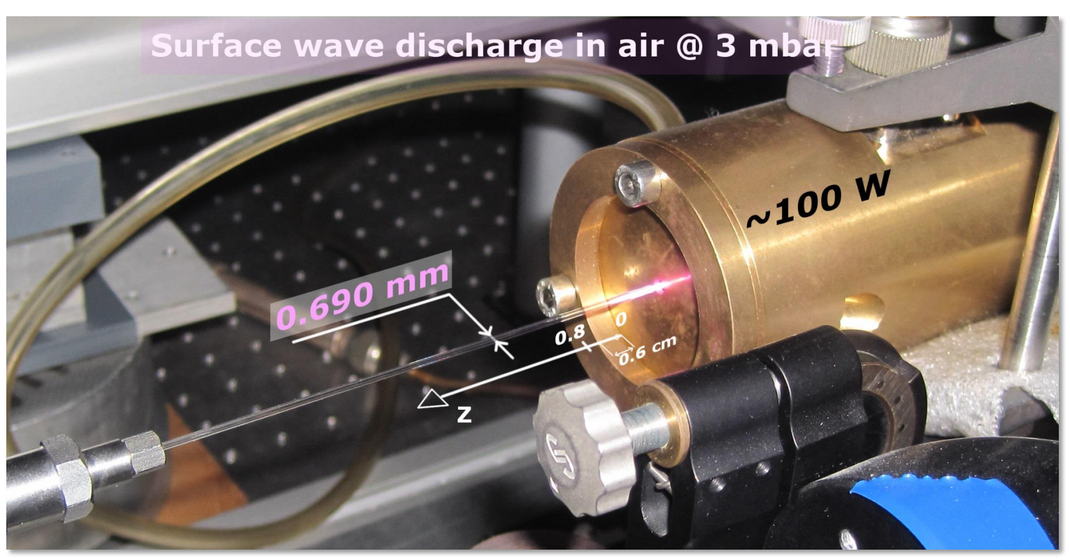
INTRODUCTION

This work uses both simulations and diagnostics to study microwave (***f* = 2.45 GHz)** micro-plasmas in dry air (**N_2 80% : O_2 20%**), confined within a small-radius capillary (***R* = 345 µm**) at low pressure (***p* = 300 Pa**) and low coupled-power (***P* ~100 W).**

Simulations are performed using the LoKI (LisbOn Kinetics) numerical code [1], which couples the homogeneous two-term electron Boltzmann equation to a set of 0D rate balance equations for the main neutral / charged species. A comprehensive kinetic scheme is adopted in the model, considering the different collisional-radiative mechanisms with the complex atomic/molecular gas/plasma system and accounting for the evolution of the mixture composition, due to the dissociation of species at constant pressure. The maintenance reduced electric field is calculated as eigenvalue solution to the problem, so as to satisfy the charged-particle gain-loss rate balance. To meet the challenge of modelling a low-pressure micro-plasma we have adopted corrected transport parameters, valid for *pR* conditions beyond the limit of the classical ambipolar theory.

The plasmas are produced using a surfatron especially adapted to the system dimensions. Axially-resolved OES diagnostics are used to determine the relative intensities of several radiative emissions (and the absolute densities of the corresponding emitting species) [N_2(B,C), N_2^+(B), N* and O*], the electron density n_e, and the gas (rotational) temperature T_g. The spectra are calibrated using a standard tungsten lamp of known spectral radiance. The absolute measurements are performed comparing experimental and synthetic (www.specair-radiation.net) ro-vibrational spectra. The measured quantities are used either as input parameters or for model validation.

[1] V. Guerra and J. Loureiro, Plasma Sources Sci. Technol. **8** (1999) 11



MODEL

Species considered in the model

N_2(X,v=0-60), **N_2**(A, B, C, B', a', a, w, a'')
O_2(X, a, b), **NO**(X, A, B), **NO_2**(X, A), **O_3**, **O_3^***
N(^{4}S, ^{2}D, ^{2}P), **O**(^{3}P, ^{1}D)
N^+,N_2^+(X, B), **N_3^+**, **N_4^+**, **O_2^+**, **O^+**, **NO^+**,**O^-**

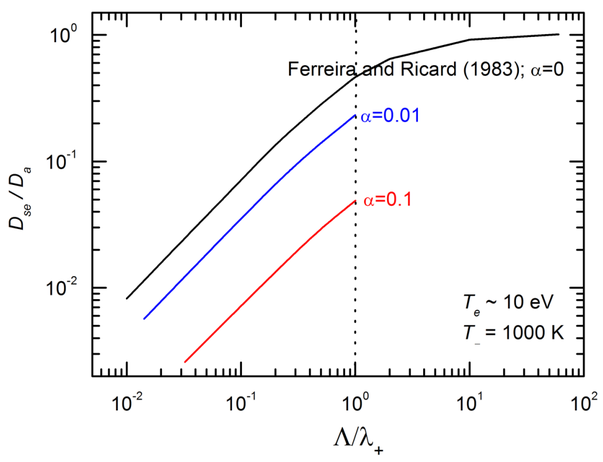
The charged-particle transport description uses an effective diffusion coefficient [2], that bridges the transition from ambipolar to free-fall regimes.

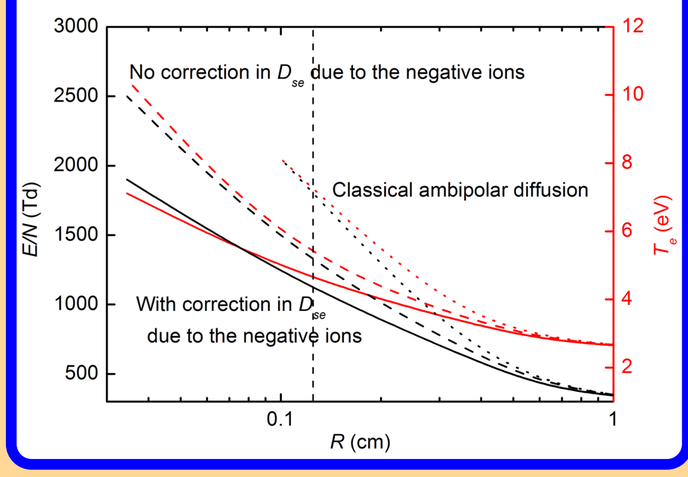
The revised transport theory accounts for multiple positive ions and a single negative ion, with low density and no net flux to the wall.

$$\frac{D_{se}}{D_a} \equiv \left(\frac{D_{se}}{D_a}\right)_{SE} \frac{1+\alpha}{\chi} \quad \text{vs} \quad \frac{\Lambda}{\lambda_+} \equiv \frac{1}{\chi^{1/2}}\left(\frac{\Lambda}{\lambda_+}\right)_{SE}$$

$$\chi \equiv \frac{1+\alpha(T_e/T_-)}{1+\alpha} \qquad \alpha \equiv \frac{n_-}{n_e}$$

[2] Self and Ewald, Phys. Fluids **9**, (1966) 2486





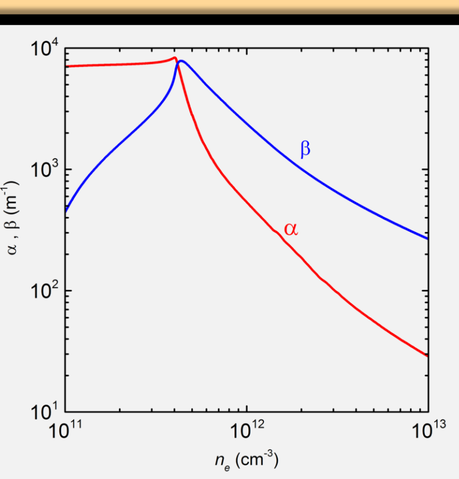
EXPERIMENTS AND SIMULATIONS

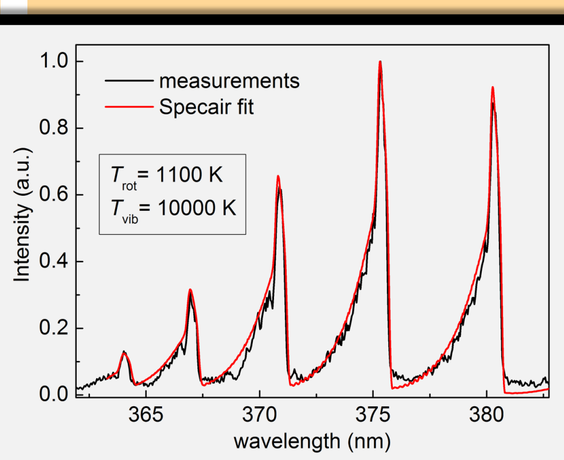
Experimental work conditions

p = 3 mbar R = 0.345 mm T_g ~ 800 K
n_e ~ 10^{12} cm^{-3} P_{coup} ~ 100 W

Second Positive System (SNS)	First Negative System (FNS)
$e + N_2(X) \rightarrow e + N_2(C)$	$e + N_2(X) \rightarrow N_2^+(B) + 2e$
$e + N_2(A) \rightarrow e + N_2(C)$	$N_2^+(B, v) \rightarrow N_2^+(X, v') + h\upsilon$
$N_2(C, v) \rightarrow N_2(B, v') + h\upsilon$	Transport losses

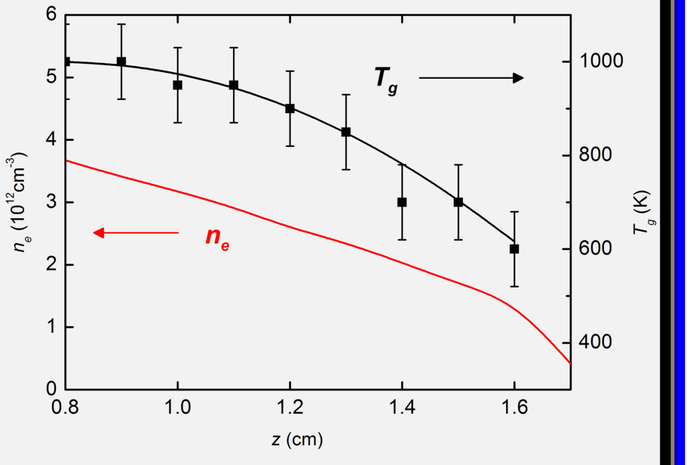
N* triplet	O* triplet
$e + N(2p^4S) \rightarrow N(3p^4S) + e$	$e + O(2p^{4\,3}P) \rightarrow O(3p^5P) + e$
$N(3p^4S) \rightarrow N(3s^4P) + h\upsilon$	$e + O_2(X) \rightarrow e + O(3p^5P) + O$
	$O(3p^5P) + O_2 \rightarrow O + O_2$
	$O(3p^5P) \rightarrow O(3s^5S) + h\upsilon$

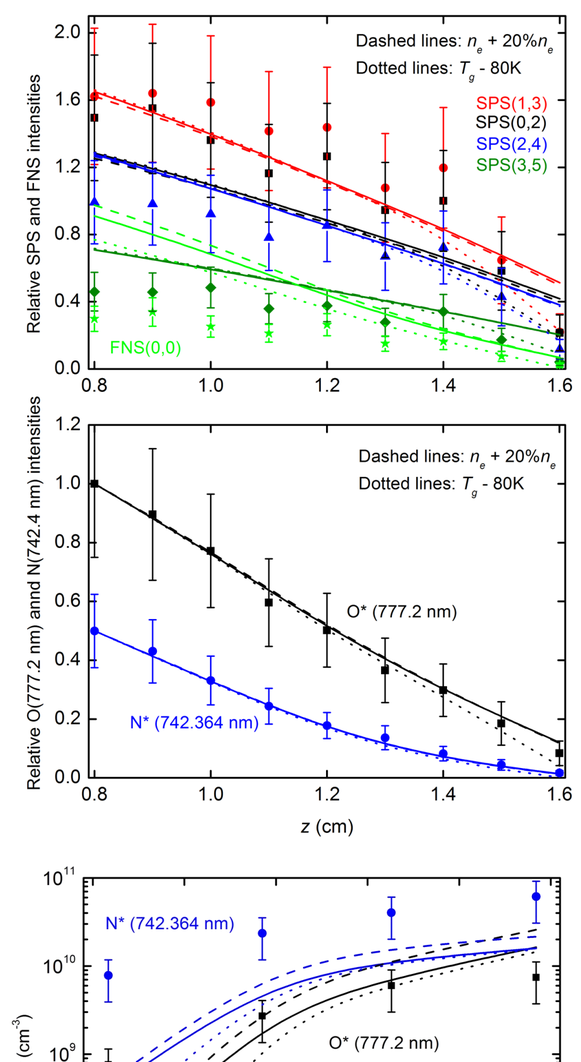


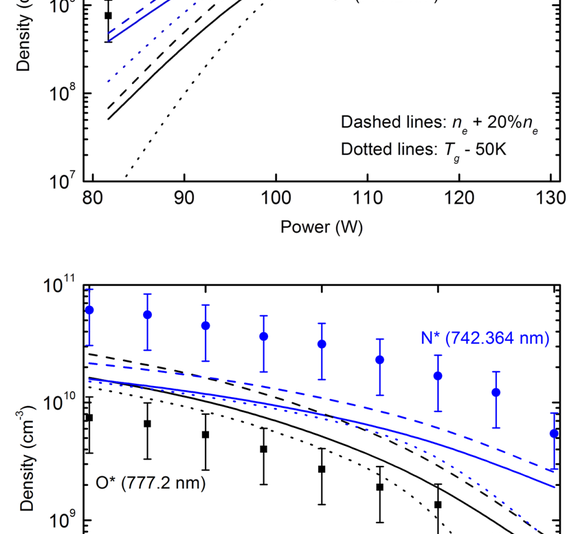


The model uses the electron density n_e and the gas temperature T_g as input parameters. The profiles of these quantities, taken between the first position of light collection for spectroscopic measurements (z = 0.8 cm) and the end of column (z = 0.8 – 1.7 cm, according to the coupled power), are estimated as follows.

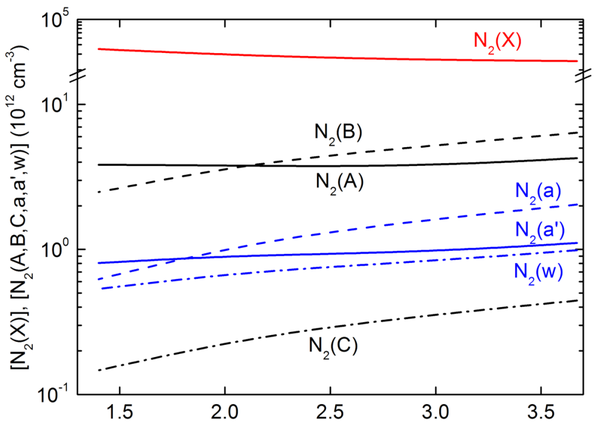
- **The $n_e(z)$ profile** is obtained from a semi-empirical analysis of the power coupled to the plasma, based on the solution to Maxwell's equations for the surface-wave propagative mode considered.
- The on-gap electron densities for different coupled powers are estimated considering the different column lengths recorded.
- Measurements of the electron density, based on the analysis of the H_β Stark broadening (taking into account the contributions of instrumental, van der Waals and Doppler broadening), yield n_e < 1.4x10^{13} cm^{-3}, in agreement with propagative estimations.
- **The $T_g(z)$ profile** is obtained by comparing, at each axial position, the measured band radiative-emission with the second positive system (SPS) $N_2(C \rightarrow B)$ and the corresponding synthetic spectrum generated by Specair software.
- The gas temperature is identified with the rotational temperature, by assuming that the distribution of N_2(C) reflects that of ground-state N_2(X) molecules, corrected by the appropriate Franck-Condon factors.

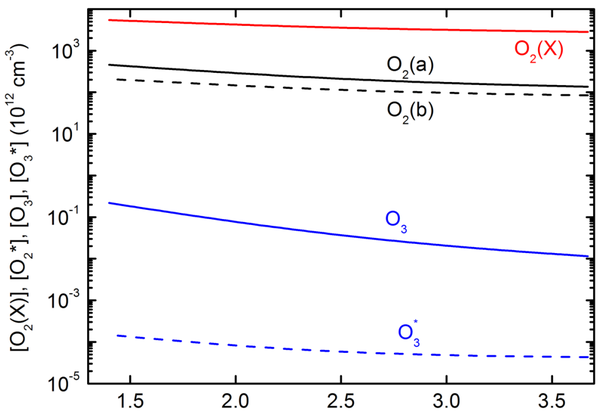


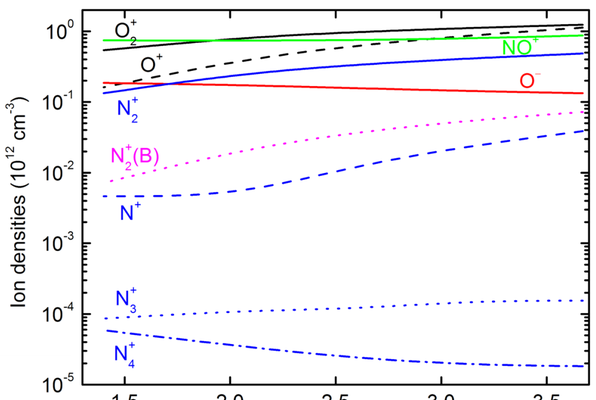


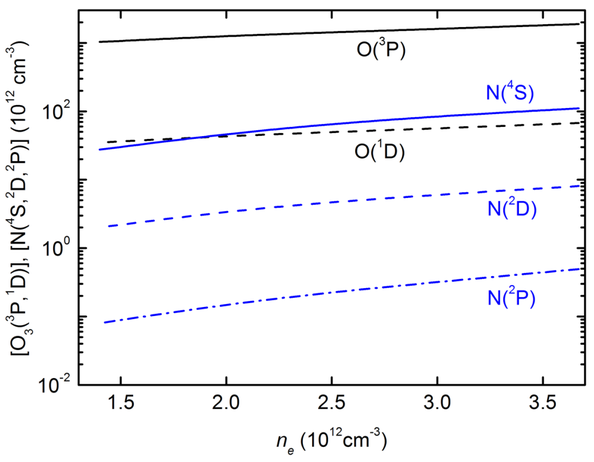


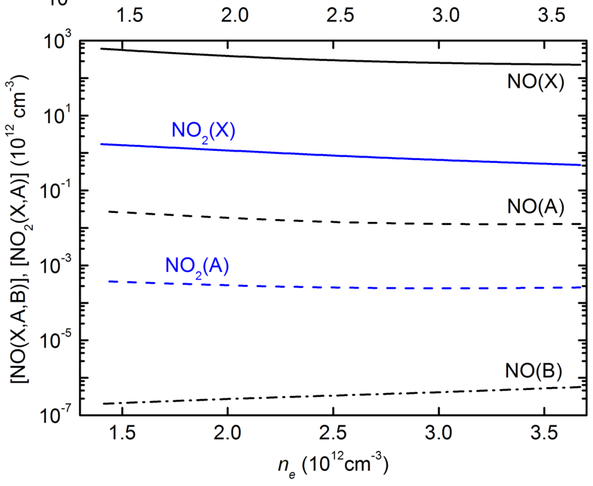
MAIN SIMULATION RESULTS

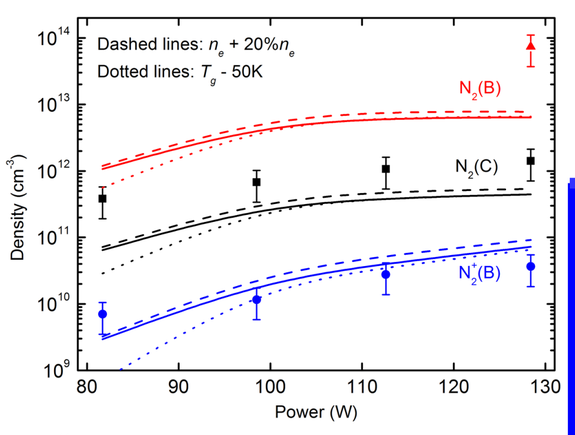


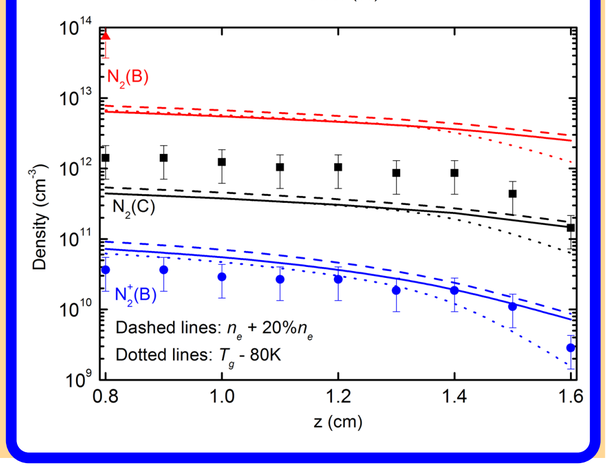












FINAL REMARKS

The charged-particle transport theory, revised to include multiple positive ions and a low-density negative ion, provides a successful description of capillary (R=0.345 mm) air plasmas at low pressure (p=3 mbar). The classical ambipolar diffusion theory fails to describe transport under these discharge conditions.

Model results predict a high dissociation degree of oxygen and negligible ozone production. The final mixture composition is 77%N_2 : 13%O_2 : 9%O : 1%NO

The creation / destruction of species is strongly dominated by electron impact mechanisms, transport losses and wall de-excitation / recombination [$\gamma_{recomb,N} = \gamma_{recomb,O} = 0.1$].

In general, the simulations are in good qualitative agreement with the measurements. The inclusion of a thermal model and of T_g-dependent wall recombination coefficients may improve simulation predictions

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