Simulation of a Non-Thermal Dielectric Barrier Discharge Plasma Reactor for CO_2 Conversion

Non-thermal plasma (NTP) in a dielectric barrier discharge (DBD) for CO_2 conversion is a technology of great interest. In this work, a reactor with argon (Ar) as ionized gas is studied, coupled with previous contributions on thermodynamic / fluid-dynamic behaviors and experimental results.

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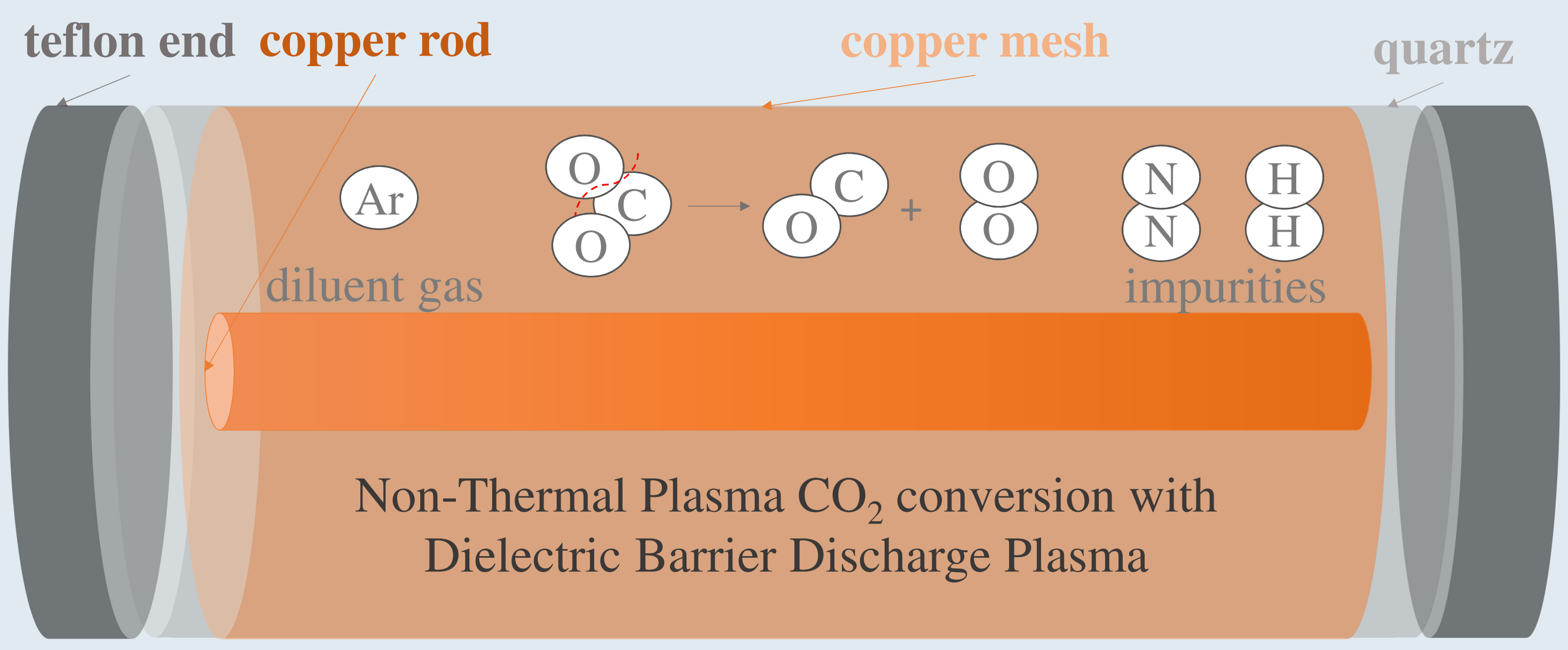
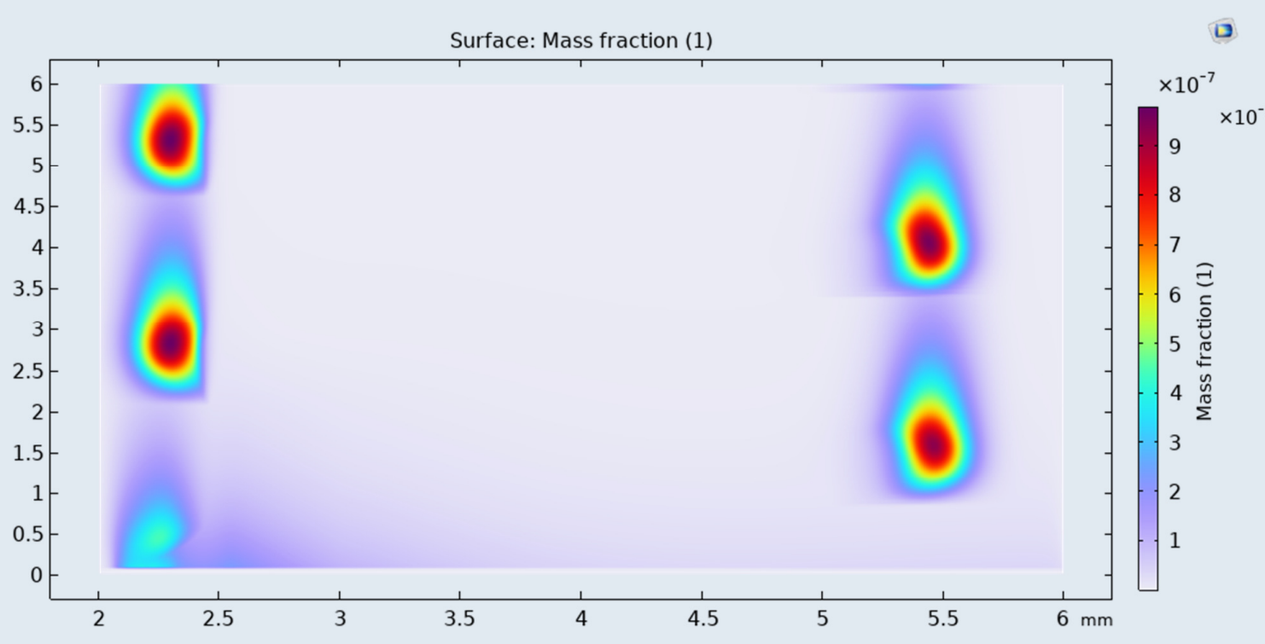
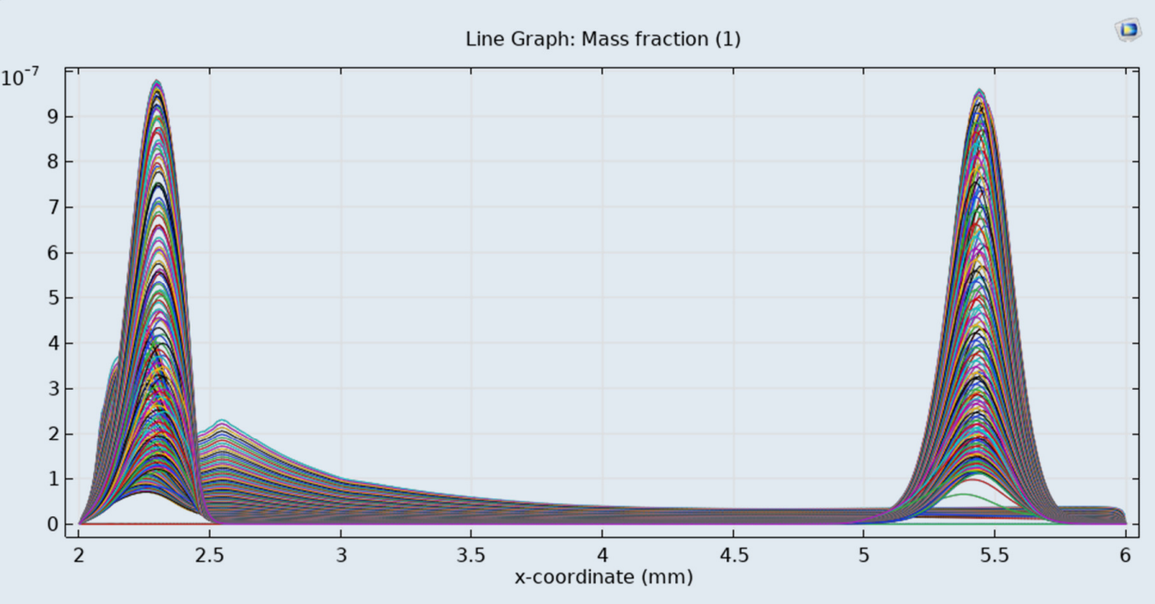






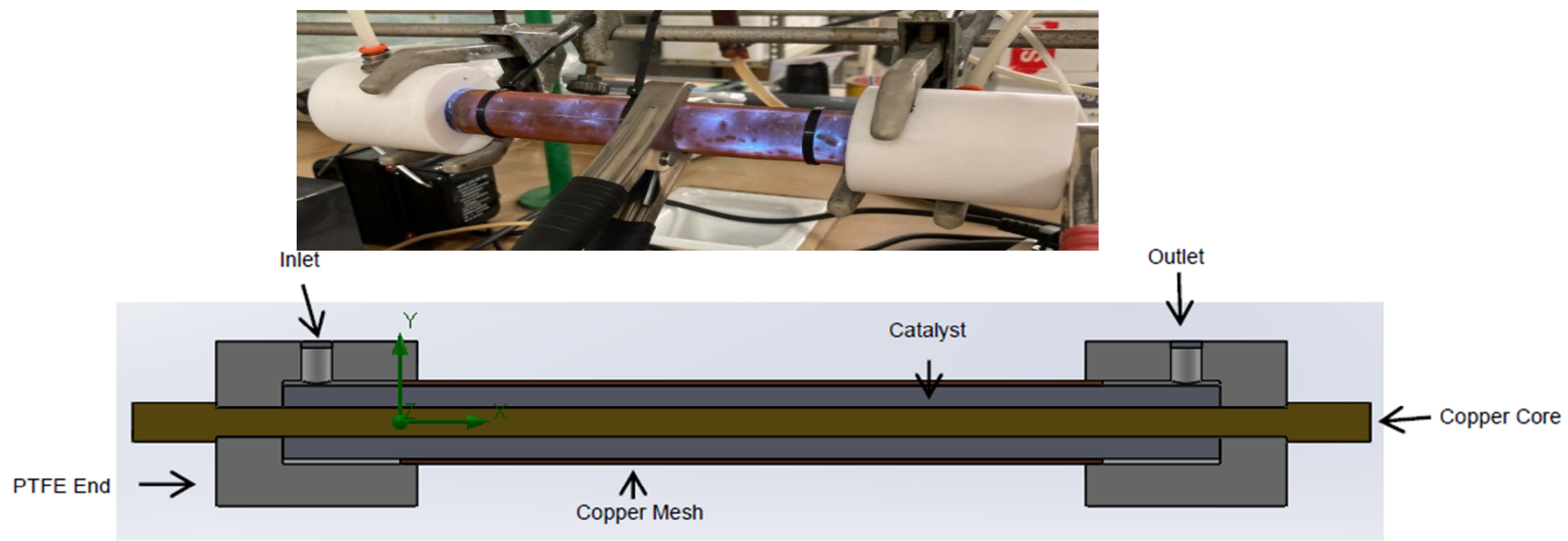
Introduction

Increasing energy demands in society have led to intensive fossil fuel usage, resulting in increasing carbon dioxide (CO_2) emissions. An important technology for CO_2 conversion is non-thermal plasma (NTP).

In this work, an NTP reactor with a dielectric barrier discharge (DBD) with argon (Ar) as diluent gas is studied, coupled with previous contributions tackling thermodynamic / fluid-dynamic behaviors[1] in the reactor and experimental results[2].

The obtained results present a preliminary view of the plasma behavior involving Ar, allowing further reactor optimization to maximize CO conversion with limited computational burden.

Future work of this plasma model could aim at: introducing user-default thermodynamic characterization of involved compounds, modelling a 2D geometry, inserting a Laminar Fluid Flow and providing a comparison to available experimental data.



Main Measurements	Length (mm)	R_{Inlet} (mm)	R_{Core} (mm)	R_{Mesh} (mm)
Reactor	210	4.5	4.5	12.5

FIGURE 1. CO_2 conversion reactor image (experimental data[2]) and Geometry and Dimensions for COMSOL simulation

Methodology

An understanding of the phenomena inside the DBD plasma reactor is obtained with the following assumptions:

1) Reactor as a 1D geometry (coordinates).
2) Dielectric material is specified with relative permittivity of quartz.
3) Input variables: applied frequency, voltage, reactor dimensions, plasma temperature, Ar molecular model, etc.
4) Ar cross-section (imported: Phelps database), and additional reactions and boundary conditions included.
5) Mesh with sufficient element size for Time Dependent Study

Governing Equations: Drift Diffusion, Heavy Species Transport, Poisson's Equation

Results and Discussion

The plasma behavior can be understood with a simplified 1D model using Argon as ionized gas as simulated:

Excited Ar Mass Fraction (Fig. 2**a)**) shows the generation of plasma after the first start-up cycle. The discharge reaches a periodic state solution only after two RF cycles. The plasma is fully formed after the second start-up cycle at the right dielectric barrier.

The Electric Potential (Fig. 2**b)**) and Electric Field (Fig. 2**d)**) indicate a homogeneous behavior across the discharge gap. The Electric Field is of a larger magnitude at the right dielectric barrier.

The Electron Density (Fig. 2**c)**) shows a large initial spike, at the start of the plasma, then reduced to a continuous flow.

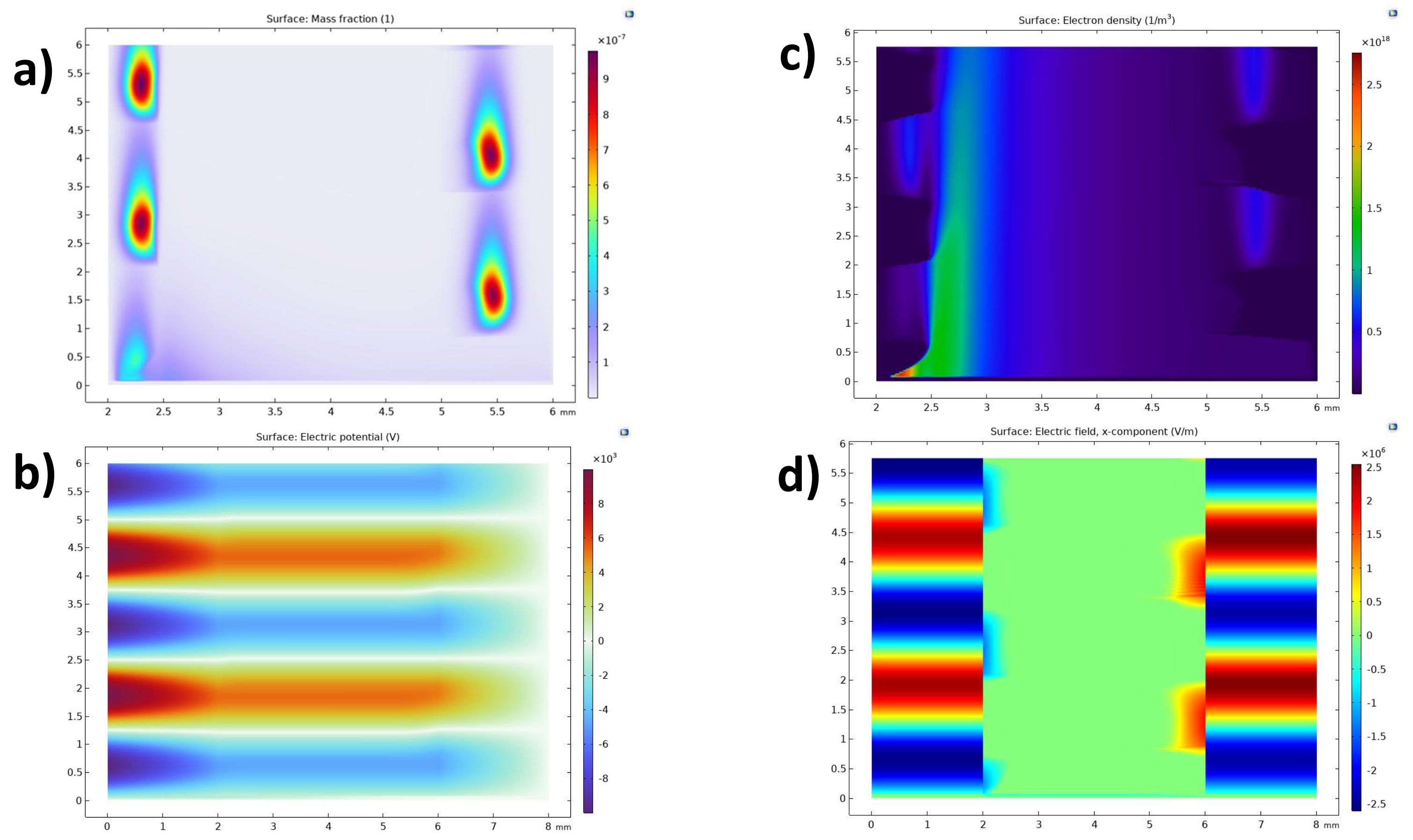


FIGURE 2. Plasma behavior represented as: **a)** Excited Ar Mass Fraction, **b)** Electric potential (V), **c)** Electron density ($1/m^3$), **d)** Electric field (V/m)

REFERENCES

1. C. Mas-Peiro, H. Quinteros-Lama, J. O. Pou, F. Llovell, "Thermodynamic Characterization of Gas Mixtures for Non-Thermal Plasma CO2 Conversion Applications with Soft-SAFT", *Journal of Chemical & Engineering Data,* 68 (6), 1376-1387, 2023

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