Modelling Homogeneous DBD for CO_2 Conversion

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Introduction

Throughout the last century, Carbon Dioxide (CO_2) has been released to the atmosphere in huge quantities. The ability to reuse CO_2 is, therefore, an important goal that humanity should stride towards. One use of CO_2 is the production of Oxygen (O_2) and Carbon Monoxide (CO) through chemical processes such as thermochemical conversion and electrochemical conversion. Although efficient, these processes lack in throughput. Non-equilibrium low-temperature plasmas offer a solution by facilitating chemical dissociation. At Instituto de Plasmas e Fusão Nuclear (IPFN), CO_2 plasma kinetics and conversion at low pressure are well researched, however, such understanding remains poorly developed for atmospheric pressure CO_2 plasmas. In this study, we aim at simulating and understanding homogeneous dielectric barrier discharges for CO_2 conversion at atmospheric pressures similar to the ones presented in [1].

LoKI-1D Fluid Model

A Dielectric Barrier Discharge (DBD) is a discharge between two electrodes with a single or multiple dielectric barriers in between as shown in Figure 1 (a).

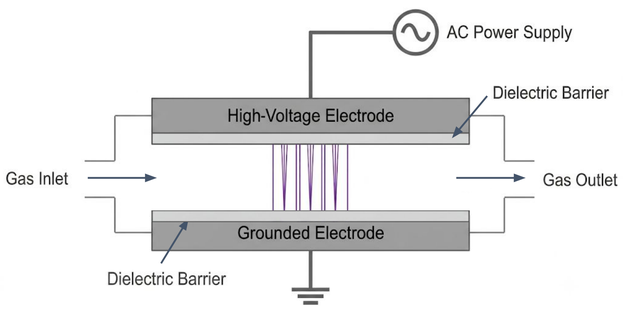

Figure 1: Schematic diagram of a DBD.

$$\frac{\partial n_k}{\partial t} + \nabla \cdot \mathbf{\Gamma}_k = S_k$$

$$\mathbf{\Gamma}_k = \frac{q_k}{|q_k|}\mu_k n_k \mathbf{E} - D_k \nabla n_k$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho$$

To compute the electronic energy, an extra equation is required to be solved. LoKI-B [2] is used to compute the rate coefficients and electrons mobility coefficient.

$$\vec{\Gamma}_k = \frac{1}{4} n_k v_{th,k}$$

$$v_{th,k} = \left(\frac{8 k_B T_k}{\pi m_k}\right)^{1/2}$$

$$\frac{\partial \sigma_s}{\partial t} = j_i + j_e$$

The discharge is captured using a 1D Drift-Diffusion model coupled with the Local Mean Energy Approximation (DD-LMEA). For consistent electric field calculations, poisson's equation is solved at the same time.

$$\frac{\partial n_\varepsilon}{\partial t} + \nabla \cdot \mathbf{\Gamma}_\varepsilon = S_\varepsilon$$

$$S_\varepsilon = -e\mathbf{\Gamma}_e \cdot \mathbf{E} - \frac{3}{2} n_e k_B (T_e - T_g) \frac{2m_e}{m_g} \nu - \sum_i \Delta E_i r_i$$

Thermal flux boundary conditions are used for all particle losses at dielectric boundaries.
To account for charged particle losses at the dielectric boundaries, a surface charge continuity equation is used.

RF - CCP Discharge Benchmark

As a more thorough benchmark, the case 4 RF-CCP discharge described in Turner *et al.* 2013 [4] is simulated as a way to verify the local mean energy approximation (LMEA), secondary electron emission and a varying boundary potential.
Our model's result is similar to previously established fluid models.

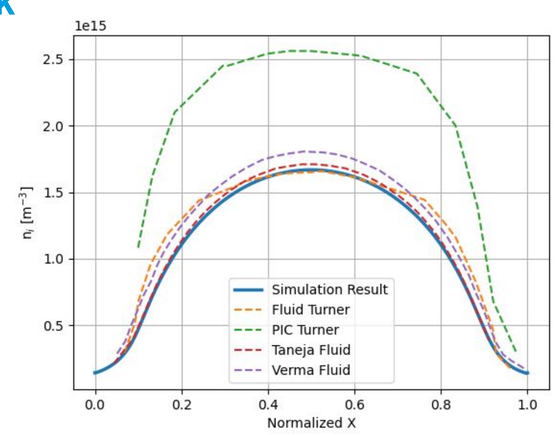

Figure 3: Comparison of the simulated ion density, at t = 0.1 ms between various benchmarks [4-6] and simulated results.

Modelling CO_2 Discharge

Dielectrics: ε_r = 2 / 10, L = 1 mm, 20 cells.
Gas Gap: L = 67 mm and 513 cells.
Discharges: f = 13.56 MHz / 1.00 MHz, 240 V peak-to-peak.
Gas Mixture: 0.98 CO_2, 0.01 CO, 0.01 O_2, P = 133 Pa, Simplified Chemistry.
Time: time-step ~10^{-11}s, T = 0.1 ms.
Numerical Methods: Implicit Poisson, Explicit Continuity, Scharfetter-Gummel Scheme.

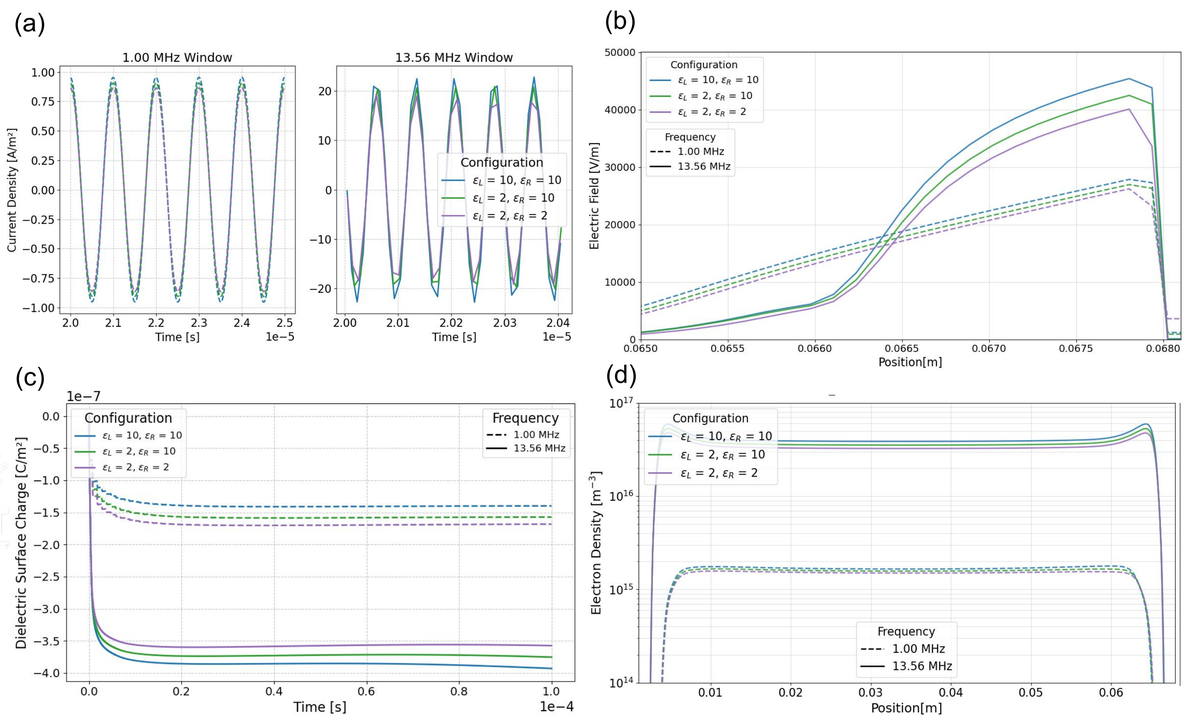

Figure 4(a): Comparison between current densities.
Figure 4(b): Comparison between electric fields at U = 0V;
Figure 4(c): Comparison between right dielectric surface charges.
Figure 4(d): Comparison between electron densities.

Time Integration Methods and Flux Schemes Benchmark

As a first benchmark for the general flux and chemistry solver, the cases presented by Teunissen 2020 [3] are used. A good agreement is found between both various time integration methods as well as various flux schemes.
The small discrepancies seen in both figures 2(a) and 2(b) can be attributed to implementation and numerical errors. In Figure 2(a), The large difference between the fully implicit model and the other schemes is due to the flux scheme used being the Scharfetter-Gummel. This is supported by Figure 2(b) which shows the same discrepancy when compared to other flux schemes.

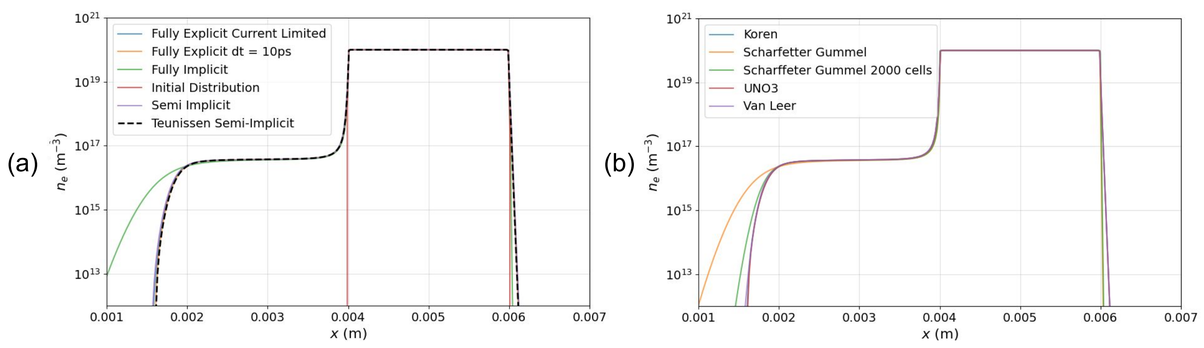

Figure 2(a): Electron density comparison between time integration schemes.
Figure 2(b): Electron density comparison between flux integration schemes.

Conclusions:

- Successfully implementing a 1D Drift-Diffusion model coupled with the Local Mean Energy Approximation (DD-LMEA) and validating it against rigorous standard benchmarks proves the model is accurate and numerically stable.
- The preliminary CO_2 discharge simulation successfully captures the expected transient behavior of a low-pressure AC Dielectric Barrier Discharge. While simplified, this establishes a verified computational framework capable of handling discharge dynamics and surface charge accumulation at dielectric boundaries.

Perspectives:

- The CO_2 reaction scheme used was extremely limited when compared to full reaction schemes, to properly capture all interactions a more complete set of reactions need to be considered.
- The regimes showed were all in low pressure. To study CO_2 for industrial application an atmospheric pressure regime should be simulated and studied.
- Reproduce results presented by Bajon *et al* (2023) [1] which show a diffusive regime for CO_2 at atmospheric pressures. This will help understand CO_2 discharges at atmospheric pressure and the mechanisms behind homogeneous DBDs.

References:

[1] Bajon *et al.* (2023). *Plasma Sources Sci. Technol.* **32** 045012;
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