Development of a 1D fluid model for gas discharge plasmas

A. Filipe, D. Franco, B. Kolling, V. Guerra and P. Viegas

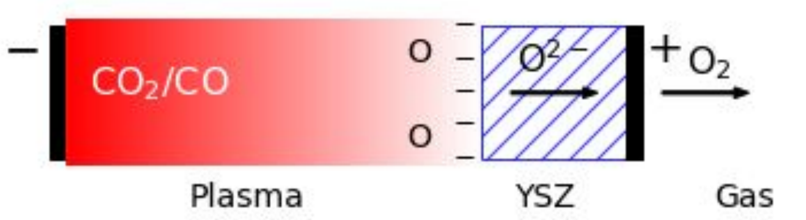
Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal

andre.g.filipe@tecnico.ulisboa.pt diogo.m.lopes.franco@tecnico.ulisboa.pt bianca.kolling@tecnico.ulisboa.pt

Abstract

A new low temperature plasma fluid model is being developed entirely from scratch as part of the PARADiSE project at IPFN, which aims to develop plasma-membrane systems for renewable fuel production. In this model, a fluid description of the plasma is used to simulate both the explicit and implicit time evolution of plasma/gas species. This is achieved by implementing the Full Fluid Moment (FFM) and Drift-Diffusion (DD) models, along with local field approximation (LFA) and local mean energy approximation (LMEA). The main goal of this work, which is still under development, is to give a self-consistent description of the plasma under glow, and "homogeneous" dielectric barrier discharges (DBD) as well as separation membranes that may be coupled to the plasma, providing a full physical picture of such systems.

Introduction: Physical Problem



$$\frac{\partial n_s}{\partial t} + \frac{\partial \Gamma_s}{\partial x} = S_s \quad (1)$$

$$\Gamma_s = \frac{q_s}{|q_s|} n_s \mu_s E - D_s \frac{\partial n_s}{\partial x} \quad (2)$$

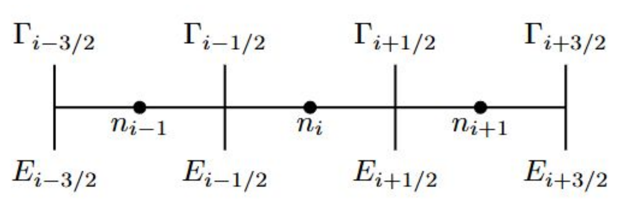
$$\frac{\partial^2 V}{\partial x^2} = -\frac{q}{\varepsilon_0} \cdot (n_i - n_e) \quad (3)$$

1. Continuity Equation 2. Flux Equation 3. Poisson Equation

- In the context of green fuel production, we wish to separate the constituents of a CO2 plasma with a YSZ membrane.
- In order to develop the theoretical model for this problem, we aim to accurately describe the physical picture through a fluid model as follows.

Mathematical Model

- Finite Volume Method (FVM) is used for spatial discretization



$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} n\,dx = n_i\,\Delta x \qquad \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial F}{\partial x}\,dx = F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}$$

- Temporal discretization: $$\int_t^{t+\Delta t} n\,dt = f \cdot n^t + (1-f)\cdot n^{t+\Delta t}$$

➢ f=1 corresponds to the Fully Explicit approach (RK4, RK3 and Trapezoidal)

➢ f=0.5 corresponds to an Explicit-Implicit approach (Crank-Nicolson)

- Explicit schemes have a limited time-step given by:

$$\Delta t_c = \min\left(C_c \frac{\Delta x}{v}\right) ; \ \Delta t_d = \min\left(C_d \frac{(\Delta x)^2}{D}\right)$$

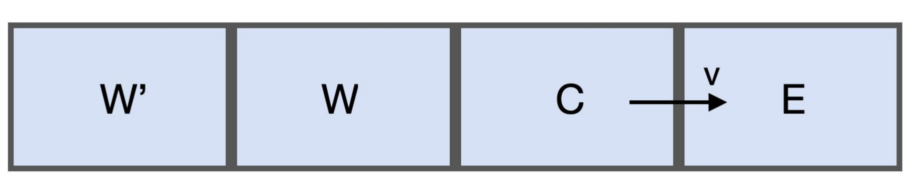
$$\tau = \min\left(\frac{\epsilon_0}{\sigma}\right), \quad \sigma = e\sum_k \mu_k n_k$$

$$\Delta t = \min\left(\Delta t_c,\, \Delta t_d,\, \tau\right)$$

- Larger time steps in the Fully Explicit method are achieved using semi-implicit and current-limited approaches.

Advection Schemes

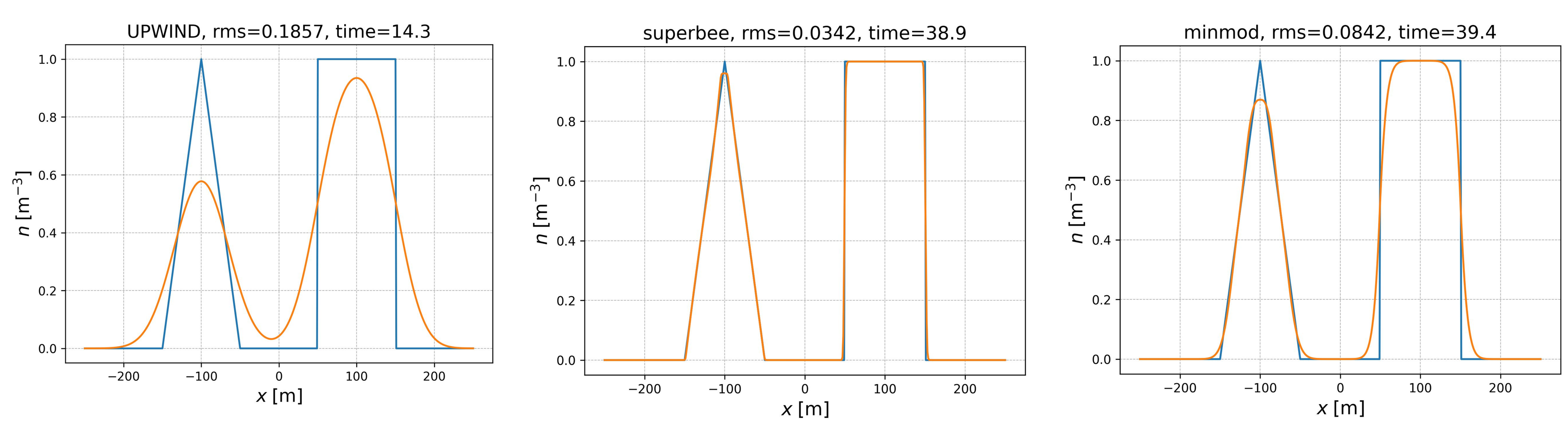
- Important to evaluate the fluxes at cell boundaries



$$\theta = \frac{n_C - n_W}{n_E - n_C}$$

$$F_{i+\frac{1}{2}} = v_{i+\frac{1}{2}}\, n_{i+\frac{1}{2}} - D_{i+\frac{1}{2}} \frac{n_E - n_C}{\Delta x} \qquad n_{i+\frac{1}{2}} = n_C + \frac{\psi(\theta)}{2}\left[1 - \frac{|v_{i+\frac{1}{2}}|\,\Delta x}{\Delta t}\right](n_E - n_C)$$

- Density average shouldn't be used to calculate the values in the walls:
  - Introduces no numerical dissipation - spurious oscillations.
  - No flow direction considered
  - Poor resolution of sharp gradients

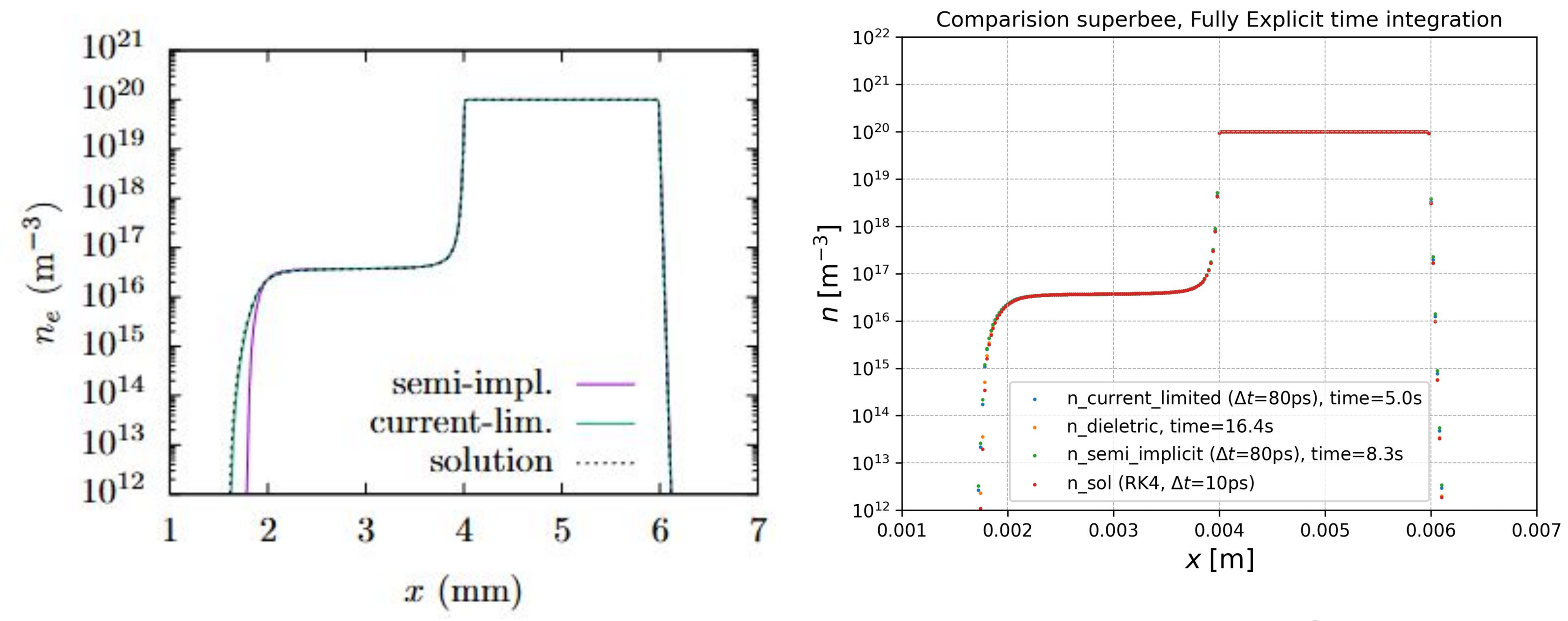


Benchmark: Initial (blue) and final (red) profiles using several advection schemes

	UPWIND	superbee	minmod
$\psi(\theta)$	0	$\max(0, \min(1, 2\theta), \min(2, \theta))$	$\max(0, \min(1, \theta))$

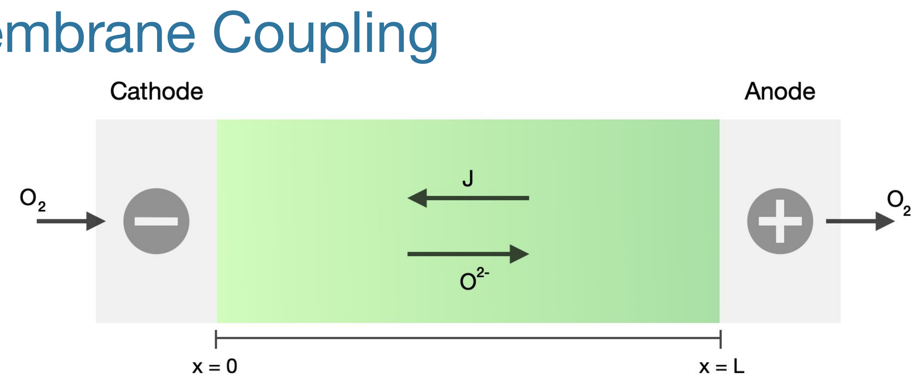
- To find the best scheme, both error and computational cost are considered.

Benchmark



Benchmark: Electric Field and electron density obtained using Poisson and Continuity equations

Membrane Coupling

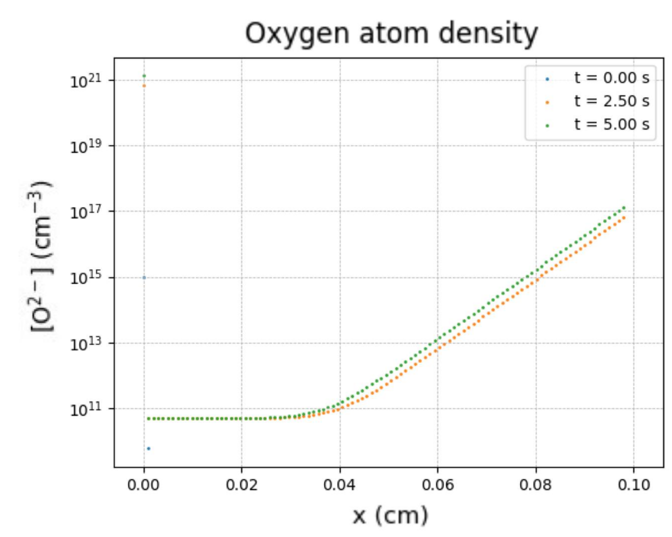


$$\frac{\partial C}{\partial t} + \nabla\cdot\mathbf{F} = 0$$

$$\mathbf{F} = D\left(\nabla C + \frac{ZeC}{k_B T}\nabla\varphi\right)$$

$$\nabla\cdot(\epsilon_r\epsilon_0\nabla\varphi) = -\rho$$

Schematic membrane model and governing equations for membrane diffusion



Membrane diffusion in large time scale fluid model simulation (t =5s)

- We are able to use the fluid model to describe species transport across the membrane, as both systems share the same governing equations (PNP system).

Full Fluid Moment (FFM):

- DD approximation:

➢ Assumes quasi-steady state for flux

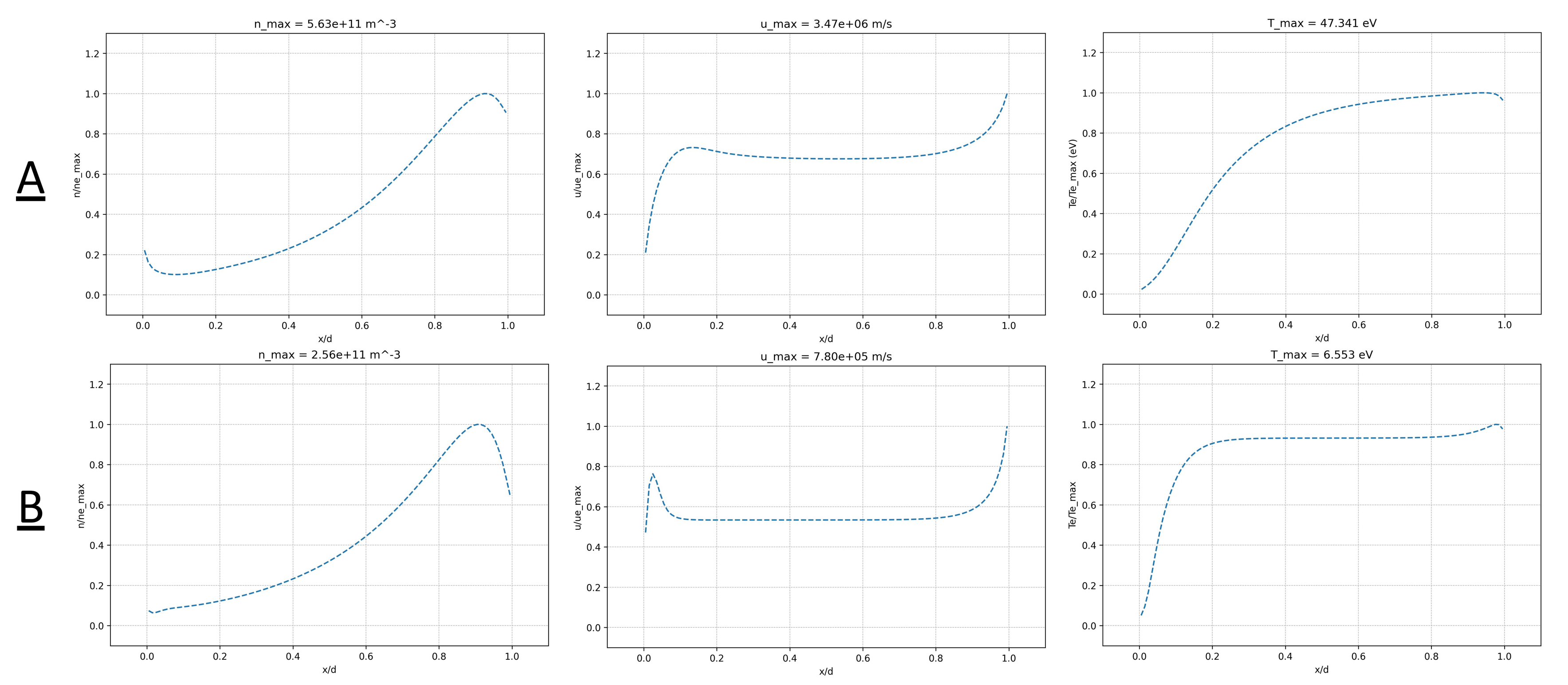
➢ Inertia terms neglected compared to collisional drag

➢ Valid when the bulk velocity is much smaller than the thermal velocity

$$\frac{\partial n_s}{\partial t} + \frac{\partial(n_s u_s)}{\partial x} = S_s,$$

$$\frac{\partial(n_s u_s)}{\partial t} + \frac{\partial}{\partial x}\left(n_s u_s^2 + \frac{p_s}{m_s}\right) = \frac{q_s}{m_s} n_s E + C_{x,s},$$

$$\frac{\partial(n_s \varepsilon_s)}{\partial t} + \frac{\partial}{\partial x}\left[\left(n_s\varepsilon_s + \frac{p_s}{m_s}\right)u_s\right] = \frac{q_s}{m_s} n_s u_s E + C_s$$



Benchmark: Density, velocity and temperature in low (A) and high (B) collisional regimes, using the Full Fluid Moment model, after reaching steady state

- A: Rarefied regime ⟶ low pd. Higher velocity and temperature.
- B: Collisional regime ⟶ high pd. Lower velocity and temperature.

References:

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[2] Viegas, P. (2018). Electric field characterization of atmospheric pressure Helium plasma jets through numerical simulations and comparisons with experiments. Université Paris-Saclay. PhD Thesis. NNT: 2018SACLX061.

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