Modélisation des décharges plasmas froids à basse pression

(Modeling of low pressure plasma discharges)

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Modelling of low-temperature plasmas

- Particles described separately per species
  - Electrons: energy absorption & ionization
  - Ions: influence electron motion, surface treatment
  - Excited neutrals: stepwise ionization, plasma chemistry
  - Gas neutrals

- Classical mechanics
  - Particle approach: Newton’s equations + averaging
  - Macroscopic approach: fluid equations

- Electromagnetic interaction described via Maxwell equations
  - Electron-ion coupling: Poisson equation
  - Applied field: DC, RF, pulsed, microwave

- Collisions treated by input data from experiments & quantum-mechanics
  Cross sections, transport coefficients, rate coefficients
  Mainly with gas
  Many uncertainties / unknowns
Particle approach

- Sample individual particles from total population
- Simulate trajectories
- Take statistical averages

- Newton’s equations of motion:
  \[
  \frac{dk}{dt} = \nu \\
  \frac{dv}{dt} = \frac{q}{m} (E + v \times B)
  \]
  Self-consistent description of plasma fields requires to follow a large number of particles simultaneously, e.g. PIC method
  macroscopic fields due to collective particles (plasma + external)

- Collision sampling from probability distributions (Monte Carlo)
  collision probability per unit time: \( \nu = N \sigma(v_{rel}) v_{rel} \) relative velocity
  target density cross section
Cross sections

Electron-neutral collisions in Argon

Momentum transfer
(isotropic scattering)

Ionization

Excitation

Threshold energy

Electron laboratory energy ≈ relative energy

\[ \varepsilon = \frac{1}{2} m_e v_e^2 \approx \frac{1}{2} m_{rel} v_{rel}^2 \]
Discharge shows instabilities, e.g. transit time oscillations:

Ion energy can exceed applied voltage

(thesis Jerome Barreilles)
Boltzmann equation

- Distribution function $f(t, x, v) = \text{density of particles in phase space}$

- Spatio-temporal evolution of $f$ described by Boltzmann equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{q}{m} (E + v \times B) \cdot \nabla_v f = \mathcal{C}[f]$$

- Simplify by approximations:
  - Homogeneous approach
  - Nonlocal approach
  - Two-term velocity expansion
  - Velocity-moment approach (fluid equations)
  - …
Homogeneous Boltzmann equation

- Electrons in homogeneous field in state steady:
  Spherical harmonics expansion
  \[ f(x, v, t) = f_0(v) + \cos \theta f_1(v) + \ldots \]
  isotropic component
  (= EEDF)
  angle
  anisotropic
  component
  with E

- Two-term homogeneous Boltzmann equation:
  \[
  -\frac{e^2 (E/ N)^2}{3m_e^2} \frac{\partial}{\partial v} \left( \frac{v}{\sigma_m} \frac{\partial f}{\partial v} \right) = C_0 [ f_0 ]
  \]
  \[
  f_i = \frac{e(E/N)}{m_e \sigma_m} v \frac{\partial f}{\partial v}
  \]

- Yields velocity distribution and all velocity-related quantities (EEDF, mean velocity, mean energy, rate coefficients) as a function of reduced field E/N
Homogeneous BE results in Argon

Freeware code BOLSIG+
www.bolsig.laplace.univ-tlse.fr

Non-Maxwellian EEDF!

E/N (Td)

Energy (eV)

Mean energy (eV)

Rate coefficient (m$^3$/s) \[ k = \langle \sigma(v) v \rangle \]

excitation

ionization

$\frac{1}{2} m \langle v^2 \rangle$
Fluid approach

- Macroscopic quantities, averaged over velocity space

  Particle density: \( n(x, t) = \iiint f(x, v, t) dv \)

  Mean velocity: \( \mathbf{w} = \langle \mathbf{v} \rangle = \frac{1}{n} \iiint f dv \)

  Mean energy: \( \varepsilon = \frac{m}{2e} \langle \mathbf{v}^2 \rangle = \frac{m}{2en} \iiint v^2 f dv \)

- Macroscopic transport equations = velocity moments of BE

\[
\iiint \left( \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f \right) v^m dv = \iiint f v^m dv
\]
Fluid equations

- **Continuity equation**: particle conservation

\[ \frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = S \]

- **Momentum equation**:

\[ m \frac{\partial \mathbf{v}}{\partial t} + m \mathbf{v} \cdot (n\mathbf{v} \otimes \mathbf{w}) + \nabla \cdot \mathbf{P} - q \mu E \mathbf{E} + \mathbf{w} \times \mathbf{B} = -m \mathbf{v}_m \mathbf{v} \]

- **Short mean free path**: drift-diffusion approximation:

\[ \text{flux} \quad n\mathbf{v} = \frac{q}{m} \nabla (nT) = \frac{q}{q} \mu n \mathbf{E} - \nabla (Dn) \]

- **Rate coefficient**:

\[ k_i = \langle \sigma_i (\mathbf{v}) \mathbf{v} \rangle \]

- **Inertia**

- **Pressure tensor**:

\[ \mathbf{P} = m f (\mathbf{v} - \mathbf{w}) \otimes (\mathbf{v} - \mathbf{w}) f \mathbf{v} \]

- **Source**

- **Mobility**

- **Flux**

- **Source**

- **Rate coefficient**

- **Pressure tensor**

- **Momentum transfer frequency**

- **Collisions**

- **Frequency**

- **Inertia**
Minimal self-consistent model (high pressure)

- Electron & ion continuity:
  \[
  \frac{\partial n_e}{\partial t} + \nabla \cdot (n_e w_e) = K N n_e \\
  \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i w_i) = K N n_e
  \]

- Electron & ion drift-diffusion:
  \[
  n_e w_e = -\mu_e n_e E - D_e \nabla n_e \\
  n_i w_i = \mu_i n_i E - D_i \nabla n_i
  \]

- Poisson (ambipolar + applied field):
  \[
  \varepsilon_0 \nabla \cdot E = -\varepsilon_0 \nabla^2 \Phi = e \eta - e \eta \\
  E = -\nabla \Phi
  \]

- Local field approximation: transport coefficients and ionization rate are functions of reduced field E/N (from experiments are homogeneous BE)

- Boundary conditions for the particle fluxes
Boundary conditions

- Particle flux toward the wall
  \[ n_{w \perp} = n_{w} - \Gamma_w \]
  - net flux

- Effective velocity of incident particles obtained from kinetic considerations
  \[ w_w = \frac{1}{4} \sqrt{\frac{8 e T}{\pi m}} + \max (\text{sgn}(q \mu E_{\perp}, 0)) \]
  - effective velocity

- Flux coming from the wall obtained from incident fluxes
  \[ \Gamma_w = \sum_{s} \gamma_s n_s w_{w,s} \]
  - sum over all species

- Equating to drift-diffusion → mixed boundary condition, e.g.
  \[ (\text{sgn}(q \mu E_{\perp} - w_w) n - \nabla_{\perp} n + \Gamma_w = 0) \]
Numerics

- Integrate equations sequentially in time: \( t^{k+1} = t^k + \Delta t \)

- Implicit update of drift-diffusion flux:
  \[
  \frac{n^{k+1} - n^k}{\Delta t} + \nabla \cdot \left( \pm \mu E n^{k+1} - D \nabla n^{k+1} \right) = S
  \]

  No CFL time step constraints: \( \Delta t < \left( \frac{W}{\Delta x} + \frac{2D}{\Delta x^2} \right)^{-1} \)

- Exponential scheme for drift-diffusion flux:
  \[
  \left( W_0 - D \frac{\partial n}{\partial x} \right)_{i+1/2} = \frac{W_{i+1/2}}{1 - \exp(-z)} n_i + \frac{W_{i+1/2}}{1 - \exp(z)} n_{i+1}
  \]
  \[
  z = \frac{W_{i+1/2} \Delta x}{D_{i+1/2}} = \frac{\pm \mu E_{i+1/2} \Delta x}{D_{i+1/2}}
  \]

  For electrons in ambipolar sheath:
  drift \( \approx \) diffusion \( \Rightarrow \) Boltzmann relation:
  \[
  \frac{n_{i+1}}{n_i} = \exp(z) \approx \exp\left( \frac{\Phi_{i+1} - \Phi_i}{T} \right)
  \]
Semi-implicit Poisson method

- Charged particle transport strongly coupled with Poisson equation:

\[ \nabla^2 \Phi^{k+1} = \frac{e}{\varepsilon_0} (n_e - n_i) \]

\[ \frac{n_e^{k+1} - n_e^k}{\Delta t} + \nabla \cdot (\mp \mu n_e^{k+1} \nabla \Phi^{k+1} - D \nabla n_e^{k+1}) = S \]

Coupling time constant (Maxwell relaxation time)
\[ \tau_d = \frac{\varepsilon_0}{e(\mu_e n_e + \mu_i n_i)} \equiv \frac{\varepsilon_0}{\mu_e n_e} \]

- Avoid time step constraint \( \Delta t < \tau_d \) by space charge prediction:

\[ \nabla^2 \Phi^{k+1} = \frac{e}{\varepsilon_0} (\tilde{n}_e^{k+1} - \tilde{n}_i^{k+1}) \]

\[ \tilde{n}_e^{k+1} = n_e^k + \Delta t \left( S - \nabla \cdot (\mp \mu n_e^k \nabla \Phi^{k+1} - D \nabla n_e^k) \right) \]

Modified Poisson equation:
\[ \nabla \cdot \left( (1 + \chi) \nabla \Phi^{k+1} \right) = \nabla \cdot \left( \chi \nabla \Phi^k \right) + \frac{e}{\varepsilon_0} \left( 2 n_e^k - n_e^{k-1} - 2 n_i^k + n_i^{k-1} \right) \]

Semi-implicit susceptibility:
\[ \chi = \frac{e \Delta t}{\varepsilon_0 (\mu_e n_e + \mu_i n_i)} = \frac{\Delta t}{\tau_d} \]

Semi-implicit terms cancel in steady state!
Microdischarges for display technology

Plasma Adressed Liquid Crystal

Plasma Display Panel (PDP)
(Philips Aachen 1998-2001)
Coplanar PDP simulation

Electric potential

Field screened by surface charges from previous discharge

Polarity change creates new discharge

UV emission rate

Discharge stopped by surface charges
Low pressure

Compare mean free path with macroscopic length scales (plasma size etc)

Mfp inversely proportional to pressure

Electron energy-transfer less efficient than momentum-transfer
Electron energy equation

- Long energy-transfer mean-free-path: local field approximation not valid
  \[ E/N \rightarrow f_0, \varepsilon, \mu_e, D_e, K \]

- Solve mean energy from energy equation:
  \[
  \frac{\partial n_e \bar{e}}{\partial t} + \frac{5}{3} \nabla \cdot \left( n_e w_e \bar{e} - n_e D_e \nabla \bar{e} \right) = -en_e w_e \cdot E + P_{\text{ext}} - n_e N_k
  \]
  thermal conduction
  work of electrostatic field
  inductive / MW power
  collisional losses

- Parametrise electron transport coefficients & rates as a function of electron mean energy
  \[ \bar{e} \rightarrow \mu_e, D_e, K, \kappa \]

- Maxwellian EEDF:
  \[ \bar{e} = \frac{3}{2} T_e \]
  \[ D_e = \mu_e T_e \]
  Einstein relation
Momentum equation

- Long momentum-transfer mean-free-path: drift-diffusion not valid, reconsider momentum equation:

\[ m \frac{\partial (nw)}{\partial t} + \nabla \cdot (nw \otimes w) + \nabla \cdot P - q \mathbf{n}(E + w \times B) = - \bar{m}_m nw \]

- Electrons: isotropic due to ambipolar trapping → neglect \( w \) terms

  Boltzmann equilibrium: \( T_e \nabla n_e \approx -e n_e E \) → \( n_e = n_0 \exp \left( \frac{\Phi - \Phi_0}{T_e} \right) \)

  Drift-diffusion equilibrium: \( D_e \nabla n_e = -\mu_e n_e E \) Boltzmann relation

- Ions: very anisotropic → neglect pressure ( & substitute continuity equation)

\[ \frac{\partial w_i}{\partial t} + (w_i \cdot \nabla) w_i + \left( \bar{\nu}_i + \frac{S_i}{n_i} \right) w_i = \frac{e}{m_i} E \]

If \( w // E \):

\[ \nabla \left( \frac{1}{2} m_i w_i^2 + eB \right) + \left( \bar{\nu}_i + \frac{S_i}{n_i} \right) m_i w_i = 0 \]
Low pressure ambipolar plasma transport

Self-consistent description of sheath & presheath: Poisson equation

Example without magnetic field:

\[ \Phi_p \approx T_e \left( 1 + \frac{1}{2} \ln \left( \frac{m}{2\pi m_e} \right) \right) \approx 4T_e \]
Dense plasmas: quasineutral approach

- Compare sheath size (Debye length) with plasma size: \[ \lambda_D = \sqrt{\frac{\varepsilon_0 T_e}{en_e}} \]

- Thin sheath \( \rightarrow \) eliminate Poisson’s equation using quasineutrality:

  Solve electric field from electron conservation / current conservation:

  \[ \nabla \cdot (-\mu_e n_e E - D_e \nabla n_e) = S_e - \frac{\partial n_e}{\partial t} = \nabla \cdot (n_e \mathbf{w}_i) \]

- Drift-diffusion ions: ambipolar diffusion:

  Separate ambipolar / external field:

  \[ E = E_{\text{amb}} + E_{\text{ext}} \]

  \[ (\mu_e + \mu_i)n_e E_{\text{amb}} = -(D_e - D_i) \nabla n_e \]

  \[ \frac{\partial n_e}{\partial t} - \nabla \cdot \left( \frac{\mu_i D_e + \mu_e D_i}{\mu_e + \mu_i} \nabla n_e \right) = S_e \]

  \[ \nabla \cdot \left( (\mu_e + \mu_i)n_e E_{\text{ext}} \right) = 0 \]

- Complications at low pressure due to inertia & boundary conditions
  But: semi-implicit Poisson method also works!
Hybrid models of magnetized discharge plasmas: fluid electrons + particle ions

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Introduction

Magnetic fields used in low-pressure discharges:
- magnetron
- electron-cyclotron resonance (ECR)
- helicon
- Hall-effect thruster
- etc… (magnetized discharges)

Magnetic field → complex physics

Insight from simple models
Plan

- Elementary physics
- Modelling
- Limits of modelling
- Illustrative model results:
  - ECR reactor
  - Hall thruster
  - Galathea trap
Elementary effects of the magnetic field

- Cyclotron motion $\rightarrow$ confinement
- Perpendicular electric field $\rightarrow$ $\textbf{E} \times \textbf{B}$ drift
- Collisions destroy magnetic confinement

\[ -e\textbf{v} \times \textbf{B} = m_e \frac{d\textbf{v}}{dt} \]

Larmor radius
\[ \rho_L = v_\perp / \omega_c \]

Cyclotron frequency
\[ \omega_c = \frac{eB}{m} \]
## Typical conditions

<table>
<thead>
<tr>
<th>plasma</th>
<th>pressure</th>
<th>0.1 – 10 mTorr</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>plasma density</td>
<td>$10^{15} – 10^{19}$ m$^{-3}$</td>
</tr>
<tr>
<td></td>
<td>magnetic field</td>
<td>0.001 – 0.1 T</td>
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<tr>
<td></td>
<td>electron temperature</td>
<td>2 – 20 eV</td>
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</table>

<table>
<thead>
<tr>
<th>lengths</th>
<th>Debye length</th>
<th>$10^{-5} – 10^{-3}$ m</th>
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<tr>
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<td>electron Larmor radius</td>
<td>$10^{-4} – 0.01$ m</td>
</tr>
<tr>
<td></td>
<td>ion Larmor radius</td>
<td>0.02 – 5 m</td>
</tr>
<tr>
<td></td>
<td>mean free path</td>
<td>0.01 – 1 m</td>
</tr>
<tr>
<td></td>
<td>plasma size</td>
<td>0.02 – 1 m</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>frequencies</th>
<th>electron cyclotron</th>
<th>$3 \times 10^8 – 2 \times 10^{10}$ s$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>electron collision</td>
<td>$3 \times 10^5 – 10^8$ s$^{-1}$</td>
</tr>
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</table>

Long mean free path
Electrons are magnetized $\Rightarrow$ collisions + ionization
Ions have only few collisions
Magnetic field not influenced by plasma
Modelling

Low pressure $\rightarrow$ particle-in-cell (PIC):
- electron and ion trajectories
- space charge electric fields


Magnetized PIC models cumbersome:
- high plasma density $\rightarrow$ small time steps, small cells
- important 2D effects

$\rightarrow$ interest in simpler faster models
$\rightarrow$ describe electrons by collisional fluid equations
Electron fluid equations

- Electron conservation
  \[ \frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = S \]
  - ionisation source
  - density flux

- Anisotropic flux
  \[ \Gamma_e = \mu n_e \nabla \Phi - \mu \nabla (n_e T_e) \]
  - drift diffusion

- Mobility tensor (classical theory)
  \[ \mu_\perp = \frac{\nu^2}{\nu^2 + \omega_c^2} \quad \mu_\parallel = \frac{e\nu/m_e}{\nu^2 + \omega_c^2} \]
  - perpendicular mobility \( \ll \) parallel mobility
  - collision frequency
  - cyclotron frequency
Magnetized drift-diffusion equation

Hall parameter

\[ n_e w_e - \mu B \times (n_e w_e) = \mu n_e \nabla \Phi - \mu \nabla (n_e T_e) \equiv G \]

Take cross product and dot product with \( B \) and combine

\[ n_e w_e = \frac{1}{1 + (\mu B)^2} \left( G - \mu B \times G + \mu^2 (B \cdot G) B \right) \equiv \left( \mu / \mu \right) \cdot G \]

Mobility tensor components:

- \( \mu_{\parallel} = \mu \)
- \( \mu_{\perp} = \frac{1}{1 + (\mu B)^2} \mu \)
- \( \mu_\times = \pm \frac{\mu B}{1 + (\mu B)^2} \mu \)

Parallel transport unaffected
Perpendicular confinement
Magnetic drifts
Hybrid models

Non-quasineutral scheme:
- ion particles $\rightarrow n_i$
- electron fluid $\rightarrow n_e$
- Poisson $\rightarrow \Phi$

$$\varepsilon_0 \nabla^2 \Phi = e (n_e - n_i)$$

Quasineutral scheme:
- ion particles $\rightarrow n_i = n_e$
- electron fluid $\rightarrow \Phi$

$$\nabla \cdot (\mu n_e \nabla \Phi - \mu \nabla (n_e T_e)) = \nabla \cdot \Gamma_i$$ (Ohm’s law)

Limits of the electron equations

- Anomalous transport $\perp \mathbf{B} \Rightarrow$ empirical parameters
  \[ \frac{e v}{m_e} \left( v^2 + \omega_c^2 \right) < \mu_\perp < \frac{1}{16} B \]
  classical mobility $? \Rightarrow$ Bohm mobility

- Non-local effects $\parallel \mathbf{B}$: inertia, mirror confinement
  But: flux $\parallel \mathbf{B}$ limited by boundaries
  \[ \mu_\parallel n_e \nabla_\parallel \Phi \approx \mu_\parallel \nabla_\parallel (n_e T_e) \]
  drift diffusion
  \[ \Phi(\mathbf{r}) = \Phi^*(\lambda) + T_e(\lambda) \ln \left( \frac{n_e(\mathbf{r})}{n_0} \right) \] (Boltzmann)
  potential = constant + diffusion term

Magnetic field lines approximately equipotential
Extreme anisotropy $\Rightarrow$ numerical errors tend to destroy the magnetic confinement

\[
\Gamma_{e,x} = \frac{1 + \Omega_x^2}{1 + \Omega^2} \left[ \mu_0 n_e \frac{\partial \Phi}{\partial x} - \mu_0 \frac{\partial n_e T_e}{\partial x} \right] + \frac{\Omega_x \Omega_y}{1 + \Omega^2} \left[ \mu_0 n_e \frac{\partial \Phi}{\partial y} - \mu_0 \frac{\partial n_e T_e}{\partial y} \right]
\]

Electron flux

Hall vector

\[
\Omega = \frac{eB}{m_e v}
\]

\[|\Omega| = \omega_e / v >> 1\]
Numerical issues (2)

\[ \nabla \cdot (\mu n_e \nabla \Phi) = 0 \]

potential profile at mid height

\[ |\Omega| = \frac{\text{cyclotron frequency}}{\text{collision frequency}} \]

electron flux in the middle of the channel
Numerical issues (3)

Iterative flux scheme:
interpolate transverse flux rather than transverse field

\[
\Gamma^{k+1}_{e,x} = \frac{1}{1 + \Omega_y^2} \left[ \mu_0 n_e \frac{\partial \Phi}{\partial x} - \mu_0 \frac{\partial n_e T_e}{\partial x} \right]^{k+1} + \frac{\Omega_x \Omega_y}{1 + \Omega_y^2} \Gamma^{k}_{e,y}
\]

average of 4 surrounding transverse fluxes
Numerical issues (4)

Coupling with Poisson’s equation:
severe time step constraint for explicit scheme

\[
\Delta t < \frac{\varepsilon_0}{en_c \mu_{ii}} = \frac{\nu}{\omega_{pe}^2} < 10^{-11} \text{ s}
\]
(vs. ion CFL-time $10^{-8} - 10^{-6}$ s)

Semi-implicit scheme:
Poisson’s equation includes prediction of space charge

\[
\nabla \cdot \left((\varepsilon_0 + e\Delta t \mu_{ee}) \nabla \Phi - e\Delta t \mu \nabla (n_e T_e)\right) = e(n_e - n_i)
\]
Examples of model results

Non-quasineutral hybrid model → sheaths resolved

Fixed:
- Gaussian ionisation source
- uniform electron temperature (diffusion)
- electron collision frequency

Calculated:
- electron/ion densities
- electron/ion fluxes, currents
- self-consistent potential
Example I: Diffusion in ECR reactor

- Source chamber
- Grounded or insulator wall
- Insulator wall
- Ionisation source
- Cylinder axis
- Grounded wall 0 V
- Process chamber
ECR reactor with dielectric wall

Magnetic confinement reduces loss to source wall
ECR reactor with grounded wall

Magnetic confinement shortcircuited by walls

Example II: Hall-effect thruster

cathode -300 V

ionisation source
gas
anode 0 V
dielectric
dielectric
plasma
cylinder axis
Hall-effect thruster

Equipotential lines ~ magnetic field lines
Applied voltage penetrates in plasma bulk

cathode sheath negligible
acceleration region
ion beam
trapped low-energy ions
Example III: semi-Galathea trap

Semi-Galathea trap

Potential well reduces ion wall loss and guides ions to exit negative plasma potential! (inverted presheath)

70% of ions guided to exit

electron current from emissive cathode to walls

Potential well reduces ion wall loss and guides ions to exit
Semi-Galathea trap without emission

Potential well disappears because of cathode sheath
Conclusions

- In magnetized discharges, charged particle transport and space charge fields are different

- This can be studied in 2D by hybrid models

- No predictive simulations, but insight in physical principles