Kinetic simplified model for electron's distribution function in glow discharge regime

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Introduction

Plasma : ionized gaz

$\longrightarrow$ Force term bc of the presence of electric field E

Electrons verify the **drift-diffusion** equation

$$\partial_t n - \nabla \cdot (n\,\mu\,E + \nabla\,(D\,n)) = S$$

with n the electron density, D the **diffusion** coefficient and μ the **mobility** coefficient

$\longrightarrow$ They are proportional to each other

Goal : write a kinetic model to use **LB schemes** for electrons

What is a plasma ?

→ Ionized gas : mixture of charged particles

→ Quasi-neutrality : **Debye length** $\lambda_D \propto \frac{1}{n_e}$

→ **Degree of ionization** : $\delta_e = n_e / n_{\text{tot}}$

→ Classification :

- Thermal plasma
- Cold plasma : full ionized, partially ionized

→ Glow discharge :

atmospheric pressure, cold plasma

$$\lambda_D \approx 10^{-6} m \quad \text{and} \quad \delta_e \approx 10^{-4}$$

electron temperature $\approx 1\,\text{eV}$ $(10^4\,K)$ and heavy species temperature $\approx 300K$

Two term approximation

f verifies Boltzmann equation :

$$\partial_t f + v \cdot \nabla_x f - \frac{e}{m} E \nabla_v f = \left(\frac{\delta f}{\delta t} \right)_c$$

with $\left(\frac{\delta f}{\delta t} \right)_c$ **collision term**

f is expanded in spherical harmonics (Legendre expansion)

$$f \approx f_0(|v|) + \frac{v}{|v|} \cdot f_1(|v|)$$

where f_0 is **isotropic** and dominant

$\longrightarrow$ replacing in Boltzmann equation and integrating over angles $1, \frac{v}{|v|}$

Two term approximation

$$\partial_t f_0 + \frac{v}{3}\nabla_r . f_1 - \frac{e}{3m|v|^2} E \cdot \frac{\partial(|v|^2 f_1)}{\partial v} = \left(\frac{\delta f_0}{\delta t}\right)_c$$

$$\partial_t f_1 + |v| \nabla_r f_0 - \frac{e}{m} E \frac{\partial f_0}{\partial v} = \left(\frac{\delta f_1}{\delta t}\right)_c$$

collision terms are given by swarm experiments

→ Assumption : $f_i(v) = n(x,t) F_i(|v|^2/2)$ with $i = 0, 1$

→ This allows to write an equation over F_0 only (energy electron distribution function or EEDF)

→ Transport coefficients depend only on F_0

→ approach used in BOLSIG+ solver[1]

1. Hagelaar, G. J. M., & Pitchford, L. C. (2005). Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models. *Plasma sources science and technology*, *14* (4), 722.

Notations

Electron distribution function (**EDF**)

$$f(t,x,v), \qquad (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3$$

will often be denoted by

$$f(t,x,v) = f(v) = f_e(v)$$

it's moments will be denoted by

$$\begin{aligned} \rho &= \int_{\mathbb{R}^3} f dv \\ u &= \frac{1}{\rho}\int_{\mathbb{R}^3} f v dv \\ \frac{1}{2}\rho(u^2+3T) &= \int_{\mathbb{R}^3} f \frac{v^2}{2} dv \end{aligned}$$

Degond et al. model

Model given by Degond et al.[2]

Three species : positive ions, neutrals and electrons

$$\partial_t f_\alpha + v_\alpha \cdot \nabla_x f_\alpha + \frac{F_\alpha}{m_\alpha} \cdot \nabla_{v_\alpha} f_\alpha = Q_\alpha(f_e, f_i, f_n)$$

for $\alpha = n, i, e$

F_α force term such as electric force

$$Q_e(f_e, f_i, f_n) = Q_{ee}(f_e, f_e) + Q_{ei}(f_e, f_i) + Q_{en}(f_e, f_n) + Q_{e,ir}(f_e, f_i, f_n)$$

$\longrightarrow$ Elastic and inelastic collisions, ionization processes

2. Isabelle Choquet, Pierre Degond, et Brigitte Lucquin-Desreux. A hierarchy of diffusion models for partially ionized plasmas. *Discrete & Continuous Dynamical Systems-B*, 8(4):735, 2007.

Elastic collisions

Between two charged particles : **Fokker-Planck**

$$Q_{e\beta}(f_e, f_\beta) = \frac{\mu_{e\beta}^2}{m_e} \nabla_{v_e} \cdot \left[\int_{\mathbb{R}^3} \sigma_{e\beta} |v_e - v_\beta|^3 S(v_e - v_\beta) \left(\frac{1}{m_e} \nabla_{v_e} f_e f_\beta - \frac{1}{m_\beta} \nabla_{v_\beta} f_\beta f_e \right) \right] dv_\beta$$

where $S(v) = \mathrm{Id} - \frac{v \otimes v}{|v|^2}$, $\beta = e, i$

Collisions with neutrals : **Boltzmann**

$$Q_{en}(f_e, f_n)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2_+} B_{en}(v_e - v_n)(f_e' f_n' - f_e f_n) dv_n \, d\omega$$

where

$$\mathbb{S}^2_+ = \{\omega : (\omega, v) > 0\}$$

Inelastic collisions

Ionization-recombination reactions

$$N + e^- \leftrightarrows N^+ + e^- + e^-$$

Special operator involving the 3 distribution functions

$$\begin{aligned} Q_{e,ir}(f_e, f_i, f_n)(v_e) &= \int_{\mathbb{R}^{12}} \delta_v \delta_{\mathcal{E}}\, \sigma^r (f_e' f_e^\star f_i - \mathcal{F}_0 f_e f_n) dv_e' dv_e^\star dv_i dv_n \\ &+ 2 \int_{\mathbb{R}^{12}} \delta_v' \delta_{\mathcal{E}}'\, \sigma^{r\prime} (\mathcal{F}_0 f_e' f_n - f_e f_e^\star f_i) dv_e' dv_e^\star dv_i dv_n, \end{aligned}$$

with

$$\begin{aligned} \delta_{\mathcal{E}} &= \delta(m_e|v_e|^2 + m_n|v_n|^2 - [m_e|v_e'|^2 + m_e|v_e^\star|^2 + m_i|v_i|^2 + 2\Delta]), \\ \delta_v &= \delta(m_e v_e + m_n v_n - [m_e v_e' + m_e v_e^\star + m_i v_i]). \end{aligned}$$

Scaling and dimensionless equation

The chosen parameter is

$$\varepsilon = \sqrt{\frac{m_e}{m_n}} = \sqrt{\frac{m_e}{m_e + m_i}} \ll 1, \qquad x \to \varepsilon x, \qquad t \to \varepsilon^2 t$$

Hilbert expansion of each operator

$$Q_{e\alpha}(f_e, f_\alpha) = Q^0_{e\alpha}(f_e, f_\alpha) + \varepsilon Q^1_{e\alpha}(f_e, f_\alpha) + \varepsilon^2 Q^2_{e\alpha}(f_e, f_\alpha) + O(\varepsilon^3)$$

The dimensionless equation then write

$$\begin{aligned} \partial_t f_e + \frac{1}{\varepsilon}(v_e \cdot \nabla_x + F_e \cdot \nabla_{v_e}) f_e \; &= \; \frac{1}{\varepsilon^2} Q^0_{en}(f_e, f_n) + \frac{1}{\varepsilon} Q^1_{en}(f_e, f_n) + Q_{ee}(f_e, f_e) \\ &+ \; Q^2_{en}(f_e, f_n) + Q^0_{ei}(f_e, f_i) + Q^0_{e,ir}(f_e, f_i, f_n) + O(\varepsilon) \end{aligned}$$

Fluid equations obtained

→ Ions and neutrals share the same velocity u_n and temperature T_n

→ Both verify Euler equations without source terms except of

$$\partial_t \rho_i + \mathrm{div}\,(\rho_i\, u_n) = R_i$$

where R_i comes from the ionization-recombination collisions

Electrons verify :

$$\begin{aligned} \partial_t \rho_e + \mathrm{div}\,(\rho_e(u_n + u_J)) &= R_e \\ \partial_t\left(\frac{3}{2}\rho_e T_e\right) + \mathrm{div}\left[\frac{5}{2}\rho_e u_n T_e + \rho_e v_J\right] - \rho_e(u_n + u_J)\cdot F_e &= S_e^E \end{aligned}$$

with $R_e = R_i$ and f_e^0 isotropic

$$u_J = -\frac{1}{6\rho_n}\left[\frac{1}{\rho_e}\nabla_x\left(\int_{\mathbb{R}^3}\frac{|v|^2}{\alpha(v)} f_e^0 dv\right) + \frac{F_e}{\rho_e}\left(\int_{\mathbb{R}^3}\frac{|v|^2}{\alpha(v)} D_W f_e^0 dv\right)\right]$$

Simplification

Assumptions :

- f_i and f_n are **maxwellians** and $u_n = 0$
- Collisions with ions are **ignored** $Q_{ei} \approx 0$
- $F_e = -E$ with E the dimensionless electric field
- $Q_{ee} \approx$ **BGK** and **rescaled** by a factor $\frac{1}{\varepsilon}$ (as suggested by Degond et. al[3])
- Collision cross-sections $=$ **constant**
- Q_{ee} and $Q_{e,ir} \approx$ **BGK**

3. Isabelle Choquet, Pierre Degond, et Brigitte Lucquin-Desreux. A hierarchy of diffusion models for partially ionized plasmas. *Discrete & Continuous Dynamical Systems-B*, 8(4):735, 2007.

Simplified equation

The EDF equation becomes

$$\begin{aligned}\partial_t f + \frac{1}{\varepsilon}(v\cdot\nabla_x - E\cdot\nabla_v)f &= \frac{1}{\varepsilon^2}Q_{en}^0(f) + \frac{1}{\varepsilon}[Q_{en}^1(f) + Q_{ee}(f)] \\ &+ Q_{en}^2(f) + Q_{e,ir}^0(f) + O(\varepsilon)\end{aligned}$$

Assumption : $B_{en}(v_e - v_n) = \text{constant}$

Then computing Hilbert expansion[4]

$$Q_{en}(f) = Q_{en}^0(f) + \varepsilon^2 Q_{en}^2(f) + O(\varepsilon^3)$$

$\rightarrow$ $u_n = 0$ implies that $Q_{en}^1(f) = 0$

4. Pierre Degond et Brigitte Lucquin-Desreux. The asymptotics of collision operators for two species of particles of disparate masses. *Mathematical Models and Methods in Applied Sciences*, 6(03):405–436, 1996.

Properties of Q^0_{en}

$$Q^0_{en}(f) = \rho_n \sigma \int_{\{\omega:(v,\omega)>0\}} [f(v - 2(v,\omega)\omega) - f(v)] d\omega$$

Proposition 1

- $\mathrm{Ker}(Q^0_{en}) = \{\text{isotropic functions}\}$
- Q^0_{en} *self-adjoint in* $L^2_{f_n}(\mathbb{R}^3)$
- *Find* ψ *st* $Q^0_{en}(\psi) = \phi$ *have a solution if and olny if* $\phi \in \mathrm{Ker}(Q^0_{en})^\perp \Leftrightarrow$

  for all $W = \frac{v^2}{2}$, $S_W = \{v \quad \text{st} \quad v^2/2 = W\}$

$$\int_{S_W} \phi(v) dN(v) = 0$$

Same properties as in [1]

Properties of Q_{en}^2

Computing Q_{en}^2 is too complicated

$\longrightarrow$ Instead of trying to calculate, we use a property, similar to what is find in [2][5] :

Proposition 2

For f_0 and ϕ isotropic, we have

$$\int_{\mathbb{R}^3} Q_{en}^2(f_0)\phi\, dv = 16\sqrt{2}\pi^2\sigma\rho_n T_n \int_0^\infty \partial_W\left(W^{3/2}\left[\frac{f_0}{T_n} + \partial_W f_0\right]\right)\phi\, dW$$

$\longrightarrow$ We can now compute it's moments !!

5. P Degond, A Nouri, et C Schmeiser. Macroscopic models for ionization in the presence of strong electric fields. *Transport theory and Statistical Physics*, 29(3-5):551–561, 2000.

Electron-electron collisions

We replace with **BGK** operator

$$Q_{ee}(f) = M(f) - f$$

where

$$M(f) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|u-v|^2}{2T} \right)$$

This will allow us to obtain a result on EDF at order 0

Remark. If we expand f in terms of ε, $f = f_0 + O(\varepsilon)$, we remark that

$$\rho = \rho_0 + O(\varepsilon), \quad u = u_0 + O(\varepsilon), \quad T = T_0 + O(\varepsilon)$$

→ We now take $\rho_0 = \rho$, etc…

Properties of $Q_{e,ir}$

In [1], Hilbert expansion of $Q_{e,ir}$ gives

$$Q^0_{e,ir}(f)(v) = \int_{\mathbb{R}^6} \delta_{\mathcal{E}}\, \sigma^r (f' f^\star \rho_i - \mathcal{F}_0 f \rho_n) dv' dv^\star - \int_{\mathbb{R}^6} \delta'_{\mathcal{E}}\, \sigma^{r\prime} (\mathcal{F}_0 f' \rho_n - f f^\star \rho_i) dv' dv^\star,$$

with

$$\delta_{\mathcal{E}} = \delta(v^2 - [v^{\star 2} + v'^2 + 2\Delta])$$

→ heavy species share the same speed due to the limit in ε

→ The solution of energy equation cannot be written like in binary collision case with a sphere parametrization

The following property comes from [1]

Proposition 3

$$\int_{\mathbb{R}^3} Q^0_{e,ir}(f)(v) \begin{pmatrix} 1 \\ v^2/2 \end{pmatrix} dv = \begin{pmatrix} R_e \\ -\Delta R_e \end{pmatrix}$$

In the case where EDF is maxwellian we can compute R_e and it is given by

$$R_e = \frac{256}{15}\pi^3 \frac{\rho}{(2\pi T)^{3/2}} I \sigma^r \left[\mathcal{F}_0 \rho_n - \rho_i \frac{\rho}{(2\pi T)^{3/2}} \exp\left(\frac{\Delta}{T}\right) \right]$$

with

$$I = \int_{\sqrt{2\Delta}}^{\infty} \exp\left(-\frac{r^2}{2T}\right) (r^2 - 2\Delta)^{5/2} r^2 \, dr$$

Properties of $Q_{e,ir}$

$Q^0_{e,ir} \approx$ **BGK** operator using previous property and assuming that **EDF is maxwellian**

$$Q^0_{e,ir}(f_0) = \frac{1}{\tau}(M_{e,ir} - f_0)$$

with

$$\begin{aligned}
M_{e,ir} &= \frac{\tilde{\rho}}{(2\pi\tilde{T})^{3/2}}\exp\left(-\frac{v^2}{2\tilde{T}}\right), \\
\tilde{\rho} &= \tau R_e + \rho, \\
\tilde{T} &= \frac{1}{\tilde{\rho}}\left(\rho T - \tau\frac{2}{3}\Delta R_e\right), \\
\tau &= \min\left(\frac{3\rho T}{4|R_e|\Delta}, \frac{\rho}{2|R_e|}\right) > 0
\end{aligned}$$

$\longrightarrow$ τ is defined st $\tilde{T}$ is non negative

Identification

We expand f and try to identify terms of the same order in the simplified equation

$$f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + O(\varepsilon^3)$$

At ε^{-2} order we have :

$$\begin{aligned} \partial_t f_0 + \frac{1}{\varepsilon}(v \cdot \nabla_x - E \cdot \nabla_v)(f_0 + \varepsilon f_1) &= \frac{1}{\varepsilon^2} Q^0_{en}(f_0) + \frac{1}{\varepsilon}[Q_{ee}(f_0) + Q^0_{en}(f_1)] + Q^0_{en}(f_2) \\ &+ Q^2_{en}(f_2) + Q_{ee}(f_1) + Q^0_{e,ir}(f_0) + O(\varepsilon) \end{aligned}$$

→ Hence

$$Q^0_{en}(f_0) = 0$$

→ This implies by proposition 1 that $\boldsymbol{f_0}$ **is isotropic**

Identification

At order ε^{-1} :

$$\begin{aligned}\partial_t f_0 + \frac{1}{\varepsilon}(v\cdot\nabla_x - E\cdot\nabla_v)(f_0+\varepsilon f_1) &= \frac{1}{\varepsilon^2}Q^0_{en}(f_0) + \frac{1}{\varepsilon}[Q_{ee}(f_0)+Q^0_{en}(f_1)] + Q^0_{en}(f_2)\\ &+ Q^2_{en}(f_0) + Q_{ee}(f_1) + Q^0_{e,ir}(f_0) + O(\varepsilon)\end{aligned}$$

gives us

$$Q^0_{en}(f_1) = (v\cdot\nabla_x - E\cdot\nabla_v) f_0 + Q_{ee}(f_0)$$

→ by proposition 1 it has a solution if and only if for all W

$$\int_{S_W} [(v\cdot\nabla_x - E\cdot\nabla_v) f_0 + Q_{ee}(f_0)]\, dN(v) = 0$$

Identification

At order ε^{-1} :

$$\begin{aligned}\partial_t f_0 + \frac{1}{\varepsilon}(v\cdot\nabla_x - E\cdot\nabla_v)(f_0+\varepsilon f_1) &= \frac{1}{\varepsilon^2}Q^0_{en}(f_0) + \frac{1}{\varepsilon}[Q_{ee}(f_0) + Q^0_{en}(f_1)] + Q^0_{en}(f_2)\\ &+ Q^2_{en}(f_0) + Q_{ee}(f_1) + Q^0_{e,ir}(f_0) + O(\varepsilon)\end{aligned}$$

gives us

$$Q^0_{en}(f_1) = (v\cdot\nabla_x - E\cdot\nabla_v) f_0 + Q_{ee}(f_0)$$

$\longrightarrow$ the first term is an odd function so necessarly for all W

$$\int_{S_W} Q_{ee}(f_0)\,dN(v) = 0$$

$\longrightarrow$ This implies that $\boldsymbol{f_0}$ is equal to it's associated **maxwellian** (with $u_0 = 0$)

Identification

Now we try to get an expression for f_1 by « inverting »

$$Q^0_{en}(f_1) = (v\cdot\nabla_x - E\cdot\nabla_v)\,f_0$$

Assuming that f_1 can be written as $\phi(v)\cdot v$ we can find an expression

$$f_1 = -\frac{1}{2\sigma\rho n\alpha}v\cdot[\nabla_x f_0 - E\partial_W f_0] + \tilde{f}_1$$

where $\tilde{f}_1$ is a function from Q^0_{en} kernel, because

$$-\frac{1}{2\sigma\rho n\alpha}v\cdot[\nabla_x f_0 - E\partial_W f_0]$$

has the same image by Q^0_{en} than f_1

Identification

At order 1 :

$$\partial_t f_0 + \frac{1}{\varepsilon}(v \cdot \nabla_x - E \cdot \nabla_v)(f_0 + \varepsilon f_1) = \frac{1}{\varepsilon^2} Q^0_{en}(f_0) + \frac{1}{\varepsilon}[Q_{ee}(f_0) + Q^0_{en}(f_1)] + Q^0_{en}(f_2) + Q^2_{en}(f_0) + Q_{ee}(f_1) + Q^0_{e,ir}(f_0) + O(\varepsilon)$$

gives us

$$\partial_t f_0 + (v \cdot \nabla_x - E \cdot \nabla_v) f_1 - Q^2_{en}(f_0) - Q_{ee}(f_1) - Q^0_{e,ir}(f_0) = Q^0_{en}(f_2)$$

→ has a solution if and only if the following is verified (**SHE-FP** equation)

$$\int_{S_W} [\partial_t f_0 + v \cdot \nabla_x f_1 - E \cdot \nabla_v f_1] dN(v) = \int_{S_W} [Q^2_{en}(f_0) + Q_{ee}(f_1) + Q^0_{e,ir}(f_0)] dN(v)$$

Final result

Taking the $1, W$ moments from previous equations leads the Energy-Transport electron equation (**ET** eq) :

$$\begin{cases} \partial_t n + \nabla \cdot (\Gamma) = S \\ \partial_t n_W + \nabla \cdot (\Gamma_W) + E \cdot \Gamma = S_W \end{cases}$$

where $n = \rho$ and $n_W = 3\rho T$ with

$$\begin{aligned} \Gamma &= -n\,\mu\,E - \nabla\,(D\,n), & \Gamma_W &= -n_W\,\mu_W\,E - \nabla\,(D_W\,n_W), \\ \mu &= \frac{1}{2\,\sigma\,\rho_n\,\alpha}, & \mu_W &= \frac{5}{6\,\sigma\,\rho_n\,\alpha}, \\ D &= \frac{T}{2\,\sigma\,\rho_n\,\alpha}, & D_W &= \frac{5T}{6\,\sigma\,\rho_n\,\alpha}, \\ S &= R_e & S_W &= -6\,\alpha\,\sigma\,\rho_n\,\rho\left[1 - \frac{T}{T_n}\right] - \Delta\,R_e. \end{aligned}$$

Conclusion

→ Try to simplify Q_{en}^0 and Q_{en}^2

→ Comparison with 2016 [Hagelaar][6]

→ LB schemes

6. Hagelaar, G. J. M. (2015). Coulomb collisions in the Boltzmann equation for electrons in low-temperature gas discharge plasmas. *Plasma Sources Science and Technology*, *25*(1), 015015.

More precisions about α

$$
\begin{aligned}
v\sigma\alpha &= \int_{\{(\omega,v)>0\}} B_{en}(v)(v,\omega)\omega d\omega \\
&= v\sigma \int_{\{(\omega,v)>0\}} \frac{(v,\omega)^2}{|v|^2} d\omega
\end{aligned}
$$

where

$$B_{en}(v) = \sigma$$

α is constant, if we change the cross-section for example

$$B_{en}(v) = \sigma |v|$$

then

$$\alpha = |v| \int_{\{(\omega,v)>0\}} \frac{(v,\omega)^2}{|v|^2} d\omega = \beta |v|$$

$\rightarrow$ This has an impact on transport coefficients values

Bibliographie

[1] Isabelle Choquet, Pierre Degond, et Brigitte Lucquin-Desreux. A hierarchy of diffusion models for partially ionized plasmas. *Discrete & Continuous Dynamical Systems-B*, 8(4):735, 2007.

[2] P Degond, A Nouri, et C Schmeiser. Macroscopic models for ionization in the presence of strong electric fields. *Transport theory and Statistical Physics*, 29(3-5):551–561, 2000.

[3] Pierre Degond et Brigitte Lucquin-Desreux. The asymptotics of collision operators for two species of particles of disparate masses. *Mathematical Models and Methods in Applied Sciences*, 6(03):405–436, 1996.