Implementation of a cold plasma model in YALES2

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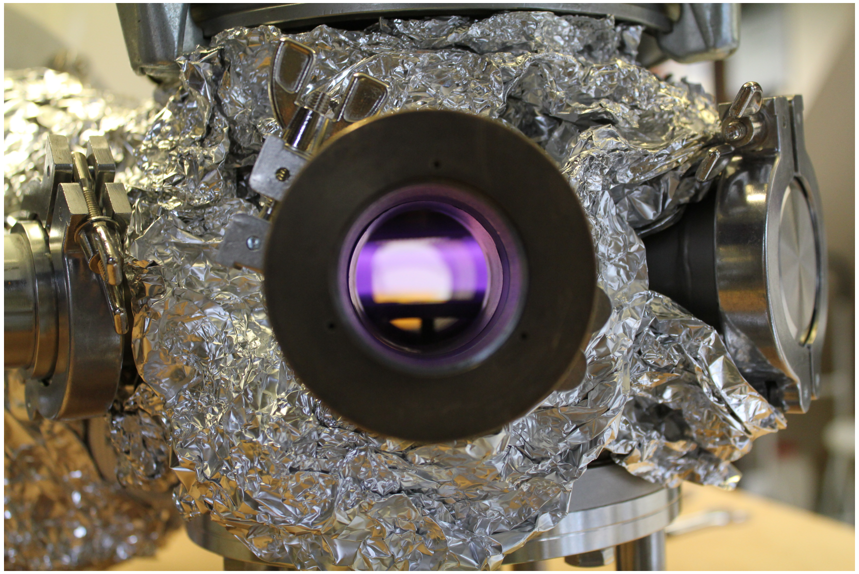
Plasma Enhanced Chemical Vapor Deposision



Silane radio-frequency (RF) discharges for photovoltaic devices [Orlac'h PhD 2017]

- Complex chemistry
- Translational non-equilibrium
- Charged species drift
- Nanoparticles
- Expensive computations
  - ➢ Need HPC code

Plasma solver

- Electron temperature equation
- Implementation of electron collision kinetics

Base test case: 1D Townsend discharge

Charged species transport equation (k=e,Ar,Ar^+)

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \boldsymbol{V}_k) = W_k \dot{\omega}_k = \alpha \frac{W_k}{W_e} |\rho_e \boldsymbol{V}_e|$$

Poisson's equation

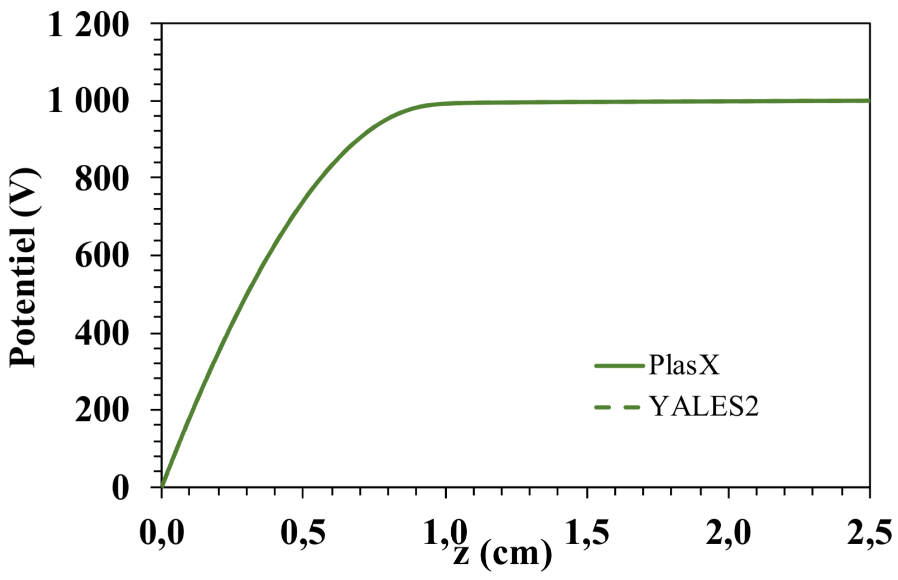
$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = \sum_k \frac{n_k q_k}{\varepsilon_0}$$

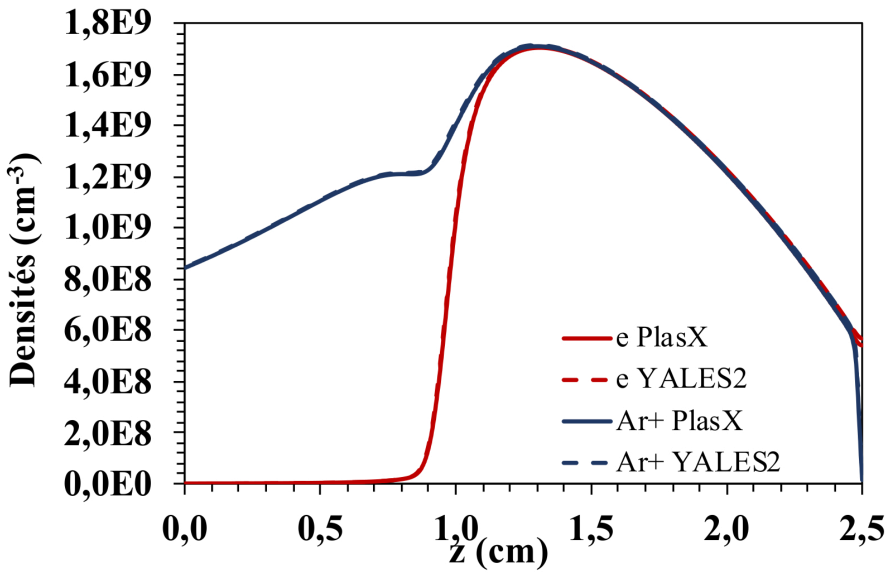
Drift-diffusion approximation

$$\boldsymbol{V}_k = -D_k \boldsymbol{\nabla} \ln Y_k + \mu_k \boldsymbol{E}$$

Townsend ionization rate [Ward 1962]

$$\alpha = p\, A \exp(-B (p/E)^{0.5})$$





- The two codes are in perfect agreement (≤ 0.3 %)

Electron temperature equation

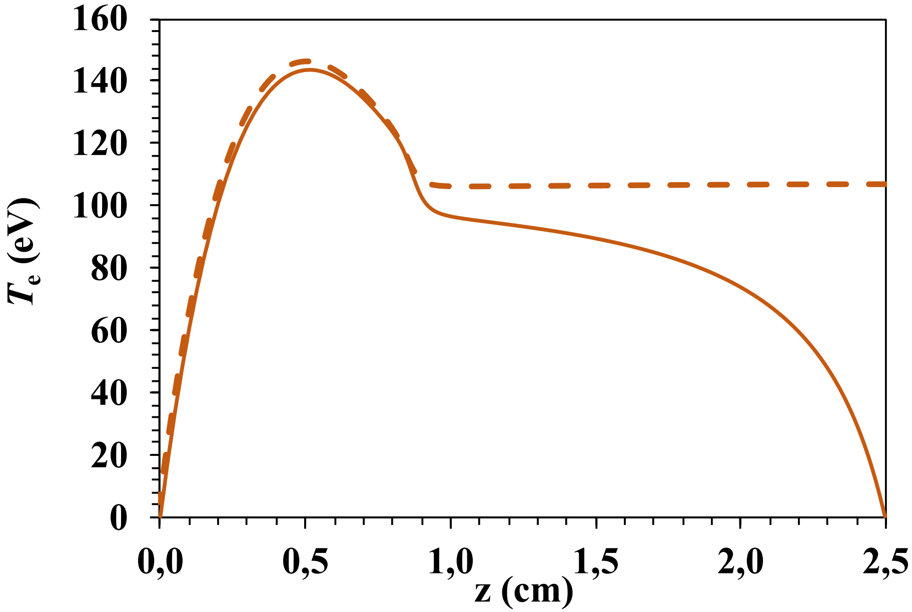
Strong translational non-equilibrium

$$T \propto 300 \text{ K} \quad \ll \quad T_e \propto 1 - 10 \text{ eVs}$$

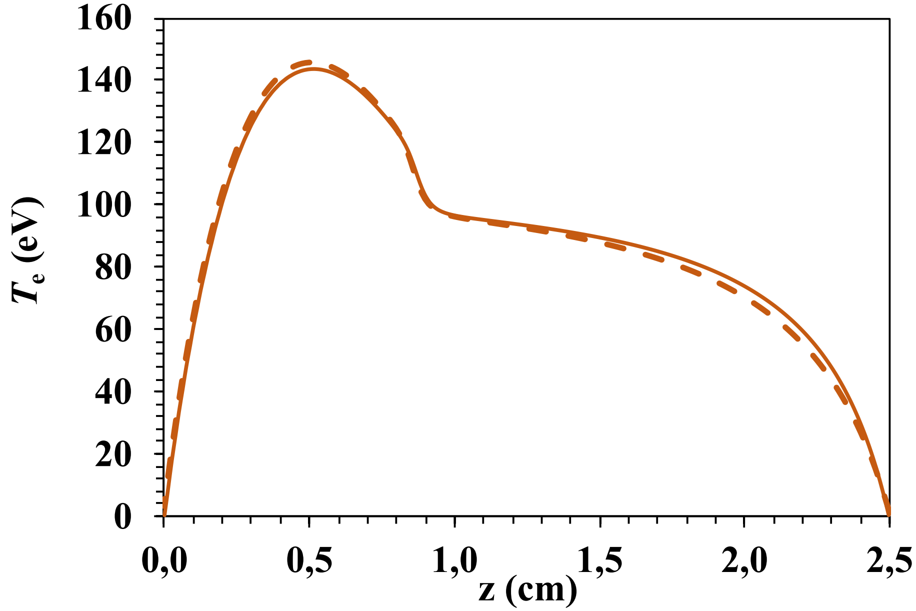
The electron temperature is needed to compute the reaction rates

$$\frac{\partial(\frac{3}{2} n_e k_B T_e)}{\partial t} + \nabla \cdot \boldsymbol{Q}_e = \boldsymbol{J}_e \cdot \boldsymbol{E} = \dot{E}_{eh}$$

Electron heat flux	Electric current	Energy exchange
$\boldsymbol{Q}_e = -\lambda_e \boldsymbol{\nabla} \ln T_e + \rho_e h_e \boldsymbol{V}_e$	$\boldsymbol{J}_e = n_e q_e \boldsymbol{V}_e$	$\dot{E}_{eh} = -E_{\text{ioniz}} \dot{\tau}_{\text{ioniz}}$



Flux boundary conditions



Dirichlet boundary conditions

Two-temperature chemistry

Fast reactions

e + heavy

$$\dot{\tau} = A\, T_e^{\beta} \exp(-E_A/T_e)$$

Slow reactions

$$heavy + heavy$$

$$\dot{\tau} = A\, T^{\beta} \exp(-E_A/T)$$

r	**Reaction**	A_r **(mol,cm³,s)**	β_r	$\mathfrak{E}_r$ **(cal.mol⁻¹)**
	Cluster growth			
19	$SiH_3^- + SiH_4 = Si_2H_5^- + H_2$	6.020×10^{11}	0.000	0
20	$SiH_2^- + SiH_4 = H_3SiSiH^- + H_2$	6.020×10^{11}	0.000	0
	Neutralization reactions			
21	$SiH_3^- + SiH_3^+ = SiH_3 + SiH_3$	1.232×10^{18}	−0.500	0
22	$SiH_2^- + SiH_3^+ = SiH_2 + SiH_3$	1.359×10^{18}	−0.500	0
23	$Si_2H_5^- + SiH_3^+ = Si_2H_5 + SiH_3$	9.648×10^{17}	−0.500	0
24	$H_3SiSiH^- + SiH_3^+ = H_3SiSiH + SiH_3$	1.001×10^{18}	−0.500	0
	Neutral-neutral reactions			
25	$SiH_4 + H = SiH_3 + H_2$	1.510×10^{13}	0.000	2,484
26	$Si_2H_6 + H = Si_2H_5 + H_2$	9.630×10^{13}	0.000	2,484
27	$Si_2H_6 + H = SiH_3 + SiH_4$	4.820×10^{13}	0.000	2,484
28	$SiH_2 + H_2 = SiH_4$	5.260×10^{10}	0.000	0
29	$SiH_2 + SiH_4 = Si_2H_6$	3.620×10^{13}	0.000	0
30	$SiH_3 + SiH_3 = SiH_2 + SiH_4$	9.030×10^{13}	0.000	0
31	$H_2 + H_2 = 2H + H_2$	8.610×10^{17}	−0.700	52,530
	Reverse rate	1.000×10^{17}	−0.600	0
32	$H_2 + H = 3H$	2.700×10^{16}	−0.100	52,530
	Reverse rate	3.200×10^{15}	0.000	0
	Additional hydrogen reactions			
33	$H_2^+ + H = H^+ + H_2$	3.850×10^{14}	0.000	0
	Reverse rate	1.900×10^{14}	0.000	21,902
34	$H_2 + H_2^+ \rightharpoonup H_3^+ + H$	1.270×10^{15}	0.000	0
35	$H^+ + 2\,H_2 \rightharpoonup H_3^+ + H_2$	1.950×10^{20}	−0.500	0

r	**Electron collision**	A_r **(mol,cm³,s)**	β_r	$\mathfrak{E}_r$ **(cal.mol⁻¹)**
	Ionization			
1	$SiH_4 + e \rightharpoonup SiH_3^+ + H + 2e$	1.510×10^{32}	−2.930	553,910
2	$SiH_3 + e \rightharpoonup SiH_3^+ + 2e$	1.355×10^{12}	0.900	188,396
3	$H_2 + e \rightharpoonup H_2^+ + 2e$	8.007×10^{10}	1.100	392,574
4	$H + e \rightharpoonup H^+ + 2e$	1.080×10^{16}	0.000	178,210
	Dissociation			
5	$SiH_4 + e \rightharpoonup SiH_3 + H + e$	1.102×10^{21}	−1.000	245,421
6	$SiH_4 + e \rightharpoonup SiH_2 + 2H + e$	5.394×10^{21}	−1.000	245,421
7	$H_2 + e \rightharpoonup 2H + e$	1.023×10^{16}	0.000	238,347
8	$H_3^+ + e \rightharpoonup H^+ + 2H + e$	1.220×10^{17}	0.000	179,380
9	$H_2^+ + e \rightharpoonup H^+ + H + e$	1.460×10^{17}	0.000	37,460
	Dissociative attachment			
10	$SiH_4 + e \rightharpoonup SiH_3^- + H$	2.269×10^{21}	−1.627	190,540
11	$SiH_4 + e \rightharpoonup SiH_2^- + 2H$	2.269×10^{21}	−1.627	190,540
12	$SiH_3 + e \rightharpoonup SiH_2^- + H$	3.440×10^{15}	−0.500	44,740
	Detachment			
13	$SiH_3^- + e \rightharpoonup SiH_3 + 2e$	1.900×10^{14}	0.500	32,425
14	$SiH_2^- + e \rightharpoonup SiH_2 + 2e$	1.900×10^{14}	0.500	25,921
	Recombination and dissociative recombination			
15	$H^+ + 2e \rightharpoonup H + e$	3.630×10^{37}	−4.000	0
16	$H_3^+ + e \rightharpoonup 3H$	8.000×10^{17}	−0.404	0
17	$H_3^+ + 2e \rightharpoonup H + H_2 + e$	3.170×10^{21}	−4.500	0
18	$H_2^+ + 2e \rightharpoonup 2H + e$	3.170×10^{21}	−4.500	0

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Perspectives

Plasma solver

- Validation of electron collision kinetics
- Coupling with flow and neutral kinetics
- Implementation of 2D axisymmetric meshing
- Other test cases: ionic wind, turbulent micro-wave discharges for CO2 conversion

Modeling of nanoparticles

- Nucleation
- Coagulation
- Charging