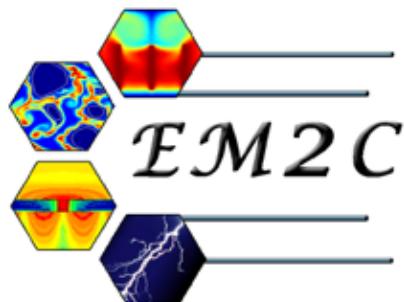


Implementation of a cold plasma model in YALES2

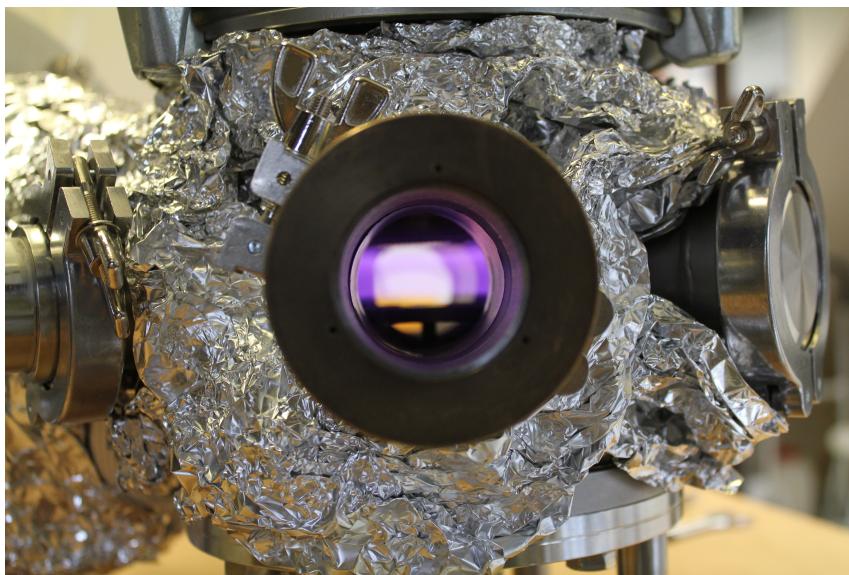
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Plasma Enhanced Chemical Vapor Deposition



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

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

Plasma solver

- Electron temperature equation
- Implementation of electron collision kinetics

Base test case: 1D Townsend discharge

Charged species transport equation ($k=e, \text{Ar}, \text{Ar}^+$)

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

Poisson's equation

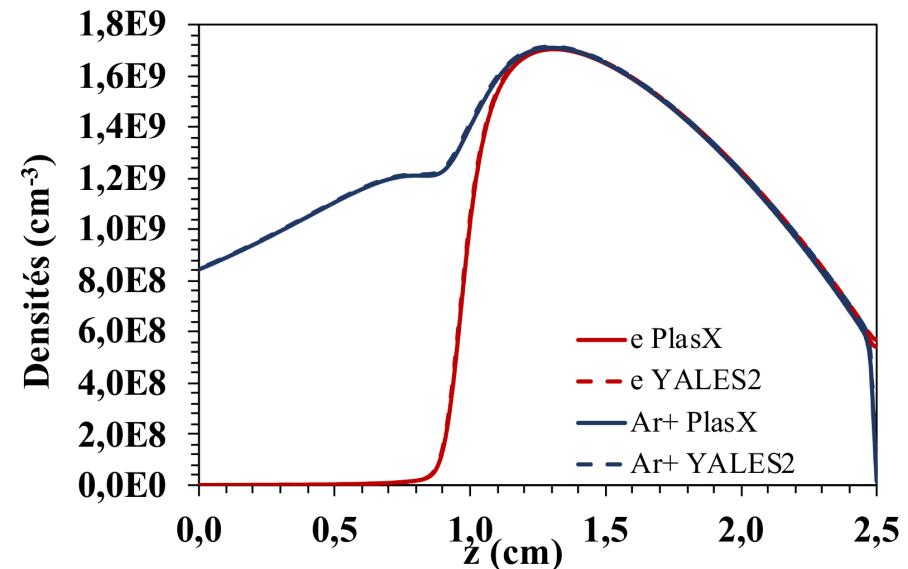
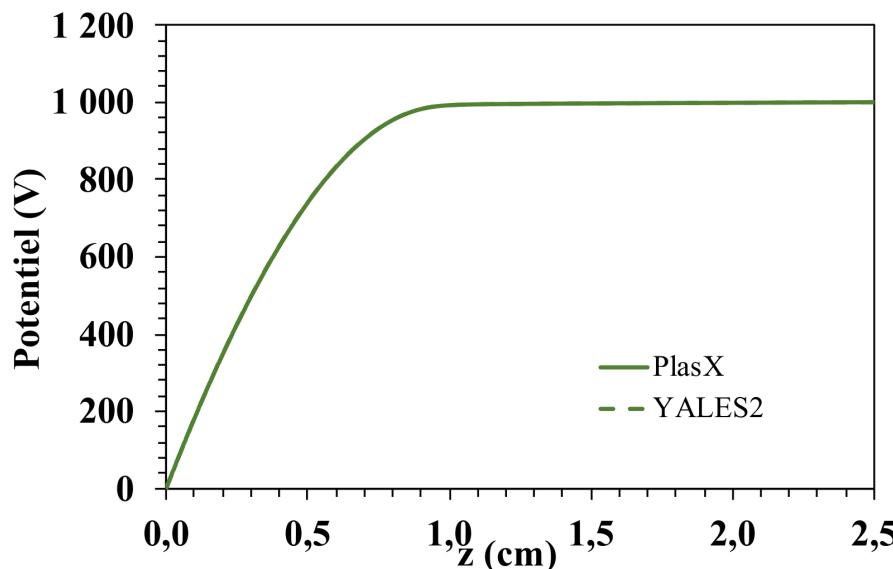
$$\nabla \cdot \mathbf{E} = \sum_k \frac{n_k q_k}{\epsilon_0}$$

Drift-diffusion approximation

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

Townsend ionization rate [Ward 1962]

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



- The two codes are in perfect agreement ($\leq 0.3 \%$)

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

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

Electron heat flux

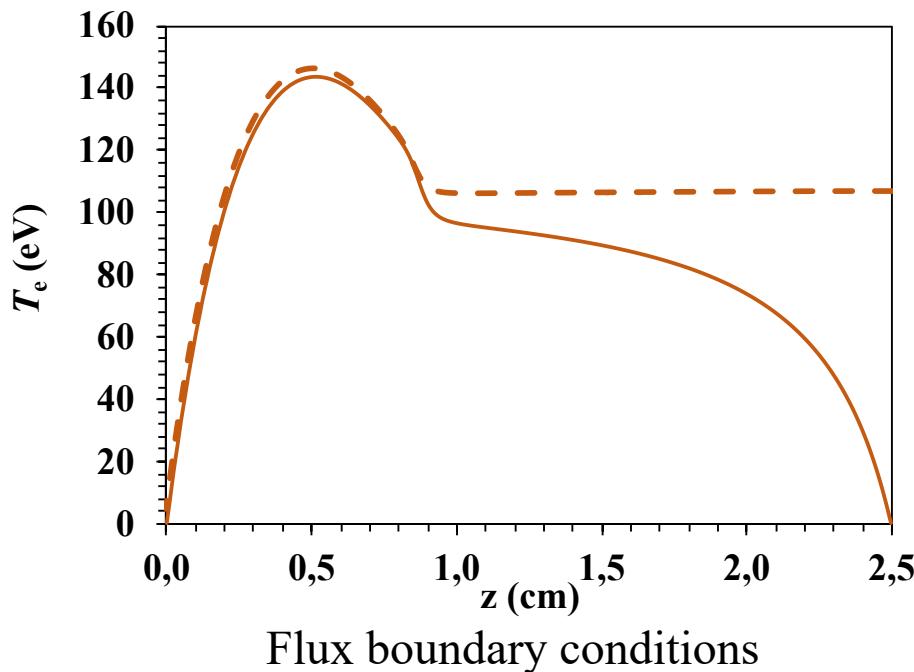
$$\mathbf{Q}_e = -\lambda_e \nabla \ln T_e + \rho_e h_e \mathbf{V}_e$$

Electric current

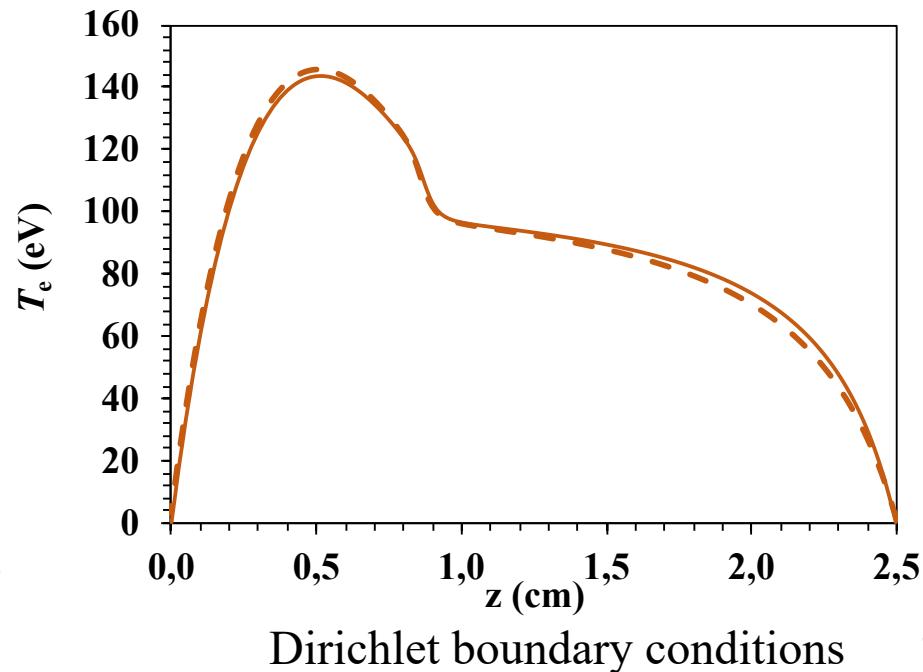
$$\mathbf{J}_e = n_e q_e \mathbf{V}_e$$

Energy exchange

$$\dot{E}_{eh} = -E_{\text{ioniz}} \dot{t}_{\text{ioniz}}$$



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*

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

<i>r</i>	Reaction	<i>A_r</i> (mol.cm ³ .s)	<i>β_r</i>	<i>E_r</i> (cal.mol ⁻¹)
Cluster growth				
19	$\text{SiH}_3^- + \text{SiH}_4 \rightarrow \text{Si}_2\text{H}_5^- + \text{H}_2$	6.020×10^{11}	0.000	0
20	$\text{SiH}_2^- + \text{SiH}_4 \rightarrow \text{H}_3\text{SiSiH}^- + \text{H}_2$	6.020×10^{11}	0.000	0
Neutralization reactions				
21	$\text{SiH}_3^- + \text{SiH}_3^+ \rightarrow \text{SiH}_3 + \text{SiH}_3$	1.232×10^{18}	-0.500	0
22	$\text{SiH}_2^- + \text{SiH}_3^+ \rightarrow \text{SiH}_2 + \text{SiH}_3$	1.359×10^{18}	-0.500	0
23	$\text{Si}_2\text{H}_5^- + \text{SiH}_3^+ \rightarrow \text{Si}_2\text{H}_5 + \text{SiH}_3$	9.648×10^{17}	-0.500	0
24	$\text{H}_3\text{SiSiH}^- + \text{SiH}_3^+ \rightarrow \text{H}_3\text{SiSiH} + \text{SiH}_3$	1.001×10^{18}	-0.500	0
Neutral-neutral reactions				
25	$\text{SiH}_4 + \text{H} \rightarrow \text{SiH}_3 + \text{H}_2$	1.510×10^{13}	0.000	2,484
26	$\text{Si}_2\text{H}_6 + \text{H} \rightarrow \text{Si}_2\text{H}_5 + \text{H}_2$	9.630×10^{13}	0.000	2,484
27	$\text{Si}_2\text{H}_6 + \text{H} \rightarrow \text{SiH}_3 + \text{SiH}_4$	4.820×10^{13}	0.000	2,484
28	$\text{SiH}_2 + \text{H}_2 \rightarrow \text{SiH}_4$	5.260×10^{10}	0.000	0
29	$\text{SiH}_2 + \text{SiH}_4 \rightarrow \text{Si}_2\text{H}_6$	3.620×10^{13}	0.000	0
30	$\text{SiH}_3 + \text{SiH}_3 \rightarrow \text{SiH}_2 + \text{SiH}_4$	9.030×10^{13}	0.000	0
31	$\text{H}_2 + \text{H}_2 \rightarrow 2\text{H} + \text{H}_2$ Reverse rate	8.610×10^{17} 1.000×10^{17}	-0.700 -0.600	52,530 0
32	$\text{H}_2 + \text{H} \rightarrow 3\text{H}$ Reverse rate	2.700×10^{16} 3.200×10^{15}	-0.100 0.000	52,530 0
Additional hydrogen reactions				
33	$\text{H}_2^+ + \text{H} \rightarrow \text{H}^+ + \text{H}_2$ Reverse rate	3.850×10^{14} 1.900×10^{14}	0.000 0.000	0 21,902
34	$\text{H}_2 + \text{H}_2^+ \rightarrow \text{H}_3^+ + \text{H}$	1.270×10^{15}	0.000	0
35	$\text{H}^+ + 2\text{H}_2 \rightarrow \text{H}_3^+ + \text{H}_2$	1.950×10^{20}	-0.500	0

<i>r</i>	Electron collision	<i>A_r</i> (mol.cm ³ .s)	<i>β_r</i>	<i>E_r</i> (cal.mol ⁻¹)
Ionization				
1	$\text{SiH}_4 + \text{e} \rightarrow \text{SiH}_3^+ + \text{H} + 2\text{e}$	1.510×10^{32}	-2.930	553,910
2	$\text{SiH}_3 + \text{e} \rightarrow \text{SiH}_3^+ + 2\text{e}$	1.355×10^{12}	0.900	188,396
3	$\text{H}_2 + \text{e} \rightarrow \text{H}_2^+ + 2\text{e}$	8.007×10^{10}	1.100	392,574
4	$\text{H} + \text{e} \rightarrow \text{H}^+ + 2\text{e}$	1.080×10^{16}	0.000	178,210
Dissociation				
5	$\text{SiH}_4 + \text{e} \rightarrow \text{SiH}_3 + \text{H} + \text{e}$	1.102×10^{21}	-1.000	245,421
6	$\text{SiH}_4 + \text{e} \rightarrow \text{SiH}_2 + 2\text{H} + \text{e}$	5.394×10^{21}	-1.000	245,421
7	$\text{H}_2 + \text{e} \rightarrow 2\text{H} + \text{e}$	1.023×10^{16}	0.000	238,347
8	$\text{H}_3^+ + \text{e} \rightarrow \text{H}^+ + 2\text{H} + \text{e}$	1.220×10^{17}	0.000	179,380
9	$\text{H}_2^+ + \text{e} \rightarrow \text{H}^+ + \text{H} + \text{e}$	1.460×10^{17}	0.000	37,460
Dissociative attachment				
10	$\text{SiH}_4 + \text{e} \rightarrow \text{SiH}_3^- + \text{H}$	2.269×10^{21}	-1.627	190,540
11	$\text{SiH}_4 + \text{e} \rightarrow \text{SiH}_2^- + 2\text{H}$	2.269×10^{21}	-1.627	190,540
12	$\text{SiH}_3 + \text{e} \rightarrow \text{SiH}_2^- + \text{H}$	3.440×10^{15}	-0.500	44,740
Detachment				
13	$\text{SiH}_3^- + \text{e} \rightarrow \text{SiH}_3 + 2\text{e}$	1.900×10^{14}	0.500	32,425
14	$\text{SiH}_2^- + \text{e} \rightarrow \text{SiH}_2 + 2\text{e}$	1.900×10^{14}	0.500	25,921
Recombination and dissociative recombination				
15	$\text{H}^+ + 2\text{e} \rightarrow \text{H} + \text{e}$	3.630×10^{37}	-4.000	0
16	$\text{H}_3^+ + \text{e} \rightarrow 3\text{H}$	8.000×10^{17}	-0.404	0
17	$\text{H}_2^+ + 2\text{e} \rightarrow \text{H} + \text{H}_2 + \text{e}$	3.170×10^{21}	-4.500	0
18	$\text{H}_2^+ + 2\text{e} \rightarrow 2\text{H} + \text{e}$	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

