Modeling negative ion kinetics in a PIC-MCC algorithm

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Scope: ITER Neutral beam injector (NBI)



Laplace Scope: Negative ion sources for fusion applications





Numerical model: Particle in Cell (PIC) with Monte-Carlo-Collisions (MCC)



- The model is fully "homemade"
- Parallelized (hybrid MPI and OpenMP)
- Poisson solver is a multi-grid (geometric)
- Magnetic field is prescribed





Physical chemistry of hydrogen including negative ions

- Vibrational excitation of H_2 needs a high T_e (~10 eV)
- Dissociative attachment of H_2 (#17, table I) occurs for $T_e \sim 1 \text{ eV}$

Table 1. Electron collisions.

#	Reaction	Cross section reference
1	$e + H \rightarrow e + H$ (elastic)	[71-75]
2	$e + H \rightarrow e + H$ (inelastic, 4 proc.)	[32]
3	$e + H \rightarrow 2e + H^+$	[32]
4	$e + H_2 \rightarrow e + H_2$ (elastic)	[76]
5	$e ~+~ H_2 ~\rightarrow~ 2e ~+~ H_2^+$	[32]
6	$e ~+~ H_2 ~\rightarrow~ 2e ~+~ H^+ ~+~ H$	[32]
	(2 proc.)	
7	$e + H_2 \rightarrow e + H_2$ (inelastic,	[32-38]
	16 proc.)	
8	$e + H_2 \rightarrow e + 2H (3 \text{ proc.})$	[32, 77]
9	$e + H_3^+ \rightarrow 3H$	[32]
10	$e ~+~ H_3^+ ~\rightarrow~ H~+~ H_2$	[32]
11	$e ~+~ H_3^+ ~\rightarrow~ e ~+~ H^+ ~+~ 2H$	[32]
12	$e \ + \ H_3^+ \ \to \ e \ + \ H^+ \ + \ H_2$	[32]
13	$e ~+~ H_2^+ ~\rightarrow~ 2H$	[32]
14	$e ~+~ H_2^+ ~\rightarrow~ e ~+~ H^+ ~+~ H$	[32, 77]
	(2 proc.)	
15	$e ~+~ H_2^+ ~\rightarrow~ 2e ~+~ 2H^+$	[77]
16	$e + H^- \rightarrow 2e + H$	[32]
17	$e + H_2^* \rightarrow H^- + H (1\% \text{ of } H_2)$	[77]
18	$e \ + \ H_2^+ \ \rightarrow \ e \ + \ H_2^+$	(Coulomb)[22]
19	$e ~+~ H^+ ~\rightarrow~ e ~+~ H^+$	(Coulomb)[22]
20	$e ~+~ H_3^+ ~\rightarrow~ e ~+~ H_3^+$	(Coulomb)[22]

~60 reactions implemented in the PIC-MCC model

Table 2. Heavy particle processes.

#	Reaction	Cross sectior reference
1	H_3^+ + H_2 \rightarrow H_3^+ + H_2 (elastic)	[78]
2	$\mathrm{H_3^+}~+~\mathrm{H}~\rightarrow~\mathrm{H_3^+}~+~\mathrm{H}$ (elastic)	
3	$H_2^+ \ + \ H_2 \ \rightarrow \ H_3^+ \ + \ H$	[43, 78]
4	$H_2^+ \ + \ H_2 \ \rightarrow \ H_2 \ + \ H_2^+$	[78]
5	$H_2^+ + H \rightarrow H_2^+ + H$ (elastic)	[79]
6	$\mathrm{H^+}$ + H \rightarrow H + $\mathrm{H^+}$	[80]
7	$\mathrm{H^{+}}~+~\mathrm{H}~\rightarrow~\mathrm{H^{+}}~+~\mathrm{H}$ (elastic)	[80]
8	$H^+ + H_2 \rightarrow H^+ + H_2$ (elastic)	[78]
9	$H^+ + H_2 \rightarrow H^+ + H_2$ (inelastic,	[41-43, 78]
	4 proc.)	
10	$H^- + H \rightarrow e + 2H$	[32]
11	$\mathrm{H^-}$ + H \rightarrow e + H ₂	[32]
12	$\mathrm{H^-} + \mathrm{H_2} \rightarrow \mathrm{H^-} + \mathrm{H_2} (\mathrm{elastic})$	[43]
13	$\mathrm{H^-}~+~\mathrm{H}~\rightarrow~\mathrm{H^-}~+~\mathrm{H}~(\mathrm{elastic})$	[43]
14	$\mathrm{H^{+}}~+~\mathrm{H^{-}}~\rightarrow~~2\mathrm{H}~(2~\mathrm{proc.})$	[32]
15	$\mathrm{H^+}~+~\mathrm{H^-}~\rightarrow~\mathrm{H_2^+}~+~\mathrm{e}$	[32]
16	$\mathrm{H^-}$ + $\mathrm{H_2}$ \rightarrow $\mathrm{H_2}$ + H + e	[32]
17	$H^- + H \rightarrow H + H^-$	[81]
18	$H + H \rightarrow H + H$	[80]
19	$H \ + \ H_2 \ \rightarrow \ H \ + \ H_2$	[80]
20	$H_2 \ + \ H_2 \ \rightarrow \ H_2 \ + \ H_2$	[82]





- High brightness negative ion beams are produced on the plasma grid (PG) surface
- Cesium is added to lower the metal work function (typically Cs/Mo converters)
- A high negative ion current emitted from the PG surface may be space charge limited:
 - Formation of a virtual cathode
 - A large chunk of ions are hence reflected back onto the PG surface



G. Fubiani *et al.*, Phys. of Plasmas **25** (2018) G. Fubiani *et al.*, New Journal of Physics **19** (2017)



Examples: plasma properties of a fusion-type negative ion source



Negative ions produced in volume account for 10 to 20% of the total amount extracted



Examples: Modeling negative ion extraction; chamfered vs. bevel *slit* apertures geometries



- Extracted negative ion current is *somewhat proportional* to the grid surface area facing the plasma
 - In agreement with the experiments*
 - Aberrations are generated on the chamfered surface
 - Need a 4096×2048 mesh nodes to properly resolve the virtual cathode (<n_p>= 3.10^{17} m^{-3})

*M. Kashiwagi et al., Rev. Sci. Instrum. 85, 02B320 (2014)



Negative ion flux calculated by the model



Slight magnetization of the negative ions affect the beamlet current density profile