

# **Introduction of the GBS plasma and neutrals multispecies model**

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The GBS code *[M. Giacomin et al 2021, JCP submitted]* is based on the drift-reduced Braginskii equations

- Magnetic pre-sheath boundary conditions
- Heating and fuelling modelled self consistently by coupling with kinetic neutral model
- TCV-like geometry with rectangular poloidal cross section
- Full-device modelling (core + edge + SOL)
- Arbitrary magnetic field





Plasma described by Braginskii drift-reduced equations:

$$
\frac{\partial n}{\partial t} = \frac{1}{-\frac{1}{B}[\phi, n]} + \frac{2}{eB} \Big[ C(p_e) - enC(\phi) \Big] - \nabla_{\parallel}(nv_{\parallel e}) + \nu_{iz}n_{\rm n} - \nu_{\rm rec}n
$$
\nExpression

\nConvection to curvature term

Similar equations for 
$$
\;T_e,T_i,v_{\parallel e},v_{\parallel i},\nabla^2\phi
$$

Reaction rates taken as functions of  $T_{e}$ ,  $T_{i}$ , n



*[M. Giacomin et al 2021, JCP submitted]*

## **Kinetic mono atomic neutral species**

$$
\bigcirc \hspace{-0.5mm} \bigcirc
$$

$$
\frac{\partial f_n}{\partial t} + \mathbf{v} \cdot \frac{\partial f_n}{\partial \mathbf{x}} = -\nu_{iz} f_n - \nu_{cx} \left( f_n - \frac{n_n}{n_i} f_i \right) + \nu_{rec} f_n
$$

with:

- Ionization
- Charge exchange
- Recombination
- e-n collisions

 $\nu_{\rm ex} = n_i \langle v_i \sigma_{\rm ex} \rangle_{v_i}$  $\nu_{\rm rec} = n_e \langle v_e \sigma_{\rm rec} \rangle_{v_e}$  $\nu_{\text{en}} = n_e \langle v_e \sigma_{\text{en}} \rangle_{v_e}$ 

 $\nu_{iz} = n_e \langle v_e \sigma_{iz} \rangle_{v_e}$ 

**Boundary conditions** : emission or reflection, one neutral for each particle, ion or neutral, impacting the wall

Ion out flux to wall include **parallel** and **drift velocity**

Two limits, valid in typical SOL conditions:

- Neutral adiabatic regime  $\tau_n < \tau_{\text{turb}}$
- Neutral lengths smaller than parallel lengths  $\lambda_{\min,n} << 1/k_{\parallel}$





Integral equation for the neutral distribution function:  
\n
$$
f_n(\mathbf{x}, \mathbf{v}, t) = \int_0^{r'_b} \left[ \frac{S(\mathbf{x}', \mathbf{v}, t')}{v} + \delta(r - r'_b) f_n(\mathbf{x}', \mathbf{v}, t') \right] \exp\left( -\frac{1}{v} \int_0^{r'} \nu_{\text{eff}}(\mathbf{x}'', t'') dr'' \right) dr''
$$

Integrate in velocity space and obtain discrete matrix system for neutral density:

$$
\begin{bmatrix} n_{\rm n} \\ \Gamma_{\rm out,n} \end{bmatrix} = \begin{bmatrix} v_{\rm cx} K_{p \to p} & (1 - \alpha_{\rm refl}) K_{b \to p} \\ v_{\rm cx} K_{p \to b} & (1 - \alpha_{\rm refl}) K_{b \to b} \end{bmatrix} \begin{bmatrix} n_{\rm n} \\ \Gamma_{\rm out,n} \end{bmatrix} + \begin{bmatrix} n_{n,\rm rec} + n_{\rm n[out,i]} \\ \Gamma_{\rm out,rec} + \Gamma_{\rm out, n[out,i]} \end{bmatrix}
$$

where kernels *K* includes contribute from reflection on walls

Solve and evaluate higher moments:  $\Gamma_{n,\perp}$  ,  $\Gamma_{n,\parallel}$  ,  $\Gamma_{n}$ 

### **First diverted turbulence simulations with neutrals**

3 sim with increasing neutrals effects (same SOL input power):

- Higher ionization source in core
- Lower temperature and higher resistivity  $\nu \propto T_e^{-3/2}$

- 200 Radius  $\sim$  1/3 TCV 100 Lower single null
	- $T_e$  source in core
	- Recycling on bottom
	- No recombination in volume





### **Density shoulder formation and neutrals contribute**



With higher density source (and resistivity):

- Increasing near SOL e-folding lengths
- Increasing far SOL density and pressure



Analysis of the roles of: perpendicular flux, parallel flux, ionization source

### **Higher density due to lower parallel transport**





 $\rightarrow$  increase in far SOL density

*[D. Mancini et al 2021, Nucl. Fusion]*

 $\mathbf{I}$ 

### **New plasma model: molecular species**



Plasma described by density, velocity and temperatures of electrons, atomic ions and molecular ions :

$$
\frac{\partial n_e}{\partial t} = -\frac{1}{B} [\phi, n_e] + \frac{2}{eB} [C(p_e) - enC(\phi)] - \nabla_{\parallel} (n_e v_{\parallel e}) + \nu_{iz,D} n_D - \nu_{\text{rec},D^+} n_{D^+} \n+ \nu_{iz,D_2} n_{D_2} - \nu_{\text{rec},D^+_2} n_{D^+_2} + \nu_{\text{diss-iz},D_2} n_{D_2} + \nu_{\text{diss-iz},D^+_2} n_{D^+_2} - \nu_{\text{diss-rec},D^+_2} n_{D^+_2} \n\frac{\partial n_{D^+_2}}{\partial t} = -\frac{1}{B} [\phi, n_{D^+_2}] + \frac{2}{eB} [C(p_{D^+_2}) - en_{D^+_2} C(\phi)] - \nabla_{\parallel} (n_{D^+_2} v_{\parallel, D^+_2}) + \nu_{iz,D_2} n_{D_2} - \nu_{\text{rec},D^+_2} n_{D^+_2} \n+ \nu_{\text{cx},D_2 - D^+} n_{D_2} + n_D \nu_{\text{cx},D - D^+} + n_{D^+_2} (\nu_{\text{diss-iz},D^+_2} + \nu_{\text{diss},D^+_2} + \nu_{\text{diss-rec},D^+_2})
$$

- + quasi neutrality:  $n_{D^+} = n_e n_{D_2^+}$
- Zdhanov closure
- Low molecules density  $n_{D_2^+} << n_{D^+}$
- Magnetic boundary conditions

Page 9 *[A. Coroado et al 2021, Nuclear Fusion, accepted manuscript]*



Atomic and molecular neutrals considered:

$$
\frac{\partial f_D}{\partial t} + \mathbf{v} \cdot \frac{\partial f_D}{\partial \mathbf{x}} = -\nu_{iz,D} f_D - \nu_{cx,D} \left( f_D - \frac{n_D}{n_{D^+}} f_{D^+} \right) + \nu_{\text{rec},D^+} f_D^+ + \nu_{cx,D_2 - D^+} \left( \frac{n_{D_2}}{n_{D^+}} f_{D^+} \right) - \nu_{cx,D - D_2^+} f_D
$$
  
+  $f_{D_2} (2\nu_{\text{diss},D_2} + \nu_{\text{diss-iz},D_2}) + f_{D_2^+} (2\nu_{\text{diss-rec},D_2^+} + \nu_{\text{diss},D_2^+})$ 

$$
\frac{\partial f_{D_2}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D_2}}{\partial \mathbf{x}} = -\nu_{iz,D_2} f_{D_2} - \nu_{cx,D_2} \left( f_{D_2} - \frac{n_{D_2}}{n_{D_2^+}} f_{D_2^+} \right) + \nu_{\text{rec},D_2^+} f_{D_2^+} + \nu_{cx,D-D_2^+} \left( \frac{n_{D}}{n_{D_2^+}} f_{D_2^+} \right) \n- \nu_{cx,D_2-D} + f_{D_2} - f_{D_2} (\nu_{\text{diss},D_2} - \nu_{\text{diss-iz},D_2})
$$

**Boundary conditions** : emission or reflection for each particle impacting the wall, or association of atomic ions and neutrals in molecular neutrals

Same limits, valid in typical SOL conditions:

- Neutral adiabatic regime  $\tau_n < \tau_{\text{turb}}$
- Neutral lengths smaller than parallel lengths  $\lambda_{\min,n} << 1/k_{\parallel}$



Two coupled integral equations solved as a linear system:

$$
\begin{pmatrix} n_D \\ \Gamma_{\text{out},D} \\ n_{D_2} \\ \Gamma_{\text{out},D2} \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} & M_{13} & 0 \\ M_{21} & M_{22} & M_{23} & 0 \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{pmatrix} \begin{pmatrix} n_D \\ \Gamma_{\text{out},D} \\ n_{D_2} \\ \Gamma_{\text{out},D2} \end{pmatrix} + \begin{pmatrix} n_{\text{re},D^+} + n_D^{\text{diss},D_2^+} \\ \Gamma_D^{\text{rec},D^+} + \Gamma_{\text{out},D}^{\text{refl},D^+} \\ n_{D_2}^{\text{rec},D^+} \\ \Gamma_{\text{D}_2}^{\text{rec},D^+} + \Gamma_{\text{D}_2}^{\text{refl},D^+} \end{pmatrix}
$$

- sub-matrices **M** include the different kernel functions **K**, considering also reflection and association on walls
- Known terms comes from recombination, reflection or dissociation of ions

#### Possibility to extend the model to include any kind of species

Page 11 *[A. Coroado et al 2021, Nuclear Fusion, accepted manuscript]*

### **Densities evaluated solving one linear system**



- sub-matrices **M** include the different kernel functions **K**, considering also reflection and association on walls
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#### Possibility to extend the model to include any kind of species

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### **Test simulation with multispecies model**



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Small, lower single null configuration, as testbed:

$$
\left(\frac{\partial n_e}{\partial t}\right)_{\text{neu}} = n_D \nu_{iz, D} + n_{D_2} (\nu_{\text{diss}, D_2} + \nu_{iz, D_2}) - n_{D_2^+} (\nu_{\text{rec}, D_2^+} + \nu_{\text{diss-rec}, D_2^+})
$$
\n
$$
\frac{S_{\delta_1, iz}^e + S_{\delta_1, dss-iz}}{S_{\delta_1, iz}^e}
$$
\n
$$
\frac{S_{\delta_1, iz}^e + S_{\delta_1, dss-iz}}{S_{\delta_1, iz}^e}
$$
\n
$$
\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, iz}^e}
$$
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\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, iz}^e}
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\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, iz}^e}
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\frac{S_{\delta_1, iz}^e + S_{\delta_1, dss-iz}}{S_{\delta_2, iz}^e}
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\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, iz}^e}
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\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, iz}^e}
$$
\n
$$
\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, iz}^e}
$$
\n
$$
\frac{S_{\delta_2, iz}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, z}} = \frac{S_{\delta_2, z}^e + S_{\delta_2, dss-iz}}{S_{\delta_2, z}} = \frac{S_{\delta_2, z}^e + S_{\delta_2, dss-iz}}
$$

## **Summary**



- A neutral model coupled with the GBS plasma model is implemented
- The monoatomic neutral model is tested and used to investigate the role of neutrals in the shoulder formation, giving insights on the phenomenon
- A new framework for multispecies plasma and neutral is introduced:
	- Plasma model developed with Zdhanov closure and extended magnetic boundary conditions
	- Neutrals model developed with multiple neutral distribution functions and equations solved in a bigger linear system
- The framework is tested in a simulation with molecular and atomic ions and neutrals