Modeling of Plasmas and Neutrals Including Plasma-Wall Interaction for Long Term Tokamak Operation

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1. Background/Motivation (1)

- **Density control** of the **core/main plasma** in future fusion reactors like **ITER/DEMO** is one of the **critical issues**, especially for their long term operation.

- **Metal plasma facing materials** (**PFMs**) are expected to be one of the promising **candidates** for such **future fusion power plants**.

- Recently, **experimental studies**:
  
  the **effects** of the **long time scale plasma – PFM wall interaction** on the main **plasma density** and its control have been done in the **QUEST** tokamak [1,2,3].

  suggest that the **wall H atom-inventory play a key role** !

1. Background/Motivation (2)

- The **purpose of this study** is to **develop a simple plasma and neutral model** which includes the **long term plasma-wall interaction**, especially the interaction between the **plasma** and **metal PFMs**.

- in order to understand **basic characteristics** of the **long term behavior** of **particle balance** in the **overall system** including:
  a) **Main Plasma**, b) **SOL/Divertor/Limiter Plasma**, c) **Wall**

- **Conventional 2D/3D Edge plasma-neutral code** (e.g. SOLPS(B2.5-Eirene), EDGE2D, UEDGE, SONIC) is **too massive** to simulate **for such a long time dynamics of the system**.

  *adopt zero-dimensional (0D) approach* taking into account the profile effect from the 2D/3D code results*
2. Model (1) : Basic Model Concept

**Particle Balance** model for the **overall system**:

(a) Main Plasma, (b) SOL/Divertor/Limiter Plasma, (c) Wall

![Diagram showing model geometry](image1)

**Particle Species in the System**

i) Plasma: \(\text{elec.}, \text{H}^+, \text{H}_2^+, \text{H}_3^+\)

ii) Neutrals \(\text{H}_2, \text{H}\)

iii) Wall Material

![Diagram showing overall concept of the present model](image2)

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Fig.1 Schematic drawing of the **model geometry** (QEST limiter configuration)

Fig.2 Overall **concept of the present model**
2. Model: Plasma Model (1)

(1a) Main Plasma

\[ \frac{d\bar{n}_M}{dt} = -\frac{\bar{n}_M}{\tau_M} + \bar{S}_M, \]  

\[ \bar{n}_M : \text{Volume averaged plasma density} \]
\[ \bar{S}_M : \text{Volume averaged ionization source} \]
\[ \tau_M : \text{the particle confinement time of main plasma} \]

Plasma transport loss across the magnetic field line

\[ \bar{n}_M = \frac{1}{V_M} \int_{V_M} n_M dV \]  

\[ \bar{S}_M = \frac{1}{V_M} \int_{V_M} S_M dV \]

\[ \alpha_M : \text{profile factor which relates the density at the LCFS} \]
\[ n_{LCFS} \]
\[ \text{with the volume averaged density} \quad \bar{n}_M \]

\[ n_{LCFS} = \alpha_M \bar{n}_M \]
2. Model: Plasma Model (2)

(1b) SOL/Limiter Plasma

\[
\frac{d\bar{n}_{SOL}}{dt} = (1 - f_{wall}) \bar{S}_{Diff} - \frac{\bar{n}_{SOL}}{\tau_{\parallel}} + \bar{S}_{SOL}, \quad (1b1)
\]

\[
\bar{S}_{Diff} = \bar{n}_M \quad (1b2)
\]

Plasma Source from the main plasma

Plasma loss along the magnetic field line

Recycling Source from the limiter plate

\(\bar{n}_{SOL}\) : Volume averaged plasma density in the SOL/Limiter region

\(\bar{S}_{Diff}\) : Diffusion source from the main plasma across the LCFS

\(f_{wall}\) : fraction of \(\bar{S}_{Diff}\) to the wall

\(\bar{S}_{SOL}\) : Volume averaged ionization source

\(\tau_{\parallel}\) : the plasma confinement time in the SOL region

\[
\tau_{\parallel} = \frac{L_{\parallel}}{2\alpha_{SOL} C_s} \quad (1b5)
\]

\(L_{\parallel}\) : SOL connection length along B-field

\(C_s\) : Ion sound speed along B-field

\(\alpha_{SOL}\) : profile factor which relates the density in front of the limiter plate \(n_{LIM}\) with the volume averaged density \(\bar{n}_{SOL}\):

\[
n_{LIM} = \alpha_{SOL} \bar{n}_{SOL} \quad (1b6)
\]

\[
\bar{n}_M = \frac{1}{V_M} \int_{V_M} n_M dV \quad (1b3)
\]

\[
\bar{S}_{SOL} = \frac{1}{V_{SOL}} \int_{V_{SOL}} S_{SOL} dV \quad (1b4)
\]
2. Model: Neutral Model (1)

(2a) H2 Molecules

\[
\frac{d\bar{n}_{H_2}}{dt} = \bar{S}^{\text{Gas-Puff}}_{H_2} + \bar{S}^{\text{Wall/Lim}}_{H_2} + \bar{S}^{\text{gain}}_{H_2} - \bar{S}^{\text{loss}}_{H_2} - \bar{S}^{\text{Pump}}_{H_2} - \frac{\bar{n}_{H_2}}{\tau_{H_2}}
\]

Gas-puffing source

Recycling source from the Wall and Limiter

Gas-pumping sink

Gain and Loss due to H2 reactions in the gas phase

Neutral transport loss

\[
\tau_{H_2} = \frac{(V_V / A_V)}{\alpha_{H_2} \nu_{H_2}}
\]

Discuss later in the wall model

Table 2.1

Main reactions taken into account

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2a1)</td>
<td>H2 reactions in the gas phase</td>
</tr>
</tbody>
</table>

\( V_V \): Volume of vacuum vessel

\( A_V \): Surface area of vacuum vessel

\( \alpha_{H_2} \): Profile factor

\( \nu_{H_2} \): Average speed of H2 molecules

Profile effect is taken into account by the 2D neutral transport simulation
2. Model: Neutral Model (2)

(2b) H atom in gas phase

\[
\frac{d\bar{n}_H}{dt} = S^\text{gain}_H - S^\text{loss}_H - S^\text{CX}_H - \bar{n}_H = 0
\]  

(2b1)

Gain and Loss due to H reactions in the gas phase

Neutral transport loss

\[ \tau_H = \frac{(V_V / A_V)}{\alpha_H v_H} \]  

(2b2)

Table 2.1
Main reactions taken into account

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

- \( V_V \): Volume of vacuum vessel
- \( A_V \): Surface area of vacuum vessel
- \( \alpha_H \): Profile factor
- \( v_{H2} \): average speed of H atoms

Profile effect is taken into account by the 2D neutral transport simulation.
2. Model: Neutral Model (3)

Table 2.1 Main reactions taken into account in the model.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Eq.</th>
</tr>
</thead>
<tbody>
<tr>
<td>H ionization</td>
<td>( H(p) + e \rightarrow H^+ + 2e )</td>
</tr>
<tr>
<td>( H_2 ) dissociation</td>
<td>( H_2 (v) + e \rightarrow 2H + e )</td>
</tr>
<tr>
<td>( H_2 ) ionization</td>
<td>( H_2 (v) + e \rightarrow H_2^+ + 2e )</td>
</tr>
<tr>
<td>( H_2 ) dissociative ionization</td>
<td>( H_2 + e \rightarrow H + H^+ + 2e )</td>
</tr>
<tr>
<td>( H_2^+ ) dissociation</td>
<td>( H_2^+ + e \rightarrow H + H^+ + e )</td>
</tr>
<tr>
<td>( H_2^+ ) dissociative recombination</td>
<td>( H_2^+ + e \rightarrow 2H )</td>
</tr>
<tr>
<td>( H_3^+ ) dissociative recombination</td>
<td>( H_3^+ + e \rightarrow 3H ) (or ( H_2 + H ))</td>
</tr>
<tr>
<td>( H_3^+ ) dissociative recombination</td>
<td>( H_3^+ + e \rightarrow 2H + H^+ + e )</td>
</tr>
<tr>
<td>H, ( H^+ ) charge exchange</td>
<td>( H + H^+ \rightarrow H^+ + H )</td>
</tr>
<tr>
<td>( H_2, H^+ ) charge exchange</td>
<td>( H_2 + H^+ \rightarrow H_2^+ + H )</td>
</tr>
<tr>
<td>( H_3^+ ) production</td>
<td>( H_2 + H_2^+ \rightarrow H_3^+ + H )</td>
</tr>
<tr>
<td>H ionization by ( H^+ )</td>
<td>( H + H^+ \rightarrow 2H^+ + e )</td>
</tr>
<tr>
<td>( H_2^+ ) dissociative ionization</td>
<td>( H_2^+ + e \rightarrow 2H^+ + 2e )</td>
</tr>
</tbody>
</table>
2. Model: Neutral Model (4)

In addition to the ground-state atom modeled above, we solve a system of simultaneous rate equations for the population density of excited atoms with the quasi-steady state collisional-radiative model (QSS-CR) to compare the H$\alpha$ intensity measured in the experiments.


Model validations of the QSS-CR model have been already done in several H$^-$ ion sources (QST 10A H$^-$ source, CERN Linac4 H$^-$ source, … etc.)
2. Model : Wall & Limiter Model (1)

(3a) Wall

\[
\frac{d\tilde{n}_{Wall}}{dt} = \Gamma_{Wall} - \frac{2k_{Wall}}{d_{Wall}} \tilde{n}_{Wall}^2
\]

(3a1) \[\tilde{n}_{Wall}\] : H atom wall-inventory (in the re-deposition layer)

**Plasma in-flux to the wall**

\[
\Gamma_{Wall} = f_{wall} \Gamma_{LCFS} \left( \frac{A_{LCFS}}{A_{Wall}} \right) + \frac{A_{Wall}}{A_{Wall} + A_{Lim}} \tilde{S}_{CX} \left( \frac{V_M}{A_{LCFS}} \right)
\]

(3a2)

**H2 out-flux from the wall**

- \[k_{Wall}\] : H atom recombination rate in the re-deposition layer
- \[d_{Wall}\] : thickness of the re-deposition layer

**Ion flux from the main plasma**

Calculated by main plasma model Eq.(1a1)

**CX H atom flux**

Calculated by H atom model Eq.(2b1)

\[A_{LCFS} \quad A_{Wall} \quad A_{Lim}\] : Surface area of LCFS, Wall and Limiter, respectively
2. Model : Wall & Limiter Model \( (2) \)

\[(3b) \text{ Limiter} \]

\[
\frac{d\bar{n}_{\text{Lim}}}{dt} = \frac{\Gamma_{//,\text{Lim}}}{d_{\text{Lim}}} - \frac{2k_{\text{Lim}} n_{\text{Lim}}}{d_{\text{Lim}}} \bar{n}_{\text{Lim}}^2
\]

\( (3b1) \) \( \bar{n}_{\text{Lim}} \) : H atom limiter-inventory (in the re-deposition layer)

**Plasma in-flux to the limiter**

**H2 out-flux from the limiter**

\( k_{\text{Lim}} \) : H atom recombination rate in the re-deposition layer

\( d_{\text{Lim}} \) : thickness of the re-deposition layer

\[
\Gamma_{//,\text{Lim}} = \frac{\bar{n}_{\text{SOL}}}{\tau_{//}} \frac{V_{\text{SOL}}}{\alpha_{\text{SOL}} A_{\text{Lim}}} + \frac{A_{\text{Lim}}}{A_{\text{wall}} + A_{\text{Lim}}} \bar{S}_{\text{CX}} \left( \frac{V_{M}}{A_{\text{LCFS}}} \right) \]

\( (3b2) \)

**Ion flux from the SOL plasma**

Calculated by SOL plasma model Eq.(2a1)

**CX H atom flux**

Calculated by H atom model Eq.(2b1)
3. Initial Model Application to QUEST

(1) Main Assumptions / Calculation Conditions

- **Low density** sheath limited **attached state in front of the limiter** has been assumed
- **Wall** and **Limiter Material** are the same for simplicity

### Table 3.1 Device and Plasma Dimensions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Major radius</td>
<td>R=0.68 m</td>
</tr>
<tr>
<td>Minor radius</td>
<td>a=0.4 m</td>
</tr>
<tr>
<td>Volume of main plasma</td>
<td>Vp=1.28 m³</td>
</tr>
<tr>
<td>Volume of vacuum vessel</td>
<td>Vv=12.8 m³</td>
</tr>
<tr>
<td>Surface area of vacuum vessel</td>
<td>Av=26.5 m²</td>
</tr>
</tbody>
</table>

### Table 3.2 Gas puffing and pumping parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas puffing rate</td>
<td>3.5x10¹⁸/puffing for 10ms</td>
</tr>
<tr>
<td>Gas pumping rate</td>
<td>1.7x10¹⁷/s</td>
</tr>
</tbody>
</table>

Fig. 2 Schematic drawing of the model geometry (QEST limiter configuration)
3. Initial Model Application to QUEST(1)

Table 3.3 Initial density for each particle species

<table>
<thead>
<tr>
<th>Species</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma</td>
<td>( n_e = n_{H^+} = 1 \times 10^{17} \text{m}^{-3} )</td>
</tr>
<tr>
<td>H2 Molecule</td>
<td>( n_{H_2} = 1 \times 10^{15} \text{m}^{-3} )</td>
</tr>
<tr>
<td>H atom</td>
<td>( n_H = 1 \times 10^{10} \text{m}^{-3} )</td>
</tr>
</tbody>
</table>

Plasma particle diffusion coeff.: \( D = 0.3 \text{ m}^2/\text{s} \)

Table 3.4 Profile factor of plasma & neutral density

<table>
<thead>
<tr>
<th>Density Profile Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma profile factor</td>
</tr>
<tr>
<td>Neutral profile factor for H(_2)</td>
</tr>
</tbody>
</table>

Table 3.5 Temperature for each particle species

<table>
<thead>
<tr>
<th>Species</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron</td>
<td>( T_e = 10 \text{ eV} )</td>
</tr>
<tr>
<td>Ion</td>
<td>( T_i = 1 \text{ eV} )</td>
</tr>
<tr>
<td>H2 Molecule</td>
<td>( T_{H_2} = 0.01 \text{ eV} )</td>
</tr>
<tr>
<td>H atom</td>
<td>( T_H = 0.1 \text{ eV} )</td>
</tr>
</tbody>
</table>

Table 3.6 Wall parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>H recombination coefficient for the wall</td>
<td>( k_{\text{wall}} = 1 \times 10^{-38} \text{ m}^4/\text{s} )</td>
</tr>
<tr>
<td>Thickness of the re-deposition layer</td>
<td>( d_{\text{wall}} = 50 \text{ nm} )</td>
</tr>
</tbody>
</table>
3. Initial Model Application to QUEST

(2) Time evolution of main plasma and wall parameters

\[ T_e=10\text{eV}, \quad T_i=1\text{eV} \quad D=0.3 \text{ m}^2/\text{s} \]

\[ k_w=1.0\times10^{-38} \text{ m}^4/\text{s} \]

Fig. 3.1 (a) plasma density and \( \text{H}_\alpha \) intensity

- During early phase \( 0 \leq t \leq 30 \text{ s} \) before the saturation of the \( \text{H} \) atom wall-inventory frequency of gas puffing (corresponding to the rapid increase in \( \text{H}_\alpha \) signal) is large.

- After the saturation of wall \( \text{H} \) atom inventory \( t \geq 60 \text{ s} \)

  \( \text{H}_\alpha \) signal is almost constant and
  the plasma density is mainly sustained by the gas feed from the wall.

- Saturation level of \( \text{H} \)-atom wall inventory agrees with that estimated in the experiments with a reasonable value of wall recombination coefficient.
3. Initial Model Application to QUEST(3)

(3) Comparison with the experiments
- Effect of the wall temperature on the H atom wall-inventory

**Experimental results** [3]

- Low Wall Temp.: Room Temp
- High Wall Temp.: 373K

**Modeling results**

- Low Wall Temp.: $k_w = 0.2 \times 10^{-38} \text{ m}^4/\text{s}$
- High Wall Temp.: $k_w = 1.0 \times 10^{-38} \text{ m}^4/\text{s}$

- Quantitatively, however, time to reach the saturation in the modeling is relatively short (~ 60 -70 s) compared with those (> 100s) in the modeling.

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3. Initial Model Application to QUEST (4)

(3) Comparison with experiments: Time evolution of Hα signal

Experimental results [3]

Modeling results

- In High Wall Temp. Case, Hα signal becomes almost constant more earlier than in Low Temp. Case – main plasma density is mainly sustained/controlled not by the external gas puffing, but by the wall out-flux after the saturation

3. Initial Model Application to QUEST

(4) Our model really robust?
- Sensitivity analysis of the results on key assumptions/parameters – $T_e$

**plasma density and H$\alpha$ intensity**

**Wall H atom-inventory**

**Fig.3.4**

(a) $T_e = 10\text{eV}$

(b) $T_e = 30\text{eV}$

(c) $T_e = 50\text{eV}$
3. Initial Model Application to QUEST

(4) Our model really robust?
- Sensitivity analysis of the results on key assumptions/parameters – $D$

**plasma density and $H_\alpha$ intensity**

**Wall H atom-inventory**

**Fig. 3.6**

(a) $D=0.3 \text{ m}^2/\text{s}$
* typical value in most of 2D Edge Plasma simulations

(b) $D=0.6 \text{ m}^2/\text{s}$

(c) $D=1.2 \text{ m}^2/\text{s}$
* estimated by Bohm diffusion
$D \sim (1/16)(Te/B)$
4. Summary & Future Problem (1)

- we have developed a simple zero dimensional (0D) model which consists of the particle balance equations for the following three different particle species:

  i) hydrogen plasma (elec., H\(^+\), H\(_2\)\(^+\), H\(_3\)\(^+\)),
  ii) neutral hydrogen atoms (H) and molecules (H\(_2\)) in the gas phase
  iii) wall-stored H atoms.

- The model has been applied to a long term operation (up to \(~100\text{-}200\) s) with the limiter configuration in the QUEST tokamak.
4. Summary & Future Problem (2)

- **Modeling results** of the long time evolution (~ 100-200 s) reasonably reproduce experimental tendencies:

  - **Density feedback control** by \( \text{H} \alpha \) signal and external gas puffing is **efficient** in the **early phase** (<100s)

  - **For more long time scale** (>100s), the **particle balance** of the system is mainly **sustained**
    not by the **external particle source/pumping**, but by the **wall recycling source**.

  - Modeling results of the **H-atom wall inventory** reasonably agree well with those in the experiments with a reasonable value of wall recombination coeff.
However, **further model validation** and **improvement** will be needed:

- **More Systematic sensitivity analysis of the results on the main assumptions and input parameters:**
  - e.g. $T_e$, $T_i$, $D$, **profile factor from 2D/3D Edge simulation**, ...
  
  As for the $T_e$, $D$, the "**basic tendencies**" are **not so sensitive** on these parameters, if we change these parameters **in the reasonable range**: $T_e \sim 10$-$50$eV, $D \sim 0.3$-$1.2$ m²/s

- For **more long term phenomena** (~ several 100-1000s,)
  **further model improvement** will be necessary:
  
  e.g. taking into account **effects of the H trapping site in deposition layer**