Modeling hydrocarbon generation / transport
In fusion experiments

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First Meeting
Co-ordinated Research Program
” Atomic and Molecular Data for Plasma Modelling ”
IAEA
Vienna International Centre
September 26-28, 2005
ITER tritium retention issues
G. Federici, ITER GWS  PSIF Workshop*  
(to be published, Physica Scripta)

ITER predictions still uncertain due to
  – chemical erosion yields at high temperature and fluxes
  – effects of type 1 ELMs (ablation)
  – effects of gaps
  – effects of mixed materials
  – lack of code validation in detached plasma.

• T issues will be heavily scrutinised by licensing authorities.
• Scale-up of removal rate required is $10^4$.
• Potential options for T removal techniques for ITER.
  1) Remove whole co-deposit by:
     • oxidation (maybe aided by RF)
     • ablation with pulsed energy (laser or flashlamp).
  2) Release T by breaking C:T chemical bond:
     • Isotope exchange
     • Heating to high temperatures e.g. by laser, or ...

* “New directions for computer simulations and experiments in plasma–surface interactions for fusion”:
Fusion applications of hydrocarbon rate data
Erosion / re-deposition / tritium retention
  (DIII-D, Tore Supra, JET examples)
  - long discharges -> hydrocarbon films
  - chemical erosion and T inventory
Use of presently available data
  PISCES linear reflex arc (Erhardt-Langer)
  throat of Tore Supra neutralizer
    (compare E-L and Janev - Reiter)
  DIII-D gaps
ELMs
## Codes in use for erosion/deposition/retention

(D Coster, J Hogan PSIF Workshop Summary Nucl Fus 2005)

### a. 2/3D Kinetic codes

<table>
<thead>
<tr>
<th>Code</th>
<th>WBC</th>
<th>ERO</th>
<th>BBQ</th>
<th>DIVIMP</th>
<th>DORIS</th>
<th>MCI</th>
<th>EDDY</th>
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<tbody>
<tr>
<td>Geometry</td>
<td>3D</td>
<td>2/3D</td>
<td>3D</td>
<td>2D</td>
<td>3D</td>
<td>2D</td>
<td>3D</td>
</tr>
<tr>
<td>Model</td>
<td>TR</td>
<td>TR</td>
<td>TR</td>
<td>TR</td>
<td>TR</td>
<td>TR</td>
<td>TR</td>
</tr>
<tr>
<td>Dynamics</td>
<td>GO</td>
<td>GO</td>
<td>GC</td>
<td>GO</td>
<td>GC</td>
<td>GO</td>
<td>GC</td>
</tr>
</tbody>
</table>

### b. 2D fluid codes

<table>
<thead>
<tr>
<th>Code</th>
<th>SOLPS</th>
<th>EDGE2D</th>
<th>UEDGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry</td>
<td>2D</td>
<td>2D</td>
<td>2D</td>
</tr>
<tr>
<td>Model</td>
<td>SC</td>
<td>SC</td>
<td>SC</td>
</tr>
<tr>
<td>Dynamics</td>
<td>FL</td>
<td>FL</td>
<td>FL</td>
</tr>
</tbody>
</table>

**TR** - trace impurity in fixed background  
**SC** - self-consistent background and impurity solution  
**GO** - gyro orbit following (classical diffusion)  
**GC** - guiding center fluid (anomalous transport)  
**FL** - fluid + kinetic corrections
CD / CH Molecular Band is analyzed to determine the H/D concentration in the divertor (G. Duxbury - Univ Strathclyde)

Relation between chemical erosion processes and H/D/T retention
JET deuterium - hydrogen change-over experiment
D Hillis, J Hogan et al J Nucl Mater 2001

H wall loading
first 5 shots
Of D-->H changeover

H concentration as deduced from the CH-CD Molecular Band

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H concentration as deduced from the CH-CD Molecular Band
Tore Supra

Interior view of Tore Supra

Full toroidal limiter  CIEL
Coupled core/ SOL/PFC code system

CASTEM-TOKAFLU-IMPFLU
BBQ
ITC-SANCO-MIST

\[
\begin{align*}
\Gamma_D^+ \\
\Gamma_e^+ \\
\Gamma_T^+ \\
\Gamma_N^+ \\
\Gamma_C^{in}(Z_i) \\
\Gamma_C^{out}(Z_i)
\end{align*}
\]

Deuterium sputtering stage

=> Core C influx

Sum over processes and geometries

physical
chemical
RES
Superstructure
leading edge
neutralizer

Self-sputtering iteration

Core C influx: \( D^+\) - sputtered

Core C efflux: self-sputtered C
CASTEM-2000 sputtering
Chemical sputtering:
C erosion fluxes for two models

Self sputtering yield

Max. C-C sputtering yield
(atoms / incident ion)

Self-sputtering
sharp increase in yield
with Z_{incident}

Roth et al
11th EFPW

J. Roth et al
NF supplement, (1991)

C emission
flux distribution

Max. C flux
2.1 \times 10^{16} \text{ pt/cm}^2/\text{s}

T_{max} = 400\text{K}

6.0 \times 10^{16} \text{ pt/cm}^2/\text{s}

T_{max} = 825\text{K}
<N_C>
BBQ carbon density averaged over \( \theta, \phi \)

radius (\( \rho/a \))

< N_C >

1.2

10^{18} \text{ m}^{-3}

0.6

0

0.9

0.95

1.0

1.03

1.06

Mid SOL heating

LCFS

III

IV

V

VI

VII
System evolution for localized heating in inner, mid- and far-SOL for:
- TRIM self-sputter (TOP)
- enhanced self-sputter (BOTTOM)
Tore Supra heat, particle flux deposition is strongly influenced by magnetic field ripple (~7%)

Model for C emission from CIEL surface
Initial C flux: TOKAFLU/IMPFLU -> BBQ (physical sputtering)

$P_{rad}(R,\phi)$ BBQ
Model validation requires attention to impurity generation from non-ideal features, e.g., intra-tile gaps

Tore Supra example

Modelled C emission (TOKAFLU / BBQ)

Physical sputtering source

$T_{e,b} = 35 \text{ eV}, \ n_{e,b} = 0.67 \times 10^{19} \text{ m}^{-3}$

$P_{\text{inj}} - P_{\text{rad}} = 0.7 \text{ MW}$

Measured CII radiation (E Dufour, C Lowry et al, EPS 2005)
Sources of BBQ CD₄ Rate Data [W. Langer, A. Erhardt, PPPL Technical Report]

<table>
<thead>
<tr>
<th>#</th>
<th>Reaction</th>
<th>Product</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>e⁻ + CD₄</td>
<td>CD₄⁺ + 2 e⁻</td>
<td>M</td>
</tr>
<tr>
<td>2</td>
<td>CD₃⁺ + D + 2 e⁻</td>
<td></td>
<td>M</td>
</tr>
<tr>
<td>3</td>
<td>CD₃⁻ + D + e⁻</td>
<td></td>
<td>M</td>
</tr>
<tr>
<td>4</td>
<td>e⁻ + CD₄⁺</td>
<td>CD₃⁻ + D⁺ + e⁻</td>
<td>NM: = 1/4 R₁</td>
</tr>
<tr>
<td>5</td>
<td>CD₃⁺ + D + e⁻</td>
<td></td>
<td>NM: = 3/4 R₁</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>CD₃⁻ + D</td>
<td>Tot. R₆ + R₇</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>M for E &lt; 1 eV,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Ex (E &gt; 1 eV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>= 1/4 Rₑxp</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>CD₂⁻ + 2 D</td>
<td>As for R₆,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>R₇ = 3/4 Rₑxp</td>
</tr>
<tr>
<td>8</td>
<td>e⁻ + CD₃</td>
<td>CD₃⁺ + 2 e⁻</td>
<td>CD₃ M</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Ex (E &lt; 15 eV)</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td>CD₂⁺⁺ + D + 2 e⁻</td>
<td>From CD₃ (M)</td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>CD₂⁻ + D + e⁻</td>
<td>NM, = 3/4 R₃</td>
</tr>
<tr>
<td>11</td>
<td>e⁻ + CD₃⁺</td>
<td>CD₂⁻ + D⁺ + e⁻</td>
<td>NM, = 1/3 R₁₀</td>
</tr>
</tbody>
</table>

M = Measured, NM = Not Measured, Ex = Extrapolated, A = Assumed
Sources of the BBQ CD<sub>4</sub> Rate Data [W. Langer, A. Erhardt]

12 \[ CD_2^+ + D + e^- \] \[ NM, = 2/3 R_{10} \]
13 \[ CD_2 + D \] Total M for E < 1 eV,
\[ \text{Ex (E>1 eV)} \]
neglect other channels
14 \[ e^- + CD_2 \] \[ CD_2^+ + 2 e^- \] From CD<sub>2</sub>M(E<200eV)
and CD<sub>4</sub> for E>200eV)
15 \[ CD^+ + D + 2 e^- \] M (CD<sub>2</sub>)
16 \[ CD + D + e^- \] \[ NM, = 1/2 R_3 \]
17 \[ e^- + CD_2^+ \] \[ CD + D^+ + e \] \[ NM, = 1/2 R_{16} \]
18 \[ CD^+ + D + e^- \] \[ NM = 1/2 R_{16} \]
19 \[ CD + D \] Total M (E < 1 eV)
\[ \text{Ex (E>1eV) neglect other channels} \]
20 \[ e^- + CD \] \[ CD^+ + 2 e^- \] NM, adopted CD<sub>4</sub> data
21 \[ C^+ + D + 2 e^- \] NM total R<sub>21</sub>+R<sub>22</sub>
\[ A=1/2 R_9; \ R_{21}=1/2 \text{ total} \]
22 \[ C + D^+ + 2 e^- \] NM, total R<sub>21</sub>+R<sub>22</sub>
\[ A=1/2 R_9; \ R_{22}=1/2 \text{ total} \]
23 \[ C + D + e^- \] \[ NM = 1/4 R_3 \]
24 \[ e^- + CD^+ \] \[ C + D^+ + e^- \] \[ NM = 1/2 R_{23} \]
25 \[ C^+ + D + e^- \] \[ NM = 1/2 R_{23} \]

M = Measured, NM = Not Measured, Ex = Extrapolated, A = Assumed
PISCES - A (UCLA) experiments:
A. Pospieszczyk, FZ-Juelich

Reflex arc linear mirror plasma

Spectroscopic arrangement
Optical multi channel analyzer

Fig. (2) EXPERIMENTAL SETUP
Code - experiment comparison
BBQ - Monte Carlo multi-species simulation (Erhardt-Langer database)
OMA (A. Pospieszczyk, FZ-Juelich)

CH$_2$ axial density

Rel. density

Nozzle location

Downstream distance (cm)

PISCES-A 13417

CH axial density

Rel. density

Nozzle location

Downstream distance (cm)

Optical Multi-channel Analyzer (A. Pospieszczyk, FZ-Juelich)

BBQ
Schematic diagram of experiment on Tore Supra Midplane Limiter (Phase II)

Plasma core

scrape-off layer

E Gauthier, A Cambe J Hogan et al
J Nucl Mater 2003
Carbon production $= f(\phi_D)$
Model comparison using partial pressure
- sensitivity to sputtering model

LHCD: High $T_{\text{surf}}$

\[ P_{\text{CD4}} \propto \varphi_D^{0.73} \]

\[ P_{\text{CD4}} \propto P_{\text{D2}}^{0.70} \]

JT-60U (N. Hosogane)

Increased production of CD$_4$ with flux

OH discharges ($T_{\text{surf}} \sim 500$K)

BBQ comparison

- Roth, Garcia-Rosales
- Mech et al
- Roth PSI 13, mono-energetic
- Roth PSI 13 Maxwell averaged
- Experiment
Deuteron impact charge exchange data [Alman, Ruzic]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Product</th>
<th>Rate (10⁻⁹ cm³/s)</th>
<th>Known (total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{D}^+ + \text{nD}_m \rightarrow \text{D} + \text{nD}_4^+ )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CD₄</td>
<td>D + CD₄⁺</td>
<td>1.880</td>
<td>4.150</td>
</tr>
<tr>
<td>D + CD₄⁺</td>
<td>1.880</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D₂ + CD₃⁺</td>
<td>1.800</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D₂ + CD₂⁺</td>
<td>1.700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D₂ + CD⁺</td>
<td>1.700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₂D₂</td>
<td>D + C₂D₂⁺</td>
<td>2.250</td>
<td>6.300</td>
</tr>
<tr>
<td>D + C₂D₂⁺</td>
<td>2.250</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D₂ + C₂D⁺</td>
<td>2.250</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D₂ + C₂D⁺</td>
<td>4.358</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Heavy hydrocarbon production: dominant species from break-up of $C_2D_2$.

BBQ calculation using Alman-Ruzic database
Janev-Reiter database rates have been implemented in BBQ. A comparison, with the same background plasma conditions, for the Tore Supra pump limiter case, shows significant differences in comparison with the Erhardt-Langer rates.

Janev-Reiter profiles
$n_{e, LP} = 2 \times 10^{18} \text{ m}^{-3}$

- $Te_{LP} = 20 \text{ eV}$
- $Te_{LP} = 10 \text{ eV}$
- $Te_{LP} = 5 \text{ eV}$
Janev-Reiter profiles

CH⁺

CH⁺

CH⁺

CH⁺

CH₄

CH₄

CH₄

nₑ,LP = 6 \times 10^{18} \text{ m}^{-3}

Tₑ,LP = 20 \text{ eV}

Tₑ,LP = 10 \text{ eV}

Tₑ,LP = 5 \text{ eV}
\[
Te_{LP} = 20 \text{ eV}
\]

\[
n_{e,LP} = 6 \times 10^{18} \text{ m}^{-3}
\]

\[
Te_{LP} = 10 \text{ eV}
\]

\[
Te_{LP} = 5 \text{ eV}
\]
Given $D$ flux (or $C_{n^+}$ for self-sputter) to surface and surface temperature, calculate impurity type, rate and velocity distribution.

Mechanisms:
- physical sputtering,
- chemical sputtering (thermal, athermal)
- RES

Impurity generation models

Surface-temperature dependence of chemical and RES yields for $T_e = 10 \rightarrow 90$ eV.

- 3-D, time-dependent finite-elements thermal analysis code developed by CEA-DEMT
- Modifications (CSPUTTER) include:
  - self-consistent heat flux (includes SEE, thermionic emission)
  - local impurity redeposition generation due to $T_{surf}$-dependent mechanisms as well as physical sputtering
  - ablation cooling (Vieder model)

DIII-D intrinsic impurities before/after new tile installation

Some evidence of T-dependent processes

![Filterscope (schematic)](image)

![Carbon concentration (%)](image)

DIII-D intrinsic impurities before/after new tile installation

Some evidence of T-dependent processes
CASTEM-2000 simulation of time-dependent carbon generation from simulated DIII-D localized source

Maximum $T_{surf}$ on heated surface

$T_{surf}$ (K)

0 200 400 600 800 1000 1200

0 1 2 3 4 5

Time (s)

2.5 mm

$Y_{chem}$ @ $t \sim 4s$

when $T_{max} = 1010K$

$Y_{chem \; min} = 1.10^{-2}$

$Y_{chem \; max} = 0.14$

$C$ flux ($10^{18}$ parts/cm$^2$/s)

0 0.4 0.8 1.2 1.6

0 1 2 3 4 5

Time (s)

Chemical

0 0.4 0.8 1.2 1.6

0 1 2 3 4 5

Time (s)
BBQ comparison with spectroscopy is encouraging

C\textsubscript{2}D\textsubscript{2} calculation
- Allman-Ruzic-Brooks rates
- vicinity of the tile gap area

Band spectroscopic modeling gives molecular energies \(\sim 0.1 - 0.3\) eV (R. Isler)

BBQ calculations find near-surface molecular rotational temperatures to be in this range, when respective localization of density and temperature is considered.

Issues: Spectroscopy is averaged over several ELMs
To be quantitative: what are heavy hydrocarbon production rates?
Semi-empirical model for ELM transport enhancement

Green: ELM-affected region in the model
Red: C neutrals and ions
Yellow: D neutrals ion ions

Transport time dependence (schematic)
1. Pre-ELM (barrier)
2. Strong enhancement (100 µsec) ELM
3. Loss of barrier, 2 x pre-ELM value
4. reducing to pre-ELM value as barrier is re-established

Intra-ELM transport radial dependence (schematic)
1. barrier
2. enhancement toward SOL
3. SOL radial transport
C6+ density solps

C6+ density CER

Normalized Radius = 0.81 0.90 0.94 0.96 0.99

Shot = 119434
DIII-D experimental:
fast (CID) camera

CIII 4650.1 evolution
Roth et al
'annealing' model

Modeling
solps 5.0 / Eirene99
IPP-Garching/Greifswald,
FZ-Juelich

CIII 4650.1 evolution
solps 'standard' model
Roth et al
'annealing' model

Inner leg
pre-ELM detached
during attached
re-detching
after recovery of
detachment

CIII evolution:
M Groth et al,
J Nucl Mater 2003
Solps simulation of CIII emission seen by 240par (lower divertor) camera

W Meyer,
M Fenstermacher,
M Groth

LLNL
ELM heat flux mitigation by injection of extrinsic impurities.
Chemical sputtering of carbon materials due to combined bombardment by ions and atomic hydrogen

W Jacob, C. Hopf, M. Schlüter, T. Schwarz-Selinger
Max-Planck-Institut für Plasmaphysik Garching
CONCLUSIONS

Intrinsic (carbon) impurity sources play a key role in ITER, both as regards erosion and for tritium retention.

The ITER problem (addressed also by JET) requires a decision about the first wall material - carbon or an alternative.

Development of validated models for C generation, deposition and retention requires experimental comparison: this typically introduces multiple uncertainties; e.g., sputtering yield models vs hydrocarbon break-up rates.

ITER relevant experimental scenarios involve fast timescale ELM events, for which spectroscopy is an key tool.

The importance of hydrocarbon generation processes has been seen in many experiments, and thus a quantitative, evaluated, integrated model for break-up processes in the plasma is needed.