APPLICATION OF MONTE-CARLO METHODS FOR PHOTON TRANSPORT IN DIVERTORS

MARCH 29 2021  |  SVEN WIESEN (FZJ)
• Introduction

• Radiative transport: transport, Boltzmann equation

• EIRENE Monte-Carlo for solving radiation transport

• Applications
  Industrial: high pressure gas discharge lamps
  Fusion: C-mod, JET, ITER (DEMO)
WHAT PROCESSES CONTROL POWER DISSIPATION?

Complex physics $\rightarrow$ coupled fluid-kinetic 2D/3D edge plasma codes

Change in ionisation-recombination balance due to photon opacity, re-absorption of strong Lyman lines

Impurity radiation $\rightarrow$ Ionization and dissociation of recycling Atoms and molecules $\rightarrow$ Recombination

$P_{\text{SOL}}$

Higher neutral pressure in vertical target configurations

Horizontal target configuration with less dense divertor

1998: C-MOD - DENSE DIVERTOR CLEARLY SHOWS LYMAN-BETA TRAPPING

Terry et al 1998

![Graphs showing Ly\(_\beta\) non-opaque, Ly\(_\beta\) opaque, and D\(_\alpha\) & Ly\(_\gamma\)](image)

Figure 5. (a) Time histories of the Ly\(_\beta\) brightness compared to that predicted for the D\(_\alpha\) brightness measured with essentially the same view for a discharge where there was no trapping of Ly\(_\beta\). (b) The same as (a), but where some trapping is evident. (c) The time history of Ly\(_\gamma\) for the same discharge as (b), indicating that Ly\(_\gamma\) and D\(_\alpha\) stay in a constant ratio, unlike Ly\(_\beta\) and D\(_\alpha\).
D I VUV SPECTRA AND MEASURED LINE INTENSITY RATIOS

- Pulse 91294 is a H fuelled Ohmic density limit pulse at 2.5 T / 2.4MA.
- Opacity is seen to be important reducing Ly$_\alpha$ by $\sim$55% and Ly$_\beta$ by $\sim$6%.
- The $T_e$ dependence suggested by all the theoretical intensity ratios is not observed.
- Either the dominant emission in the line integration moves with a plasma region that has a constant $T_e$ or there are questions regarding the population modelling.
$N_2$ seeding (high $<n_e>$ edge): D emission spectroscopy $\Gamma_{N_2}$ leads to outer leg cooling, inward shift in $S_{iz}$ profile

$n_e$ from D$\delta$ Stark broadening – parameterized model [Lomanowski, NF, 2015]

Continuum (ff+fb) emission encodes high and low $T_e$ information

ff+fb model: adaslib/continuo

ADAS ADF11 ACD, SCD inverse photon efficiency:
$\Rightarrow S_{iz}$ from scanning VUV Ly-$\alpha$ (opacity corrected,
$\Rightarrow S_{rec}$ from D$\varepsilon$
Comparison with **EDGE2D synthetic spectroscopy** ⇒ qualitative agreement in profile evolution, best agreement at highest $f_{\text{RAD}}$

- EDGE2D $n_e$ underestimated (~2x)
- Low N$_2$ seeding ⇒ EDGE2D hotter $T_e$
- High N$_2$ seeding ⇒ good match in $T_e$ profiles
- Shift in ionization front reproduced ⇒ **what about particle balance?**

![Graph showing ionization and recombination profiles](image)

![Comparison of Experiment and EDGE2D with opacity correction vs. no opacity correction](image)

- $I_{\text{div,OT}} \approx S_{\text{iz}}^{\text{Ly-}\alpha} - S_{\text{rec}}$
- Exp. $S_{\text{iz}}^{\text{Ly-}\alpha}$ mediated by $\downarrow T_e$ AND photoexcitation
- EDGE2D $S_{\text{iz}}^{\text{Ly-}\alpha}$ mediated only by $\downarrow T_e$

B. Lomanowski, ITPA – DSOL24 31.05.2017 | Page 5
SIZE-SCALING FOR OPACITY IN TOKAMAKS

- Similarity parameter for opacity importance: $\eta$
- From this: opacity relevant for ITER (DEMO)
- C-mod „closer“ to ITER

$\eta \approx \bar{n}_e^{\text{div}} R \approx \bar{n}_D^{\text{div}} R$
Modelling of “ITER-like” C-mod divertor (high density, vertical targets)

- Neutral pressure & $D_\gamma$ (and $D_\alpha$) emission within x2
- Calculated neutral pressure sensitive to volume recombination, Ly$_\alpha$ opacity, viscosity and ion-molecule elastic collisions
KINETIC (TRANSPORT) EQUATION

- linearized Boltzmann-Equation
- for particles travelling in straight lines between collisions
- with no forces acting on them between collisions

Solving for $f(\vec{r}, \vec{v}, t)$ or $f(\vec{r}, E, \vec{\Omega}, t)$:

$$\left[ \frac{\partial}{\partial t} + v\vec{\Omega} \cdot \nabla \right] f(E, \vec{\Omega}) = S(E, \vec{\Omega}) - v\sigma_a(E)f(E, \vec{\Omega})$$

$$+ \int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' [v'\sigma_s(E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega})f(E', \vec{\Omega}') - v\sigma_s(E \rightarrow E', \vec{\Omega} \cdot \vec{\Omega}')f(E, \vec{\Omega})]$$

Monte-Carlo method:
- EIRENE: Solution of the kinetic transport equation by following test-particle histories
- Averaging over many particle-histories and collision types
  → approximate stochastical solution $f(\vec{r}, E, \vec{\Omega}, t)$
Mathematically, the form of the linearised transport equation for photons and for kinetic particles is identical.

### Particles (fermions)

- **Velocity** \( v \)
- **Energy** \( E_{kin} = \frac{m}{2} v^2 \)

### Photons (bosons)

- **const. lightspeed** \( c \)
- **Energy** \( E_{ph} = h \nu \)

### Solution of transport equation results in:

- **Kinetic particle (energy) flux**
  \[
  \Phi_{kin} = v \frac{m v^2}{2} f_{kin}(\vec{r}, \vec{v})
  \]

- **Specific radiation intensity**
  \[
  I = E c \cdot f_{ph}(\vec{r}, E_{ph}, \Omega)
  \]
RADIATION TRANSPORT EQUATION

\[
\frac{1}{c} \frac{\partial}{\partial t} + \mathbf{\Omega} \cdot \nabla \int (\mathbf{r}, \mathbf{\Omega}, E, t) = j(\mathbf{r}, \mathbf{\Omega}, E, t) - \alpha(\mathbf{r}, \mathbf{\Omega}, E, t) I(\mathbf{r}, \mathbf{\Omega}, E, t) + \frac{\delta I(\mathbf{r}, \mathbf{\Omega}, E, t)}{\delta r}
\]

Photons: sources & sinks

\[
\dot{j}_E^{spont} = n_2 A_{21} \frac{E_{12}}{4\pi} \psi_E
\]

\[
\alpha_E^{abs} = n_1 B_{12} \frac{E_{12}}{4\pi} \phi_E \left( 1 - \frac{n_2 g_1 \psi_E}{n_1 g_2 \phi_E} \right)
\]

Optical thickness

\[
\tau_E(z) = \int_{z_1}^{z_2} dz \alpha(z, E)
\]

\[
\begin{cases} < 1 \quad \text{opt. thin} \\ > 1 \quad \text{opt. thick} \end{cases}
\]

\[
\sim \eta = n^{div} \cdot L^{div}
\]

Doppler Lyman-\(\alpha\) line \(T_n=5\) eV, \(n_n=10^{19} \text{ m}^{-3}\)

MC source sampling distribution

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ITERATIVE PROCEDURE #1

0. Setup initial conditions: e.g. \( n_{n=1}(r)^0 = \text{const}, n_{n=2}(r)^0 = \text{const}, I_E(r)^0 = 0 \)

1. Follow photons with source \( A_{21} n_{n=2}(r)^{i-1} \) on background \( n_{n=1}(r)^{i-1} \rightarrow I_E(r)^i \)

2. Follow neutrals on background \( I_E(r)^{i-1} \rightarrow n_{n=1}(r)^i \) & \( n_{n=2}(r)^i \)

3. Calculate \textit{rate defect} \( d \), if \( d \) close to zero: \text{stop}, otherwise:

4. \( i = i + 1 \); to save memory: copy all fields into background, i.e from \( i \) to \( i - 1 \)

5. Go to step 1

\[
d = \left| \int dv^t \int d\Omega_v^t R_{atom}^{abs} - \int dE^t \int d\Omega_E^t R_{photon}^{abs} \right| \rightarrow 0
\]
FIRST TEST: SLAB PLANCK-MODEL

- Lyman-\( \alpha \)
- Periodic boundary Conditions
- \( T_1 = 1\text{eV}, n_1 = 10^{20}\text{m}^{-3} \)

\[ T \]
\[ n \]

variation of \( N_{\text{MC,A}} \)

Wiesen 2005
FIRST TEST: SLAB PLANCK-MODEL

- Lyman-α
- Periodic boundary Conditions
- $T_1=1\text{eV}, n_1=10^{20}\text{m}^{-3}$

$N_P = 1000000$

- Planck
- Iteration 1
- Iteration 20
- Iteration 70

$I(E) \left[\text{s}^{-1}\text{cm}^{-2}\right]$

$E \left[\text{eV}\right]$
V&V CONT‘D: HIGH-PRESSURE MERCURY-GAS DISCHARGES

Examples of High Intensity Discharge Lamps (HID)

CDM-75 W
Shop-Lighting
Material: PCA

D2-36 W
Automotive
Material: Quartz

R=5 mm, L_\text{el}=5 mm, P=200 W
p_{\text{Hg}}=10 \text{ bar}

p_{\text{Hg}}=100 \text{ bar}
LINE BROADENING MECHANISMS & Profiles

- Lorentz: natural ($A_{ik}$), Stark ($n_e$), Resonanz, Van-der-Waals, turbulence...
- Gaussian: Doppler ($T$)
- Voigt: convolution of Lorentz & Doppler
- Holtsmark (quasi-static)
- isotope-Mixing
- Zeeman splitting and broadening
COMPARISON FOR LYMAN LINES: NATURAL, LINEAR STARK & DOPPLER

Quasi-static ions $T_i$
Collisional elecs $T_e$
Doppler $T_n$
natural

$Ly_\alpha$

$Ly_\beta$

$Ly_\gamma$

$Ly_\delta$

Wiesen 2005
ISOTOPE EFFECT & EFFECTIVE BROADENING

0.1 eV

1 eV

10 eV

100 eV

Lyα

Wiesen 2005
(NORMAL) ZEEMAN EFFECT

\[
\phi_{DZ}(\Delta E, \theta) = \frac{1}{2} \phi_D(\Delta E, T) \sin^2 \theta + \frac{1}{4} \left[ \phi_D(\Delta E - \mu_B B, T) + \phi_D(\Delta E + \mu_B B, T) \right] (1 + \cos^2 \theta)
\]

Relevanz: Zeeman vs Doppler

\[ B[T] > E_0[eV] \sqrt{T[eV]} \]

- normal Zeeman effect leads to additional broadening of line shape → reduction of effective optical thickness \( \tau \)
- anisotropisation of radiation field

Sampling: e.g. \( T=0.5 \) eV, \( B=8T \):

Wiesen 2005

S. Wiesen, 29 March 2021

Member of the Helmholtz Association

JULICH Forschungszentrum
**Epansion of radiation field into cubic splines I^S(E) and orthonormal Y_{lm}(\Omega)**

\[ R_{\text{atom}}^{\text{abs}} = B_{12} \bar{J} = B_{12} \int dE \sum_{lm} I^{S}_{lm}(E) \int d\Omega Y_{lm}(\Omega) \phi_{DZ}(E, \nu, \Omega \cdot \Omega_{\nu}) \]

\[ \phi_{DZ}(E, \nu, \Omega \cdot \Omega_{\nu}) = \sum_{q=\pm 1,0} \sum_{k=0,2} a_{qk} Y_{k0}(\Omega) \phi^{q}(E, \nu, \Omega \cdot \Omega_{\nu}) \]

Rotation:

\[ \Omega_{\nu} \parallel B \quad \rightarrow \quad Y_{lm}(\Omega) = \sum_{m'} Y_{lm'}(\Omega_{\nu}) D_{m'm}^{l}(\nu, \theta_{\nu}, 0) \]

\[ R_{\text{atom}}^{\text{abs}} = B_{12} \int dE \sum_{lm} I^{S}_{lm}(E) \sum_{q} \sum_{k} a_{qk} \int d\Omega Y_{lm}(\Omega) Y_{k0}(\Omega) \phi^{q}(E, \nu, \cos \theta) \]

\[ \bar{\phi}_{l,qk}^{m'm''}(E, \nu) = \int d\Omega_{\nu} Y_{lm'}(\Omega_{\nu}) Y_{km''}(\Omega_{\nu}) \phi^{q}(E, \nu, \cos \theta_{\nu}) \]

Assuming azimuthal symmetry, i.e. only terms w/ \( m' = m'' = 0 \)

Analog: \( R_{\text{photon}}^{\text{abs}} = B_{12} \bar{F} \)

Here: assume isotropic Maxwell atoms
PHOTOEXCITATION IN ITER TOKAMAK

Wiesen 2005
ITER: LYMAN-ALPHA REABSORPTION IN DIVERTOR

opt.thin approx. w/ reabsorption

Fixed plasma, only iterate $D_0(n=1,2)$ & Ly$_\alpha$ photons

Isotropisation in line centre

$n_D(x)$

$n_D$ reduced $\sim 4-5$

S. Wiesen, 29 March 2021

Wiesen 2005
ITERATIVE PROCEDURE #2

• Include iteration of neutrals with plasma: coupling of EIRENE (neutrals & photons) with SOLPS-ITER or EDGE2D or equivalent → fully coupling numerically expensive

• We do not iterate photons/neutrals on themselves (as we can take into account the non-linear interaction of photons with neutrals when iterating with plasma)

• Calculate upper state of a neutral by using a collisional radiative model taking into the reabsorption rates of photons into account from iteration step before

→ That assumes that the upper stages have very short (meta-stable) lifetimes (~A_{ik}), i.e no transport for the upper state included (usually for fusion applications this seems to be a good approximation) also: neglect Zeeman-effect and only Doppler broadening
ITER DIVERTOR ENGINEERING PARAMETER: PEAK TARGET HEAT FLUX VS. DIVERTOR GAS PRESSURE

Lyman opacity not an issue for ITER divertor operational space (shift in required throughput), but change in ionisation-recombination balance and density further upstream (factor 2)

SOLPS4.3 modelling
V.Kotov, D.Reiter, S. Wiesen, A. Kukushkin et al
Figure 4.3: The “equilibrium” effective ionization rate, Formula (4.27), the “opaque” ionization rate and the optically thin ionization rate.

Opaque ionisation rates exceed ordinary ones

Kotov, Reiter, Wiesen et al, 2006
ITER CASE

Kotov, Reiter, Wiesen et al 2006

\[ x = \text{poloidal distance from target} \]
TAILORING OF THE OPTIMAL IMPURITY MIX FOR RELIABLE EXHAUST SCHEME FOR DEMO

Various seeding impurities possible
- Nitrogen: Divertor
- Neon: SOL
- Argon: SOL & pedestal
- Krypton: Pedestal & core
- Xenon: Future machines, pedestal

\[ q_{rad}^{imp} = n_e n_z L_z (n_e, T_e, \tau) l \]

DEMO: 30% core radiation w/ X-point radiator
JET-C: LYMAN-OPACITY IMPORTANT FOR STABLE X-POINT RADIATOR IN SOLPS4.3

Reduction of upstream temperature (and increased density)

\[ n_e^{mid} = 1.6 \times 10^9 \text{ m}^{-3} \]
\[ f_{rad} = 81\% \text{ (D: 28\%, C: 72\%)} \]

Ionization source ⇒ enhanced convective energy flux ⇒ reduced parallel gradient

Same drop for \( T_i \)

Deeper detachment after formation of X-point radiator

\[ n_e^{mid} = 1.62 \times 10^9 \text{ m}^{-3} \]

Model B=Model A + NNC + MAR + transport of Ly photons and photo-excitation

V. Kotov, D. Reiter, S. Wiesen
JNM2013
CONCLUSIONS

• The radiation transport MC module still exists in EIRENE

• Applications: dense tokamak divertors, also: industrial

• The module has been barely used after 2005 → now being reactivated and applied in fusion

• EIRENE photon modul is currently being revised and updated at FZJ to make it generally available (again) to community: as stand alone or as part of e.g. SOLPS)

• New interesting applications in fusion emerging, e.g.:
  - interpretation of spectroscopy → validation of edge codes
  - diagnostics (e.g. metal wall reflections)
  - ITER (with metal wall) and DEMO (at large $f_{\text{rad}}$)
MODEL NEEDS

- Revised CR models with (semi-) opaque lines, validation of opacity models (e.g. isotope effects or collisional broadening in high density - DEMO)

- Wall reflection models for photons, e.g. on W/Be or deposited layers, how to parametrise a model for inclusion into EIRENE, e.g. roughness?

- Comparison with other codes for re-verification in 3D geometries, e.g. CHERAB vs EIRENE

- Code development: Improved Hybrid models for speed up of fully coupled models → EUROfusion TSVV-5
HYBRID METHODS

Hybrid Formulation of Radiation Transport in Optically Thick Divertor Plasmas*

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Received 9 September 2015, revised 20 October 2015, accepted 22 October 2015
Published online 08 July 2016
HYBRID METHODS

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**Fig. 3** Plot of the mean number of collisions calculated using the collision estimator (Monte Carlo simulation) and the model Eq. (10). The model is in a good agreement with the simulation in highly scattering media, i.e., if the mean number of collisions is large.

**Fig. 4** A hybrid Monte Carlo simulation that combines the kinetic equation and a fluid equation can be devised, provided a suitable interfacing between the regions is done. In the second hybrid simulation, the amount of photons escaping from the diffusive region (right) to the kinetic region (left) has been estimated using an ad hoc model.