## Numerical study of the ITER divertor plasma with the B2-EIRENE code package

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## Abstract

The problem of plasma-wall interaction and impurity control is one of the remaining critical issues for development of an industrial energy source based on nuclear fusion of light isotopes. In this field sophisticated integrated numerical tools are widely used both for the analysis of current experiments and for predictions guiding future device design. The present work is dedicated to the numerical modelling of the edge plasma region in divertor configurations of large-scale tokamak fusion devices. A well established software tool for this kind of modelling is the B2-EIRENE code. It was originally developed for a relatively hot ( $\geq 10 \text{ eV}$ ) "high recycling divertor". It did not take into account a number of physical effects which can be potentially important for "detached conditions" (cold, - several eV, - high density, -  $\approx 10^{21} \text{ m}^{-3}$ , - plasma) typical for large tokamak devices. This is especially critical for the modelling of the divertor plasma of ITER: an international project of an experimental tokamak fusion reactor to be built in Cadarache, France by 2016. This present work is devoted to a major upgrade of the B2-EIRENE package, which is routinely used for ITER modelling, essentially with a significantly revised version of EIRENE: the Monte-Carlo neutral transport code.

The main part of the thesis address three major groups of the new physical effects which have been added to the model in frame of this work: the neutral-neutral collisions, the up-to date hydrogen molecular reaction kinetics and the line radiation transport. The impact of the each stage of the upgrade on the self-consistent (between plasma, the neutral gas and the radiation field) solution for the reference ITER case is analysed. The strongest effect is found to be due to the revised molecular collision kinetics, in particular due to hitherto neglected elastic collisions of hydrogen molecules with ions. The newly added non-linear effects (neutral-neutral collisions, radiation opacity) are found to be quite significant for ITER conditions (large size and density) as well, despite the fact that their experimental identification in the presently available smaller devices (including JET) is very difficult.

An experimental validation of this particular package which is used for the ITER design has been carried out for a series of discharges at the Joint European Torus (JET) tokamak (UK, Culham). A relatively good (within a factor 2) agreement for the outer divertor has been found. At the same time, a significant discrepancy between the modelling and the experiment is seen in the inner divertor. As in the case of ITER the model for molecular kinetics has a significant impact on the solution.

The new version of the coupled code (SOLPS4.2) has been made available to the ITER International Team and is now extensively used there. It has already provided significant revisions of currently predicted divertor operational scenarios.

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## **0.1 Introduction**

#### 0.1.1 Fusion research

The topic of this work is numerical modelling of the divertor plasma of tokamak fusion devices. Therefore the terms "fusion", "tokamak" and "divertor" should be explained first.

The ultimate goal of the fusion energy research is creation of a new industrial-scale energy source based on the nuclear fusion of light elements. Due to repulsive Coulomb forces acting between charged nuclei a fusion reaction can only occur if the kinetic energy of the reagents is high enough: tens of kilo-electron volts. The reaction easiest to achieve is the DT reaction D+T $\rightarrow$  <sup>4</sup>He+n+17.6 MeV. This reaction can be efficient already when the average kinetic energy (the temperature) of the reagents is around 10 keV [1], Chapter 1, [2]. For such high temperatures the matter forms a mixture of stripped ions and electrons known as a hot plasma. The principal problem of the fusion research is how to sustain the reaction which can produce industrially relevant amount of energy in a controllable way. Individual fusion reactions have been routinely demonstrated on particle accelerators since 1930th but a net positive energy gain can not be achieved in this way.

Achieving a positive energy release, that is, obtaining more energy from the fusion reactions than it was spent to create the hot plasma, is called the break-even. To reach the break-even the plasma parameters have to meet the so called Lawson criterion. It states that the  $n\tau$  product must exceed roughly  $10^{20} m^{-3} \cdot s$  [2]. Here *n* is the plasma density and  $\tau$  the time scale of the energy loss from the plasma. Presently a modified version of the Lawson criterion, the so called triple product, is used more frequently, see e.g. [2].

The Lawson criterion shows that there are basically two ways to achieve the breakeven. One can try to create an extremely dense plasma during short time. This principle is exploited in inertial confinement (inertial fusion) which is based on the compression of small pellets by intense laser radiation or ion and electron beams [3]. In such devices the plasma exists only for nano-seconds but its density can reach  $10^{30} m^{-3}$  (higher than the solid-state density).

The alternative is to confine a not so dense plasma for relatively long time, ensuring its good thermal insulation. This approach is realized in magnetic confinement devices. A charged particle in magnetic field gyrates around the filed lines due to Lorentz force. The magnetic field of several Tesla allows to "suspend" the plasma, isolating it from the solid walls. The devices of this kind have plasma densities only up to  $10^{20} m^{-3}$  but the energy confinement time is in the range of seconds.



Figure 1: The tokamak magnetic configuration (reproduced from [3]).

Different kinds of devices with magnetic confinement have been studied in the past and are studied now: tokamaks, stellarators, magnetic mirrors, reversed field pinches and others [3]. Tokamaks represent the mainstream of modern fusion research. They are the best studied and the most extensively developed devices. The first projects of fusion reactors (the devices targeting at the industrial level energy production) are based on this concept. However, a significant progress has been made recently for other types of devices as well, especially for stellarators [4].

The tokamak magnetic configuration was first proposed in the USSR by A. Sakharov and I. Tamm [5]. It became the leading type of devices in fusion research since 1967 when the electron temperature exceeding 1 keV was first observed in tokamak T-3 in Kurchatov Institute, Moscow [6]. A schematic of the tokamak geometry and magnetic field is

shown in Figure 1. A magnetic field inside a long coil (a solenoid) is parallel to its axis. In the absence of collisions the charged particles could escape from such a magnetic field only through the ends of the solenoid. To avoid these end losses, one can connect both ends of the solenoid making the geometry toroidal. This kind of magnetic field in a toka-mak, which is created by external coils is called the toroidal field  $B_{\phi}$ . The toroidal field is inherently non-uniform. In particular, it is higher at the inner side of the torus. In a non-uniform magnetic field different kinds of drift motion are possible e.g. gradient drift and curvature drift [7, 8]. The drifts can effectively transport particles across the magnetic

field even in the absence of collisions.

This drift motion can be mitigated by inducing a plasma current in the toroidal direction. This current creates a component of the magnetic field in the poloidal plane (poloidal field)  $B_{\theta}$ , Figure 1. The poloidal plane is the plane containing the torus axis. It can be shown that the presence of the poloidal magnetic field mitigates the drift motion [5], see e.g. [8]. In real devices the poloidal field is created not only by plasma current, but also by extra magnetic coils (poloidal field coils). They are used to enhance stability, to allow an active feedback control of the plasma equilibrium and to shape the magnetic field. The poloidal field is typically an order of magnitude lower than the toroidal one. The toroidal and poloidal magnetic field together form helical magnetic field lines. Most of them do not return to the initial point after a finite number of turns around the torus, but instead fill a closed surface. One speaks therefore not about the field lines but about the nested magnetic surfaces (flux surfaces).

In most of the modern tokamaks the plasma is elongated in vertical direction to make more effective use of the magnetic field (in this way the plasma is pushed towards the high field region). The distance between the axis of the torus and the centre of gravity of the poloidal projection of the plasma volume is called the major radius *R*, Figure 1. The shortest distance between this centre of gravity and the boundary of the plasma volume is called the minor radius *a*. The toroidal current in tokamaks is induced by the alternating magnetic flux created by the vertical central solenoid: the so called inductive current drive. Therefore, the tokamak is an intrinsically pulsed machine, although the duration of the pulses can be very long (up to hundreds seconds) and a non-inductive current current drive is also possible. The toroidal current can also heat the plasma (ohmic heating) but this heating becomes ineffective for temperatures higher than  $\approx 1.5$  keV because of the low plasma resistivity at high temperatures. To reach higher temperatures (10 keV and higher), the auxiliary heating is used. It can be either injection of fast neutral particles (Neutral Beam Injection, NBI) or the resonance electromagnetic waves (Electron Cyclotron and Ion Cyclotron Resonance Heating, ECRH and ICRH).

The transport of the charged particles along the magnetic field (magnetic surfaces) can be described by a theory which considers only collisions between particles, - the classical theory [9, 10, 11]. However, the experimentally observed transport across the magnetic field is much stronger (at least an order of magnitude) than predicted by the classical theory or a more advanced theory which takes into account the non-uniformity of the magnetic field (the neo-classical theory, see [1], Sections 4.4-4.11). The origins of this so-called anomalous transport are still being extensively studied. The basic reason (according to the current knowledge) is the presence of the self-consistent perturbations of electric field and magnetic fields in plasma (turbulent transport), see [1], Sections 4.16-4.23. Despite fact, that the mechanisms of the anomalous transport are still not completely understood, a significant progress has been made in past two decades in improving the plasma confinement. The conditions which satisfy Lowson criterion for the break-even have been already achieved on three machines: JET (Europe), JT-60 (Japan) and TFTR (USA), see [1], Chapter 12. The D-T operation has been tested on two of them (JET [12] and TFTR).

#### 0.1.2 Scrape-off-Layer and Divertor

One of the conditions which must be satisfied to make the fusion reactor efficient is a sufficiently low level of high-Z impurities in plasma. Here Z is the charge number of the chemical element. The major, principally unavoidable mechanisms of the power loss from the hot centre of the plasma volume (the so called core plasma) is the bremsstrahlung radiation. The radiated power for bremsstrahlung scales as ~  $Z^2$ . Therefore, even the presence of a small amount of high-Z impurities can boost up the radiation losses. The maximum tolerable concentration for carbon it is  $\approx 2$  %, for neon  $\approx 0.5$  %, for iron  $\approx 0.05$  % and for tungsten <0.01 % [13].

The main source of impurities is the sputtering of the plasma-facing components by fast particles. Plasma-facing components (the first wall) are the elements of the structure which receive directly the particle fluxes from the plasma. The amount of impurities can be controlled by reducing the amount of sputtered material and by hindering its penetration into the main plasma. The choice of the wall material itself is also important: low-Z materials (beryllium, carbon) or materials with low sputtering yield (tungsten, molybdenum)

are preferable. This is, however, only a partial solution, especially for a fusion reactor which has also inherent source of helium produced by the fusion reaction (the helium ash). The impurities, therefore, have to be constantly removed from the plasma. This can be achieved by organising a particle throughput inside the vacuum vessel: puffing in the pure hydrogen isotopes and pumping out the mixture including all impurities. In this way the amount of impurities in the plasma can be sustained on an acceptable level.



Both the effectiveness of wall sputtering and the pumping of impurities and their penetration into the plasma core are determined by the processes which take place at the plasma edge. This region is also called the Scrape-Off-Layer (SOL). It can be approximately defined as the plasma region significantly affected by the recombined and sputtered neutrals coming from the wall. The properties of this region have been extensively studied in the last 20 years on different machines. A comprehensive review of the current state of the SOL physics can be found in the book of Peter Standgeby [14].

Figure 2: Limiter configuration of SOL plasma

Two main configurations of the SOL plasma are used presently in tokamaks: a limiter configuration and a divertor configuration. The advantages and drawbacks of each configuration are outlined in [14], Section 5.1. The limiter

is a part of the wall which is "touched" by one of the magnetic surfaces, Figure 2. This surface is called the last closed magnetic surface (LCMS). Magnetic surfaces of larger radius intersect the limiter. The charged particles on those surfaces have a high probability to make it on the solid surface where they are neutralised. Most of them return to the plasma and some part can be pumped out as a neutral gas. This process of the neutralisation of charged particles with subsequent re-ionization is called "recycling". The disadvantage of the limiter configuration is that the limiter is very close to the main plasma. The plasma near the limiter surface is still hot (tens eV). As a result, the sputtering is very efficient and the sputtered material can easily contaminate the main plasma. The pumping efficiency is low because of low achievable density of the neutral gas.

These problems are solved in the divertor configuration which is shown in Figure 3. This magnetic configuration has a separatrix. The sepatartix is a surface which divides regions of the magnetic field with different topology: closed magnetic surfaces in the core and open magnetic surfaces at the edge. In the divertor configuration the area where the charged particles impinge on the wall (the area of intense plasma-wall interaction) is located farther from the main plasma. It can be shown, that in this case the heat flux from the main plasma is transported mainly by thermal conduction unlike to limiter SOL where the convection dominates, see [14] Section 5.2 or [15]. As a result, a significant temperature gradient develops and the plasma temperature in front of the solid surface drops to a few eV. This significantly reduces the target erosion (physical sputtering). In addition, the increased distance hinders the penetration of the sputtered particles into the main plasma. In the divertor configuration a relatively high neutral pressure at the entrance to the pumping slot (up to 10 Pa and more) can be achieved, thus increasing the efficiency of the pumping and removal of impurities.

Some terms related to the SOL plasma which and used throughout this Thesis are explained below. The point of the self-intersection of the separatrix in the poloidal plain is called the X-point. The configuration shown in Figure 3 has only one X-point. It is called thus a single-null divertor configuration. Configurations with two X-points (double-null configurations) are also possible. The solid surfaces intersected by the magnetic surfaces are called the divertor targets. The volumes in front of them are called the inner and the outer divertor. The region beneath the X-point is called the Private Flux Region (PFR), Figure 3. The distance from one target to another along the magnetic field is called the connection length. The toroidal field is much larger than the poloidal one, therefore this length can be an order of magnitude larger than the perimeter of the magnetic surfaces seen in the poloidal cross-sections and reaches 100 m and more for large machines. The direction normal to the magnetic surfaces is called the radial direction. The direction along the magnetic field is called the parallel direction and its projection on the poloidal plane is called the poloidal direction. In this Thesis the consideration will be focused mainly on

the divertor region. To stress this, the term "divertor plasma" will be often used instead of "SOL plasma".



Figure 3: Divertor configuration of SOL plasma

Besides the advantages listed above, the divertor configuration has one more important feature. The so called H-mode, - the operational regime with improved confinement, - was first discovered and now can be stably reproduced on divertor machines (starting from ASDEX). This to a large extent predefined the modern shift in favour to divertor configuration which is used in most of the large tokamaks. The H-modes were obtained on limiter machines as well (TORE-SUPRA, TEXTOR) but the improvement of confinement is much less pronounced there. At the same time, the divertor has some disadvantages compared to the limiter. In particular, the divertor itself takes a large part of the "expensive" magnetic volume which reduces the efficiency of machine.

A severe problem of the divertor which is especially important for the reactor conditions is a strong concentration of the target heat loads. The conductive heat flux follows the magnetic surfaces. Its radial dispersion comes mainly from the cross-field transport and therefore small. As a result, the effective wetted area which receives most of the load is much smaller than the geometrical size of the targets. The heat flux density can reach 10 MW/m<sup>2</sup> and more sig-

nificantly complicating the design. However, a significant fraction of the incoming heat flux can be disposed due to radiation. In this case it may be spread on a much larger area. The hydrogen radiation is usually not effective but the radiation of impurities can dissipate 50-70 % of the total heat flux. It can be either the radiation from the sputtered impurities (e.g. carbon) or the impurities which are seeded specially for this purpose (Ne, Ar, N<sub>2</sub>). For divertor configurations the contamination of the main plasma can still be acceptable even in this case.

A radical solution of the problem of divertor heat loads can be found in achieving the so called divertor detachment. It is known from experiment that different regimes of the divertor operation may appear depending on the level of density. In experiment this latter is usually defined as the average density along a line-of-sigh which intersects the core plasma <n>. Three different regimes can be seen as the density <n> increases:

- 1. Sheath-limited (low recycling) regime similar to the operation of limiter. The heat flux is transferred to the target mainly by convection. The density at the target  $n_t$  increases nearly linearly with < n > and the temperature at the target  $T_t$  is high (>10 eV).
- 2. Conduction-limited (high recycling) regime. The density  $n_t$  increases nearly quadratically with  $\langle n \rangle$ , the temperature  $T_t$  decreases.
- 3. Detached regime (detachment). The density  $n_t$  saturates (the so-called rollover) and then starts to decrease.

More precisely, the experimental features of detachment can be defined in the following way. Detachment is characterised by a decreasing ion flux on the divertor targets as  $\langle n \rangle$  increases, whereas the  $H_{\alpha}$  radiation continues to increase, see [14], Chapter 16. A strong pressure drop from upstream to the targets can be also seen. One distinguishes between the partial detachment, when the maximum ion flux density starts to decrease, and the full detachment, when the total ion flux starts to decrease. Detachment is observed in almost all divertor tokamaks. The plasma at the inner target of large machines is normally detached and it is possible to achieve the detachment of the outer target as well [16, 135].

Understanding the divertor detachment is still an active research area. But it is already clear that the detachment allows to reduce the peaking of the incident target heat flux. It

The SOL plasma in the case of the H-mode does in fact never reach steady-state even approximately. It is permanently perturbed by the so-called Edge Localised Modes (ELMs): periodic bursts of energy and particles expelled from the core plasma. As it is clear at present, the ELMs can carry a large fraction of energy (up to 30-40 % of the total SOL energy input, see e.g. [18]) and can be seriously dangerous (for the plasma facing components) especially for large machines. The physics of ELMs is still not completely understood and their modelling from first principles is a challenging area of research, see e.g. the recent review [19].

In this work only the steady-state modelling without any kinds of transient events is considered. The results should be thus understood as obtained for the inter-ELM period. In principal, it is possible to estimate the response of the SOL plasma on ELMs using the similar software tools as used in this work. This can be done applying periodic perturbations to the transport coefficients, see e.g. [20]. There are also other kinds of instabilities which may occur in the SOL plasma, e.g. formation of MARFE (Multifaceted Asymmetric Radiation from the Edge): strongly radiating blobs of relatively cold and dense plasma, see e.g. [14], Chapter 22. All those instabilities are not considered in this work as well, although their modelling using the same codes is possible.

It should be pointed out that the problem of plasma-wall interaction and the edge plasma is to a large extent universal for all kinds of magnetic confinement devices (tokamaks, stellarators etc.). It becomes especially serious for reactor conditions. Moreover, the progress in improving the plasma confinement makes this problem more and more severe. The findings made in this field for specific devices and specific conditions may, therefore, have a broader area of application.

#### 0.1.3 Motivation and outline of the thesis

The SOL plasma is a complex system. Its detailed description has to be at least 2D in space and includes mutual influence of plasma transport and neutral recycling. A quantitative analysis of the SOL and the prediction of its behaviour are impossible without numerical modelling. Presently the "standard" configuration which is used for such an analysis is a combination of a finite-volume fluid code describing the plasma transport and a Monte-Carlo code to describe the transport of neutral particles. Fluid-diffusion models are applied sometimes for the neutrals as well. A first 2D fluid model for the SOL and divertor plasma coupled to a Monte-Carlo code for neutrals was presented in [21]. The B2-EIRENE code used in the present work was originally developed by D. Reiter and M. Baelmans [22, 23, 24]. It is based on 2D plasma transport code B2 by B. Braams [25] and the Monte-Carlo neutral transport code EIRENE, developed by D. Reiter et al. [26, 27]. This package was later further developed at IPP Garching under name SOLPS [28]. This is the main code package which is used in the European activities on fusion edge plasma modelling. The EDGE2D code is an analogue of B2 developed for JET [29, 30]. It is currently used with a Monte-Carlo neutral code NIMBUS [31] but work is in progress to replace NIMBUS by EIRENE. In the US the fluid plasma code UEDGE [32] is usually applied for SOL modelling, sometimes in combination with the Monte-Carlo neutral code DEGAS-2 [33] (analogue of EIRENE).

The B2-EIRENE code is the software tool which is used to simulate the divertor plasma of ITER: an international project of the next-step tokamak fusion device targeting to demonstrate the technical and economical feasibility of industrial fusion power production. This code was originally designed for the so called high recycling mode of divertor operation with relatively low density ( $\approx 10^{14}$  cm<sup>-3</sup> and less) and high temperature (ten eV and more). The B2.4-EIRENE code which was used previously to model the ITER divertor plasma did not take into account some physical effects which are important for divertor conditions with higher density ( $\approx 10^{15}$  cm<sup>-3</sup>) and lower temperature (from several eV to below 1 eV). In particular, the effects related to the hydrogen molecular chemistry and the non-linear effects (neutral-neutral collisions and the line radiation opacity).

The goal of this work was an upgrade of the code which extends its range of applicability for the detached divertor conditions and hence for the current ITER divertor design concept. The corresponding options were already implemented in EIRENE separately from each-other. The task was to combine them together in one coupled code self-consistent between plasma, neutral gas and radiation field.

This thesis incorporates the results of the following previous works. The model for neutral-neutral collisions based on a so called BGK approximation [34, 35, 36, 37]. It was implemented in EIRENE by Christoph May for his PhD Thesis [38, 39]. The improved molecular reaction kinetics is based on the Sawado-Fujimoto [40, 41] model for the chemistry of hydrogen molecules, with vibrational kinetics added by D. Reiter and P. Greenland [42, 43]. The description of elastic collisions was developed by P. Bachmann and D. Reiter [44]. The photon transport model coupled to atomic kinetics was first implemented by Sven Wiesen in the framework of his PhD Thesis [45, 46, 47] and by Petra Börner for her Diploma Thesis [48, 49] for fixed plasma conditions. It had to be significantly modified for the purpose of this thesis, in which a self consistent solution is sought.

The thesis is organised as follows. Chapter 1 contains a general description of the B2 (Section 1.1) and EIRENE (Section 1.2) codes and their application for ITER, Section 1.3. Chapter 2 describes the model for neutral-neutral collisions. The up-to date model for molecular kinetics is described in Chapter 3. Chapter 4 is devoted to the model for radiation transport and its coupling with atomic kinetics. In the description of each model special attention is paid on the underlying physics and on the scope of validity. An example of the effect produced for the calculated ITER plasma (in the self-consistent modelling) is shown for each new model feature. The final impact of the upgraded model on the predicted operational scalings of the ITER divertor is shown in Chapter 5. The first experimental validation of the upgraded package is discussed in Chapter 6. Most of the technical information about implementation of the described models in the code can be found in Appendices.

The package developed in frame of this Thesis is indexed as SOLPS4.2. It is meanwhile extensively used now by the ITER International Team (without photon opacity), see recent publications [50, 51, 52].

## **Chapter 1**

# **B2-Eirene modelling**

### 1.1 The B2 code

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#### **1.1.1 Equations**

The B2.4 code solves a set of fluid equations describing the 2-dimensional radial-poloidal transport of a multi-species plasma with toroidal symmetry. The code was originally developed by Bastian Braams in the framework of his PhD thesis [25].

The general form of the fluid equations for a single-ion plasma is the following [24, 25]:

$$\frac{\partial n_i}{\partial t} + \operatorname{div}(\mathbf{V}_i n_i) = S_n^i \tag{1.1}$$

$$\frac{\partial n_e}{\partial t} + \operatorname{div}(\mathbf{V}_e n_e) = S_n^e, \tag{1.2}$$

$$\frac{\partial}{\partial t}\left(m_{i}\mathbf{V}_{i}n_{i}\right)+\nabla\cdot\left(m_{i}n_{i}\mathbf{V}_{i}\mathbf{V}_{i}\right)=-\nabla p_{i}-\nabla\cdot\Pi_{i}+Z_{i}en_{i}\left(\mathbf{E}+\mathbf{V}_{i}\times\mathbf{B}\right)+\mathbf{R}_{i}+S_{mu_{\parallel}}$$
(1.3)

$$-\nabla p_e - en_e \left(\mathbf{E} + \mathbf{V}_e \times \mathbf{B}\right) + \mathbf{R}_e = 0 \tag{1.4}$$

$$\frac{\partial}{\partial t} \left( \frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \mathbf{V}_i^2 \right) + \operatorname{div} \left( \left[ \frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \mathbf{V}_i^2 \right] \mathbf{V}_i + \mathbf{q}_i \right) + \nabla (\Pi_i \cdot \mathbf{V}_i) = (e n_i Z_i \mathbf{E} - \mathbf{R}) \cdot \mathbf{V}_i - Q_{ei} + S_E^i \quad (1.5)$$

$$\frac{\partial}{\partial t} \left( \frac{3}{2} n_e T_e \right) + \operatorname{div} \left( \frac{5}{2} n_e T_e \mathbf{V}_e + \mathbf{q}_e \right) = -e n_e \mathbf{E} + \mathbf{R} \cdot \mathbf{V}_i + Q_{ei} + S_E^e$$
(1.6)

Equations (1.1), (1.2) are the continuity equations for ions and electrons, Equations (1.3), (1.4) are the momentum balance equations and (1.5), (1.6) a the energy balance equations. The definitions of vector and tensor operations can be found in Appendix C. Note in particular that  $V_{\alpha}V_{\alpha}$  defines a tensor called dyadic but not a scalar product.

The following notations are used:

 $n_e$  and  $n_i$  are the density of the electrons and ions;

 $V_e$  and  $V_i$  are the average (drift) velocities of the electrons and ions;

 $T_e$  and  $T_i$  are the electron and ion temperatures (expressed in energy units);

 $m_i$ ,  $Z_i$  are the mass and charge number of the ion;

 $p_e = n_e T_e$ ,  $p_i = n_i T_i$  are the pressure of ion electrons and ions;

B, E are the magnetic induction and the strength of electric field;

 $\Pi$  is the divergence-free part of the stress tensor;

 $\mathbf{R}_{e}$ ,  $\mathbf{R}_{i}$  are the friction forces between electrons and ions;

 $\mathbf{q}_i$  and  $\mathbf{q}_e$  are the ion and electron heat fluxes;  $Q_{ei} = k_{ei}(T_i - T_e)$  is the energy exchange rate between ions and electrons;

 $S_n$ ,  $S_{mu_{\parallel}}$ ,  $S_E^e$ ,  $S_E^i$  are the sources of particles, parallel momentum, electron and ion energy due to interaction with neutrals.

The friction forces  $\mathbf{R}_{e}$ ,  $\mathbf{R}_{i}$  were calculated in [11]:

$$\mathbf{R} = \mathbf{R}_e = -\mathbf{R}_i = en_e \left(\frac{\mathbf{j}_{\parallel}}{\sigma_{\parallel}} + \frac{\mathbf{j}_{\perp}}{\sigma_{\perp}}\right) - 0.71n_e \nabla_{\parallel} T_e - \frac{3}{2} \frac{en_e^2}{\sigma_{\perp} B^2} \left[\mathbf{B} \cdot \nabla T_e\right]$$
(1.7)

Here  $\mathbf{j} = en_i \mathbf{V}_i - en_e \mathbf{V}_e$  is the electric current,  $\sigma$  is the electric conductivity, signs  $\parallel$  and  $\perp$  denote directions parallel and perpendicular to magnetic field.

The classical heat fluxes  $q_i$  and  $q_e$ , which were calculated in the same work [11], take the form:

$$\mathbf{q}_{\mathbf{i}} = -k_{\parallel}^{i} \nabla_{\parallel} T_{i} - k_{\perp}^{i} \nabla_{\perp} T_{i} + k_{\wedge}^{i} \left[ \frac{\mathbf{B}}{B} \cdot \nabla_{\perp} T_{i} \right]$$
(1.8)

$$\mathbf{q}_{\mathbf{e}} = -k_{\parallel}^{e} \nabla_{\parallel} T_{e} - k_{\perp}^{e} \nabla_{\perp} T_{e} + k_{\wedge}^{e} \left[ \frac{\mathbf{B}}{B} \cdot \nabla_{\perp} T_{e} \right] - 0.71 \frac{T_{e}}{e} \mathbf{j}_{\parallel} - \frac{3}{2} \frac{T_{e}}{e \omega_{e} \tau_{e} B} \left[ \mathbf{B} \cdot \mathbf{j}_{\perp} \right]$$
(1.9)

Here *k* are the thermal conductivities, subscript  $\land$  denotes diamagnetic direction which is perpendicular to both *B* and  $\nabla T_e$ . The numerical coefficient 0.71 in Equations (1.7-1.9) corresponds to ions with *Z* = 1. The values for other *Z* can be found in [11], Chapter 2.

The set of equations (1.1)-(1.6) is simplified for toroidal geometry. Quasineutrality of plasma and the absence of electric currents (ambipolarity) are assumed. The viscosity tensor  $\Pi$  is taken in Newton form with different viscosity coefficients parallel and perpendicular to magnetic field,  $\eta_{\parallel}$  and  $\eta_{\perp}$ . Therefore, the Equation (1.3) in the parallel direction takes the form of the Navier-Stokes equation. For the perpendicular direction only diffusion transport is considered, see Equation (1.13) below. This version of B2 code does not take into account classical drifts (EXB drift, curvilinear drift etc.). More recent version B2.5 [28] and later do have this additional feature, but the level of maturity of these extensions is not yet sufficient for routine "design" applications.

For numerical solution the equations are transformed to the so called "toroidal-poloidalradial" coordinate system. The detailed description of the different kinds of transformations applied for SOL modelling can be found in [24]. In the transformed coordinate system the equations are expressed using metric coefficients  $h_x$ ,  $h_y$  and g:

$$h_x = \left| \frac{\partial \mathbf{r}}{\partial x} \right|, \quad h_y = \left| \frac{\partial \mathbf{r}}{\partial y} \right|, \quad \sqrt{g} = h_x h_y$$
 (1.10)

Here  $\mathbf{r} = \{x', y', z'\}$  are the Carthesian coordinates and *x* and *y* are the poloidal and radial coordinate respectively. The poloidal coordinate surfaces are the projections of the magnetic flux surfaces to the poloidal plane, the radial coordinate is directed perpendicular to the magnetic surfaces. The velocity is represented by its two components *u* and *v*. Velocity *u* is the projection of the parallel velocity  $u_{\parallel}$  into the poloidal plane (poloidal velocity). Velocity *v* is the component of velocity perpendicular to magnetic surface (radial velocity). In the absence of drifts, the parallel velocity can be expressed as  $u_{\parallel} = \frac{B}{B_{\theta}}u$  where  $B_{\theta}$  is the projection of magnetic field into the poloidal plane.

Finally the set of equations, generalised for multi-species plasmas, takes the following form [25].

Continuity equation:

$$\frac{\partial n_{\alpha}}{\partial t} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} n_{\alpha} u_{\alpha} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} n_{\alpha} v_{\alpha} \right) = S_n^{\alpha}$$
(1.11)

Momentum balance equation for the parallel direction:

$$\frac{\partial}{\partial t} \left( m_{\alpha} n_{\alpha} u_{\parallel \alpha} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_{x}} m_{\alpha} n_{\alpha} u_{\alpha} u_{\parallel \alpha} - \frac{\sqrt{g}}{h_{x}^{2}} \eta_{x}^{\alpha} \frac{\partial u_{\parallel \alpha}}{\partial x} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_{y}} m_{\alpha} n_{\alpha} v_{\alpha} u_{\parallel \alpha} - \frac{\sqrt{g}}{h_{y}^{2}} \eta_{y}^{\alpha} \frac{\partial u_{\parallel \alpha}}{\partial y} \right) = \\ = \frac{B_{\theta}}{B} \frac{1}{h_{x}} \left[ -\frac{\partial p_{\alpha}}{\partial x} - \frac{Z_{\alpha} n_{\alpha}}{n_{e}} \frac{\partial p_{e}}{\partial x} + c_{e} \left( \frac{Z_{\alpha}}{Z_{eff}} - 1 \right) Z_{\alpha} n_{\alpha} \frac{\partial T_{e}}{\partial x} + c_{i} \left( \frac{Z_{\alpha}}{Z_{eff}} - 1 \right) Z_{\alpha} n_{\alpha} \frac{\partial T_{e}}{\partial x} \right] + \sum_{\beta} F_{\alpha\beta} + S_{mu_{\parallel}}^{\alpha} \quad (1.12)$$

Here  $c_i$  and  $c_e$  are the coefficients of the thermal force (this force can be important for impurities),  $F_{\alpha\beta}$  is the friction force between species  $\alpha$  and  $\beta$ ,  $Z_{eff}$  is the effective charge:

$$Z_{eff} = \frac{\sum_{\alpha} Z_{\alpha}^2 n_{\alpha}}{\sum_{\alpha} Z_{\alpha} n_{\alpha}}$$

Diffusion equation in the radial direction ( $D_n$  and  $D_p$  are the diffusion coefficients):

$$v_{\alpha} = -\frac{D_{n}^{\alpha}}{h_{y}} \frac{\partial}{\partial y} (\ln n_{\alpha}) - \frac{D_{p}^{\alpha}}{h_{y}} \frac{\partial}{\partial y} (\ln p_{\alpha})$$
(1.13)

Equations (1.11)- (1.13) are taken for each ion species  $\alpha$ . Energy balance for electrons:

$$\frac{\partial}{\partial t} \left(\frac{3}{2} n_e T_e\right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left(\frac{\sqrt{g}}{h_x} \frac{5}{2} n_e u_e T_e - \frac{\sqrt{g}}{h_x^2} k_x^e \frac{\partial T_e}{\partial x}\right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left(\frac{\sqrt{g}}{h_y} \frac{5}{2} n_e u_e T_e - \frac{\sqrt{g}}{h_y^2} k_y^e \frac{\partial T_e}{\partial y}\right) = \frac{u_\alpha}{h_x} \frac{\partial p_e}{\partial x} + \frac{v_\alpha}{h_y} \frac{\partial p_e}{\partial y} - k_{ei} \left(T_e - T_i\right) + S_E^e$$
(1.14)

Energy balance for ions:

$$\frac{\partial}{\partial t} \left( \frac{3}{2} n_i T_i + \sum_{\alpha} \frac{1}{2} m_{\alpha} n_{\alpha} u_{\parallel \alpha}^2 \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} \left[ \sum_{\alpha} \frac{5}{2} n_{\alpha} u_{\alpha} T_i + \sum_{\alpha} \frac{1}{2} m_{\alpha} n_{\alpha} u_{\alpha} u_{\parallel \alpha}^2 \right] - \frac{\sqrt{g}}{h_x^2} \left[ k_x^i \frac{\partial T_i}{\partial x} + \sum_{\alpha} \frac{1}{2} v_x^{\alpha} \frac{\partial u_{\parallel \alpha}^2}{\partial x} \right] \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} \left[ \sum_{\alpha} \frac{5}{2} n_{\alpha} u_{\alpha} T_i + \sum_{\alpha} \frac{1}{2} m_{\alpha} n_{\alpha} v_{\alpha} u_{\parallel \alpha}^2 \right] - \frac{\sqrt{g}}{h_y^2} \left[ k_y^i \frac{\partial T_i}{\partial y} + \sum_{\alpha} \frac{1}{2} v_y^{\alpha} \frac{\partial u_{\parallel \alpha}^2}{\partial y} \right] \right) = -\frac{u_{\alpha}}{h_x} \frac{\partial p_e}{\partial x} - \frac{v_{\alpha}}{h_y} \frac{\partial p_e}{\partial y} + k_{ei} (T_e - T_i) + S_E^i$$

$$(1.15)$$

It is assumed that all ions have the same temperature  $T_i$ ,  $n_i = \sum_{\alpha} n_{\alpha}$ .

In the Equations (1.11)-(1.15) the subscript *x* denotes the transport coefficients in the parallel direction, and the subscript *y* stands for the perpendicular direction.

The electron density and average velocity are found from the conditions of quasineutrality and ambipolarity:

$$n_e = \sum_{\alpha} Z_{\alpha} n_{\alpha}, \quad u_e = \frac{1}{n_e} \sum_{\alpha} Z_{\alpha} n_{\alpha} u_{\alpha}, \quad v_e = \frac{1}{n_e} \sum_{\alpha} Z_{\alpha} n_{\alpha} v_{\alpha}$$
(1.16)

#### **1.1.2 Transport coefficients**

Classical transport coefficients are used for the description of parallel transport. The transport coefficients for a single-ion plasma can be found in [53]. They are expressed in terms of two basic collision times. The collision time for electron-ion collision (for single-component plasma,  $n_e = Zn_i$ ):

$$\tau_e = \frac{3\sqrt{m_e}T_e^{3/2}}{4\sqrt{2\pi}n_i Z^2 e^4 \ln\Lambda} = 3.44 \cdot 10^{11} \frac{T_e^{3/2}}{Zn_e \ln\Lambda}$$
(1.17)

The collision time for ion-ion collisions:

$$\tau_i = \frac{3\sqrt{m_p m_i} T_i^{3/2}}{4\sqrt{\pi} Z^4 n_i \ln \Lambda} = 2.09 \cdot 10^{13} \frac{T_i^{3/2} \sqrt{m_i}}{Z^4 n_i \ln \Lambda}$$
(1.18)

All the formulas with reduced numerical coefficients throughout this subsection yield the result (by default) in SI units. They are given for temperatures in eV and densities in m<sup>-3</sup>. The ion mass  $m_i$  is expressed in proton masses  $m_p$  (amu). Formulas taken from [53] use CGS units.

The Coulomb logarithm  $\ln \Lambda$  is a factor which is used to take into account long range character of the collisions [9, 10]. It is calculated using the approximation:

$$\ln\Lambda = 15.2 - 0.5\ln\frac{n_e}{10^{20}} + \ln\frac{T_e}{1000}$$
(1.19)

The typical value is 10..15.

Classical thermal conductivity was calculated by Spitzer and Härm [9]. Electron thermal conductivity:

$$k_{\parallel}^{e} = 3.2 \frac{n_{e} T_{e} \tau_{e}}{m_{e}} = \frac{2.4}{\sqrt{2\pi m_{e}} e^{4}} \frac{T_{e}^{5/2}}{Z \ln \Lambda} = 3.1 \cdot 10^{4} \frac{T_{e}^{5/2}}{Z \ln \Lambda}$$
(1.20)

Ion thermal conductivity:

$$k_{\parallel}^{i} = 3.9 \frac{n_{i} T_{i} \tau_{i}}{m_{i}} = \frac{10.7}{4 \sqrt{\pi m_{p}} e^{4}} \frac{T_{i}^{5/2}}{\sqrt{m_{i}} Z^{4} e^{4} \ln \Lambda} = 1.25 \cdot 10^{3} \frac{T_{i}^{5/2}}{\sqrt{m_{i}} Z^{4} \ln \Lambda}$$
(1.21)

Formulas (1.20) and (1.21) with numerical coefficients give the result in W/(m·eV). For the hydrogen ion  $k_{\parallel}^i$  is a factor  $\approx 30$  smaller than  $k_{\parallel}^e$ .

The formula for parallel viscosity was obtained by Braginskii [11]:

$$\eta_{\parallel} = 0.96n_i T_i \tau_i = \frac{0.406\sqrt{m_p}}{e^4} \frac{\sqrt{m_i} T_i^{5/2}}{Z^4 \ln \Lambda} = 3.2 \cdot 10^{-6} \frac{T_i^{5/2}\sqrt{m_i}}{Z^4 \ln \Lambda}$$
(1.22)

This is the dynamic viscosity expressed in kg/m<sup>3</sup>  $\cdot$ s (P $\cdot$ s).

Expressions (1.20)-(1.22) can be generalised for the case of multi-species plasma [25]:

$$k_{\parallel}^{e} = 3.2 \frac{n_{e} T_{e} \tau_{e}}{m_{e}} = \frac{2.4}{\sqrt{2\pi m_{e}} e^{4}} \frac{T_{e}^{5/2}}{Z_{eff} \ln \Lambda}$$
(1.23)

$$k_{\parallel}^{i} = \frac{10.7}{4\sqrt{\pi m_{p}}e^{4}} \sum_{\alpha} \frac{Z_{\alpha}^{-2} n_{\alpha}}{\sum_{\beta} \left( Z_{\beta}^{2} n_{\beta} \sqrt{\frac{2m_{\alpha}m_{\beta}}{m_{\alpha} + m_{\beta}}} \right)} \frac{T_{i}^{5/2}}{\ln \Lambda}$$
(1.24)

$$\eta_{\parallel}^{\alpha} = \frac{0.406\sqrt{m_p}}{e^4} \frac{Z_{\alpha}^{-2} n_{\alpha}}{\sum_{\beta} \left( n_{\beta} Z_{\beta}^2 \sqrt{\frac{2}{m_{\alpha} + m_{\beta}}} \right)} \frac{T_i^{5/2}}{\ln\Lambda}$$
(1.25)

Formulas (1.23)-(1.25) represent a simplification of the complete multi-species transport theory. They are valid for the case if one species dominates [25].

Energy exchange coefficient  $k_{ei}$  is taken from [53] and generalised for the multi-species case:

$$k_{ei} = \frac{4\sqrt{2\pi m_e}e^4}{m_p} \left(\sum_{\alpha} \frac{Z_{\alpha}^2 n_{\alpha}}{m_{\alpha}}\right) \frac{n_e \ln \Lambda}{T_e^{3/2}} = 4.75 \cdot 10^{-9} \left(\sum_{\alpha} \frac{Z_{\alpha}^2 n_{\alpha}}{m_{\alpha}}\right) \frac{n_e \ln \Lambda}{T_e^{3/2}}$$
(1.26)

Formulas (1.17) and (1.18) allow to estimate the Mean Free Path (MFP) and thus to evaluate the validity of the fluid approximation. Corresponding expressions for electrons and hydrogen ions are:

$$MFP_e = v_T^e \cdot \tau_e = 2.5 \cdot 10^{17} \frac{T_e^2}{n_i \ln \Lambda}, \quad MFP_i = v_T^i \cdot \tau_i = 2.05 \cdot 10^{17} \frac{T_i^2}{n_i \ln \Lambda}$$
(1.27)

Here  $v_T^e = \sqrt{\frac{3T_e}{m_e}}$  and  $v_T^i = \sqrt{\frac{T_i}{m_i}}$  are the estimates if the electron and ion thermal velocities. Three characteristic regions can be discussed for the SOL plasma of a JET or ITER size devices. In the upstream region the density is relatively low and the temperature is relatively high. Substituting  $n_e = 10^{19} m^{-3}$  and  $T_e = 100 \ eV$  into formula (1.27) one gets MFP<sub>e</sub>  $\approx 18 \ m$ . This is smaller than connection length which can be 50-200 m for large machines. At the entrance to the divertor region the plasma cools down and the density becomes somewhat higher. Substituting  $n_e = 10^{20} m^{-3}$  and  $T_e = 10 \ eV$  yields  $MFP_e = 2.4 \ cm$ . This is small compared to the expected spatial scale of the variation of plasma parameters:  $\approx 10 \ cm$  in parallel direction. Finally, in front of the target the gradients can be very strong but the MFP becomes smaller than one millimeter because the plasma there is cold and dense. Indeed, substituting  $n_e = 10^{21} m^{-3}$  and  $T_e = 1 \ eV$  yields  $MFP_e = 3.5 \cdot 10^{-5} \ m$ . This simple estimate shows that one should expect the fluid approach for the plasma transport to be valid at least as a first approximation.

However, the transport of heat and momentum takes place mainly not due to the particles with thermal energies as it was assumed in the above estimates, but due to fast particles with much larger MFP. Using the fluid approximation for the parallel heat fluxes and viscosity lead to nonphysical results in case of steep gradients [14], Chapter 26. To take this into account, while remaining in the frame of the fluid model (without full kinetic description) the corrections for the classical (fluid) transport coefficients are introduced. In B2 the following expression with so called "flux limits" are used for the electron heat conductivity and viscosity:

Here  $k_{\parallel SH}^{e}$  is the Spitzer-Härm coefficient given by Formula (1.23) and  $\eta_{\parallel}^{\alpha}$  is calculated by Formula (1.25). The values of the flux limiting factors  $F_{e}$  and  $F_{mom}$  used in this work were 0.2 and 0.5 respectively. They are the values which yield the best fitting to the results of the full kinetic simulations (solving the Fokker-Plank equation for the model problems where such simulations are possible, see [14], Chapter 26).

The transport coefficients in the perpendicular direction are anomalous: no robust and usable theory exists at the moment to calculate them. They are usually taken as constants. Their values are the values which give the best fitting to the experimental radial profiles. The typical values are  $\chi_y^e = \chi_y^i = 1 \ m^2/s$ ,  $v_y = 0.2 \ m^2/s$  and  $D_y^n = 0.3..0.5 \ m^2/s$ . Here  $\chi$  is the thermal diffusivity (*k* divided by thermal capacity) and *v* is the kinematic viscosity ( $\eta$  divided by mass density).

#### **1.1.3 Boundary conditions**

For the combination of the continuity equation (1.11) and diffusion equation (1.13) one needs two boundary conditions on the radial boundaries and only one boundary condition on the poloidal boundary. Here and below the term "poloidal boundary" means the boundary across the magnetic surfaces (x = const) and "radial boundary" means the boundary along magnetic surfaces (y = const). On the boundaries which represent the wall of the vacuum chamber a constant e-folding length is usually specified (derivative of the logarithm in normal direction). Typical value for tokamaks is 3 cm. On the boundary with the Core plasma (Core-Edge Interface, CEI) either density or the particle flux can be specified. For the poloidal boundaries the zero density gradient at the guard cell (see below in Section 1.1.4) is usually prescribed on both boundaries. This "technical" boundary condition does not really affect the solution, because upwind scheme is used for this equation [24], Section 3.4.1.

On the radial surfaces e-folding length, temperature or the heat flux density can be specified for the energy equations (1.14), (1.15). The e-folding length is typically 3 cm as for the density.

To specify the boundary conditions on the poloidal surfaces which are intersected by the magnetic field lines (targets) one has to consider the properties of the plasma sheath. This is a thin layer of uncompensated charge forming between the plasma and the solid surface. Its thickness is estimated by the Debye length: that is ~  $10^{-5}..10^{-4}$  cm for a tokamak SOL.

It can be shown, see e.g. [14], Sections 2.3-2.4, that the sheath layer can be stable only if the parallel velocity of the incident plasma is larger than the sound speed  $u_{\parallel} \ge c_s$ . This inequality is usually reduced to an equality (strict Bohm criteria). The boundary condition which is used in B2 has the form:

$$u_{\parallel} = \sqrt{\frac{n_e T_e + T_i \cdot \sum_{\alpha} n_{\alpha}}{\sum_{\alpha} m_{\alpha} n_{\alpha}}}$$
(1.29)

Thus, the isothermal sonic velocity is assumed. This is the most primitive form of this boundary condition: in particular, it assumes equal velocity for all species. B2 has also an option to specify the condition  $u_{\parallel} \ge c_s$ . In this case a zero second derivative of  $u_{\parallel}$  in poloidal direction is enforced. This option was not used in the present work.

The boundary conditions for the energy equations at the targets read:

$$q_{\parallel}^{e} = \gamma_{e} T_{e} n_{e} u_{\parallel}^{e}, \quad q_{\parallel}^{i} = \gamma_{i} T_{i} n_{e} u_{\parallel}^{e} \tag{1.30}$$

Here  $\gamma_e$  and  $\gamma_i$  are the so called sheath transmission factors. They can be found from the kinetic description of sheath and pre-sheath, see [14], Sections 2.8, 25.5. This consideration includes the interaction of the particles with the floating potential which forms at any contact between a solid wall and plasma. The values which were used in this work:  $\gamma_i = 3.5$  for ions and  $\gamma_e = 2 + \gamma_{\Phi}$  for electrons(see e.g. [24]). Here  $\gamma_{\phi}$  is describes acceleration by the floating potential  $\Delta\Phi$  [27], chapter 1.5.1:

$$\gamma_{\phi} = -\frac{e\Delta\Phi}{T_e} = \ln\left[\sqrt{\frac{2\pi m_e}{kT_e}} \frac{\sum_{\alpha} Z_{\alpha} n_{\alpha} u_{\parallel}^{\alpha}}{n_e}\right]$$
(1.31)

This relation neglects the plasma current and the electron emission from the surface. For a pure deuterium plasma  $\gamma_{\Phi} = 2.8$  (for  $T_e = T_i$ ).

The sheath boundary conditions as the are described here valid only if the angle between the surface and the magnetic field line is not too small. It it is less than  $1^{\circ}$  than they have to be modified (funnelling model) [14], Sections 25.2, [54].

#### 1.1.4 Numerical algorithm

The numerics of the B2 code are largely described in [25], some more detail about the implementation of the boundary conditions can be found in [24]. Here only a brief description is given.

B2 uses finite-volume discretisation on a topologically rectangular mesh (drawn along the magnetic surfaces). The description of the basic ideas of this method can be found in [55]. From the mathematical point of view equations (1.11)-(1.15) are a set of convection-diffusion equations. The general form of such an equation is:

$$\nabla \cdot (\rho \mathbf{u} \Phi - \Gamma \cdot \nabla \Phi) = S \tag{1.32}$$

Here  $\Phi$  and **u** are unknown quantities, the scalar  $\rho$  and the tensor  $\Gamma$  are coefficients (which may depend on  $\Phi$  and **u**) and *S* is the source term. The discretisation is based on the conservation of the physical quantities in a grid cell. The scalar quantity  $\Phi$  is discretized in cell centres and the velocity **u** is discretized at the cell faces. The calculated quantities are in fact the averages over the cell volume or over the cell face. The discrete coefficients depend continuously on the local Peclet number (Pe). The dependence gives central difference for small Pe and upwind difference for large Pe. This scheme thus combines the second order of approximation of the former with stability of the latter. A special correction procedure is applied to the continuity equation to handle the case of low Mach number when the flow becomes effectively incompressible.

B2 applies source linearization to the sources obtained from the neutral transport code . The source S is split into two parts:

$$S = S_v \Phi + S_c, \quad S_v = \frac{\max(0, S) - |S| \cdot R}{\Phi_0}, \quad S_c = \min(0, S) + |S| \cdot R \tag{1.33}$$

Here  $\Phi_0$  is the value for which the source *S* was calculated (at the beginning of time step). The factor R=5 is usually taken. Notation (1.33) allows a very flexible way of implementing the boundary conditions. In B2 they are specified giving equivalent sources in the small extra cells attached to the grid boundaries: so called guard cells [24]. For example if *A* is the area of the guard cell face, then imposing  $S_v = 0$  and  $S_c = -QA$  defines the constant flux density *Q* to the boundary (Neumann condition). Analogously, imposing  $S_v = -h$  and  $S_c = h\Phi_d$  where *h* is very large ("infinite") defines Dirichlet condition  $\Phi = \Phi_d$ . The mixed condition (linear combination of  $\Phi$  and its flux) can be specified in the same way.

To obtain the steady-state solution of the discretized system (1.11)-(1.15) the equations are iterated on each time-step in a cyclic order until convergence is achieved. Time-stepping is applied to get some underrelaxation. The discretisation is fully implicit in time. Each iteration (internal iteration on one time-step) consists of the following actions (quotation from [25]):

- 1. The source terms  $S_n$ ,  $S_{mu_{\parallel}}$ ,  $S_E^e$ ,  $S_E^i$  are computed (by the neutral transport code);
- 2. The momentum balance equations (1.12) are relaxed by changing the field  $u_{\parallel \alpha}$  for each species  $\alpha$ ;

- 3. The total momentum equation is relaxed through identical changes in the velocities of all species;
- 4. The fields  $v_{\alpha}$  are adjusted to satisfy the diffusion equations (1.13);
- 5. The continuity equations (1.11) are relaxed through simultaneous changes to  $n_e$ ,  $u_{\parallel \alpha}$  and  $v_{\alpha}$  for each species  $\alpha$ ;
- 6. The electron and ion energy equations (1.14), (1.15) are relaxed separately by changes to the fields  $T_e$  and  $T_i$  respectively;
- 7. The total energy equation (sum of (1.14) and (1.15)) is relaxed by identical changes to  $T_e$  and  $T_i$ ;
- 8. The continuity equations (1.11) are relaxed once more as in step 2.

This procedure includes the pressure correction which was mentioned before

The "Strongly Implicit Procedure" of Stone [56] based on incomplete  $L \cdot U$  decomposition is used to relax the discrete equations (five-point equations). Relaxation of the equations for the total momentum and total energy is done in order to increase the convergence rate in the presense of mutual momentum and energy exchange terms: interspecies friction forces  $F_{\alpha\beta}$  in equation (1.12) and the term  $k_{ei}(T_e - T_i)$  in equations (1.14), (1.15).

### **1.2 The EIRENE code**

#### **1.2.1** Monte-Carlo method for transport problems

This section describes the general ideas of applying Monte-Carlo methods for linear transport problems. The main advantage of the Monte-Carlo methods is their ability to handle a complicated geometry and make a detailed description of the system on a kinetic level. It is sometimes the only tool which can be used for the 2D and 3D problems which involve kinetic transport effects and complex chemistry. The main drawback of the method is that the computation time must be large to achieve a low level of numerical error. The underlaying theory has been well developed for the purposes of nuclear engineering (transport of neutrons) [57]. The consideration below follows [27] and tries to highlight mainly the issues which are important from the practical point of view.

The primary quantity of interest in the kinetic modelling is the one-particle distribution function:  $f(\mathbf{r}, \mathbf{v}, i, t)$ . This is a probability density in phase-space of the test particle which is characterised in general by a position vector  $\mathbf{r}$ , a velocity vector  $\mathbf{v}$ , a species index *i* (*i* stands for, e.g., *H*, *D*, *T*, *D*<sub>2</sub> etc.) and the time *t*.

The basic equation for the distribution function f(x) is the Boltzmann kinetic equation (see e.g. [58]):

$$\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}, \mathbf{v}, t) = \int \int \int \sigma(\mathbf{v}', \mathbf{V}'; \mathbf{v}, \mathbf{V}) |\mathbf{v}' - \mathbf{V}'| f(\mathbf{v}') f_b(\mathbf{V}') d\mathbf{v}' d\mathbf{V} - \int \int \int \sigma(\mathbf{v}, \mathbf{V}; \mathbf{v}', \mathbf{V}') |\mathbf{v} - \mathbf{V}| f(\mathbf{v}) f_b(\mathbf{V}) d\mathbf{v}' d\mathbf{V}' d\mathbf{V} - (1.34)$$

Equation 1.34 is written for the case of only one test species  $i_0$ , which can interact with species b, therefore the species index is omitted. The triple integrals denote the integration over the whole velocity space.  $\sigma(\mathbf{v}', \mathbf{V}'; \mathbf{v}, \mathbf{V})$  is the cross section for a binary particle collision. The first two arguments in  $\sigma$ , namely the velocities  $\mathbf{v}', \mathbf{V}'$  of the first integral, correspond to the velocity of the species  $i_0$  and b, prior to the collision. These are turned into the post collision velocities  $\mathbf{v}, \mathbf{V}$ , again for species  $i_0$  and b, respectively. The first integral, therefore, describes transitions ( $\mathbf{v}', \mathbf{V}' \rightarrow \mathbf{v}, \mathbf{V}$ ) into the velocity space interval [ $\mathbf{v}, \mathbf{v} + d\mathbf{v}$ ] for species  $i_0$ , and the second integral describes the loss from that interval for this species. The collisions are assumed to be point events. The equation (1.34) as it is written here does not take into account any external force (external force field): the particle motion between collision events is governed only by inertia. The particles with distribution functions  $f(\mathbf{v})$  and  $f_b(\mathbf{V})$  will be called further "the test particles" and "the background particles".

For linear transport problems the distribution  $f_b(\mathbf{V})$  is given. The function  $f(\mathbf{v})$  can then be taken out of the second integral in (1.34). One arrives to the following equation:

$$\frac{\partial f(\mathbf{r}, \mathbf{v}, i, t)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}, \mathbf{v}, i, t) + \nu_t(\mathbf{r}, \mathbf{v}, i) f(\mathbf{r}, \mathbf{v}, i, t) = \int d\mathbf{v}' C(\mathbf{r}; \mathbf{v}', i^* \to \mathbf{v}, i) |\mathbf{v}' - \mathbf{V}'| f(\mathbf{r}, \mathbf{v}, i, t) + Q(\mathbf{r}, \mathbf{v}, i, t)$$
(1.35)

Here  $v_t(\mathbf{r}, \mathbf{v})$  is the total collision frequency,  $C(\mathbf{r}; \mathbf{v}', i' \rightarrow \mathbf{v}, i)$  is the kernel of the collision operator and  $Q(\mathbf{r}, \mathbf{v}, i, t)$  is the primary source. Collision frequency is the number of collisions which the test particle experiences during a unit time interval:

$$\nu_t(\mathbf{r}, \mathbf{v}, i) = \sum_k \nu_k(\mathbf{r}, \mathbf{v}, i), \quad \nu_k(\mathbf{r}, \mathbf{v}, i) = \int \int \int \sigma_k(\mathbf{v}, \mathbf{V}, i; \mathbf{v}', \mathbf{V}', i') |\mathbf{v} - \mathbf{V}| f_b(\mathbf{V}) d\mathbf{v} d\mathbf{V}' d\mathbf{V}$$
(1.36)

Here  $v_k(\mathbf{r}, \mathbf{v}, i)$  is the collisions frequency for the specific process *k*. The collision kernel is the number of particles of species *i'* with velocity (**v**') which emerge from the collisions as the particles of species *i* with velocity **v**:

$$C(\mathbf{r}; \mathbf{v}', i' \to \mathbf{v}, i) = \sum_{k} v_k(\mathbf{r}, \mathbf{v}', i') c_k(\mathbf{r}; i', \mathbf{v}' \to \mathbf{v}, i)$$

$$c_k(\mathbf{r}; \mathbf{v}', i' \to \mathbf{v}, i) = \frac{\int \int \sigma(\mathbf{v}', \mathbf{V}', i'; \mathbf{v}, \mathbf{V}, i) |\mathbf{v}' - \mathbf{V}'| f_b(\mathbf{V}') d\mathbf{V}' d\mathbf{V}}{\int \int \int \sigma(\mathbf{v}', \mathbf{V}', i'; \mathbf{v}, \mathbf{V}, i) |\mathbf{v}' - \mathbf{V}'| f_b(\mathbf{V}') d\mathbf{v}' d\mathbf{V}' d\mathbf{V}}$$
(1.37)

The factor  $c_k(\mathbf{r}; \mathbf{v}', i' \to \mathbf{v}, i)$  is the conditional probability distribution for the post-collision *i* and **v** for the specific collision process *k*. The collision frequency and the collision kernel can include not only collisions in the volume but surface collisions as well. The absorption can be formally taken into account introducing a special kind of collisions which turn the test particle into an artificial "empty" species.

Equation (1.35) can be further transformed into an integral equation of the Fredholm type with the kernel consisting of the collision kernel  $C(\mathbf{r}; \mathbf{v}' \to \mathbf{v})$  and the transport kernel (by integrating over characteristics) [27, 57, 59]. This approach is used for rigorous mathematical analysis of the Monte-Carlo method and it is not considered here.

The simplest Monte-Carlo approach of solving the Equation (1.35) can be derived straight from its physical meaning. Indeed, this equation describes the distribution function of the particles, which start from the source  $Q(\mathbf{r}, \mathbf{v}, i, t)$ . They travel along the straight lines and undergo collisions with background particles and the wall with frequencies  $v_k(\mathbf{r}, \mathbf{v})$ . In each collision the particle changes its velocity and type according to the distribution  $c_k(\mathbf{r}; \mathbf{v}', i' \rightarrow \mathbf{v}, i)$ . The process continues until the test particle disappears due to absorption. Solving the Equation (1.35) by reproducing this process "in a computer" for a finite number of trajectories using machine generated pseudo-random numbers is called "analog sampling". The pseudo-random numbers are deterministic sequences which possess some properties of real random numbers (e.g. have the same distribution function). It has to be pointed out that all "random processes" generated by a computer are, in fact, deterministic and can be exactly reproduced.

To proceed with analog sampling one does not in fact even have to know about the existence of Equation (1.35). But using a formal mathematical description allows in some cases to show that it is possible to build an algorithm which does not mimic exactly the physical processes behind the transport but leads to the same solution as Equation (1.35). The algorithms of such kind are called "non-analog sampling" and some examples of them will be shown below.

The following issues have to be resolved to build a Monte-Carlo sampling procedure: i) sampling from the source  $Q(\mathbf{r}, \mathbf{v}, i, t)$ ; ii) tracking the test particles in space; iii) sampling from the distribution  $c_k(\mathbf{r}; \mathbf{v}', i' \rightarrow \mathbf{v}, i)$ ; iv) calculating the estimates over the trajectories. The issues i) and iii) are largely problem dependent. The issue ii) is in opposite common for all kinds of the transport problems.

For the test particle which emerges from the primary sources or from a collision the distance to the next collision L (free path) can be sampled from the inverse cumulative distribution F(L) [33, 57, 59]:

$$F(L) = 1 - \exp\left[-\int_0^L \frac{v_t}{|\mathbf{v}|} dl\right], \quad \int_0^L \frac{v_t}{|\mathbf{v}|} dl = -\ln u \tag{1.38}$$

Here *u* is a random number distributed uniformly between 0 and 1. At the point of collision the type of the collision event is sampled from the discrete probability distribution  $p_k = \frac{v_k}{v_l}$ . After that the post collision velocity is sampled from the distribution  $c_k$  or the particle is absorbed.

To use the relation (1.38) in practice one samples first the number  $\ln u$  and then updates the integral  $\int_0^L \frac{v_i}{|\mathbf{v}|} dl$  until it meets the last equality of (1.38) or until the test particle reaches a surface. The parameters of the background (they are required to calculate  $v_k$  and to sample the post-collision state from  $c_k$ ) are usually specified on a discrete grid. The routine which controls the tracking of the test particles have to ensure that the position on the grid is known at each moment.

Sampling the free path L is an example of the general method of sampling the random variable with given distribution function. It can be applied if the inverse cumulative distribution can be easily calculated. If this is not the case, then the rejection sampling technique can be applied, see e.g. Section B.1.

For practical problems it is usually not necessary to know the distribution function  $f(\mathbf{r}, \mathbf{v}, i, t)$  itself but it is necessary to calculate some moments of this distribution. As it was already mentioned above, the procedure of calculating those moments is called "the estimation". Two kinds of estimates (or "estimators") are usually used in Monte-Carlo codes: collision estimator and track-length estimator. Let  $\omega^n = \{x_0, x_1, x_2 \dots x_n\}$  denotes a trajectory in the one-particle phase space  $x = (\mathbf{r}, \mathbf{v}, i, t)$ . The points  $x_j$  are the coordinates of the collisions. In general an estimate *R* calculated over *N* trajectories  $\omega_i$  is the following sum:

$$R = \frac{1}{N} \sum_{i=1}^{N} X(\omega_i)$$
 (1.39)

The function  $X(\omega_i)$  depends on the type of the estimator. For the collision estimator:

$$X_{C}(\omega_{i}) = \sum_{j=1}^{n} g_{c}(x_{j})w(x_{j})$$
(1.40)

Here  $g_c$  is the detector function which is calculated for each collision and  $w(x_j)$  is the so called statistical weight. In the simplest case  $g_c = 1$  this estimation yields the total number of collisions. It can be shown that  $X_C$  gives unbiased estimation of the sum of  $g_c$  over all collisions [57].

For the track-length estimator the function  $X(\omega_i)$  has the following form:

$$X_T(\omega_i) = \sum_{j=1}^n \int_{x_j}^{x_{j+1}} \frac{ds}{|\mathbf{v}(s)|} w(s) g_t(s)$$
(1.41)

Here  $g_t(s)$  is the detector function which is defined in each point of the particle's trajectory. This estimator gives the unbiased estimation of the corresponding moment of the distribution function:

$$\int f(\mathbf{r}, \mathbf{v}) g_l(\mathbf{r}, \mathbf{v}) d\mathbf{v}$$
(1.42)

In particular, if  $g(\mathbf{r}, \mathbf{v}) = 1$  it yields the total number of particles. In other words, the sum over the residence time of the particles in a volume is proportional to the number of particles in this volume. In neutron physics the estimator (1.41) is usually expressed in terms of integral  $\int_{x_j}^{x_{j+1}} ds$  (without dividing by velocity). In this case for  $g(\mathbf{r}, \mathbf{v}) = 1$  it yields the volume integral over the particle flux density. Estimators (1.40) and (1.41) can be applied to any control volume. In particular, to each cell of the computational grid to get the spatially resolved estimation.

The statistical error of the calculations: the deviation from the mean expectation, can be estimated in the same way as in the case of multi-dimensional integration, see e.g. [59] or [60], Chapter 7.6. It is given by the estimate of the statistical variance:

$$\operatorname{var}[\mathbf{X}] = \frac{1}{N-1} \sum_{i=1}^{N} \left( X_i - \frac{1}{N} \sum_{i=1}^{N} X_i \right)^2 = \frac{1}{N-1} \left\{ \sum_{i=1}^{N} X_i^2 - \frac{1}{N} \left[ \sum_{i=1}^{N} X_i \right]^2 \right\}$$
(1.43)

Here  $\mathbf{X} = \{X_i\}$  is a set of *N* points sampled to estimate the expectation of the mean value of  $X_i$ . The variance can serve as an estimate of the numerical error, based on the Central Limit Theorem:  $\sqrt{\text{var}[\mathbf{X}]/N}$ . One has to keep in mind, however, that the calculated var $[\mathbf{X}]$  is only an estimate of the true variance. An extra analysis is required in some cases to find out how close those are to each over, e.g. when the calculated var $[\mathbf{X}]$  is too large [59].

Introducing the statistical weight w into estimators (1.40) and (1.41) allows to use different kinds of the non-analog sampling. The most well known are Russian roulette and splitting. Russian roulette is applied if at some point it is not desirable to sample a test particle further. For example if it is out of the region of interest. In this case one can "kill" the particle with a probability P. If the particle was not "killed", then its statistical weight is multiplied by 1/P. In the opposite case it may be necessary to increase the amount of the test particles in some regions. To do this one can split the test particle into n particles. The correct estimation will be obtained if the weight of each particle is divided by n. Another kind of the non-analog sampling which is often used, is the suppression of absorption: reducing the test particle statistical weight instead of absorbing ("killing") it. The non-analog methods mentioned here are special cases of more general techniques. Their description and rigorous mathematical derivation can be found in [57].

The design of a typical Monte-Carlo transport code can be considered as consisting of two principal parts: the geometry module and the physical module. The geometry module performs the particle tracking and it is to a large extent independent of the particular problem to be solved (neutron transport, radiation transport etc.). This subsection was mainly dealt with this common part. The physics of the problem is defined by the source Q, the post-collision distribution  $c_k$  and the collision rates  $v_k$ . This problem-specific part of the code is called the physical module. The physical module of EIRENE code will be briefly described in the next section.

#### **1.2.2** Description of the code

EIRENE is a linear Monte-Carlo solver developed specifically for the transport of neutral particles in plasma. The thorough information on the code and its databases can be found on the web-page <u>www.eirene.de</u>. In this section the physical model will be described and some technical information about the code will be given.

The code can handle a full 3D geometry defined on a tetrahedral grid [49, 48]. For divertor applications the 2D toroidal geometry is mainly used. For this case two options are available at the moment. The simplest and the oldest option is that the code uses the same quasi-orthogonal grid consisting of quadrangles as the plasma code. This grid is called "the standard grid". The boundaries of the standard grid which coincide with the boundaries seen by the plasma code are called "non-default standard surfaces" ("standard surfaces" are the surfaces which form the standard grid). Extra physical boundary surfaces (for example the wall of the vacuum vessel) are called "the additional surfaces".

The disadvantage of the standard grid is that the scoring (calculating the estimators) outside the defined plasma volume is impossible. To overcome this drawback the geometry module of the code was extended to work on a triangular grid. This grid is similar to the grids which are used for Finite Element calculations. It can fill the volume between the plasma grid and the additional surfaces. The plasma grid is divided into triangles as well and the both grids are attached to each other forming one continuous triangular grid. The properties of the wall material can be specified for the additional and non-default standard surfaces. These surfaces can have some absorption coefficient and semi-transparency as well.

Several types of sources of the test particles are available. The most important for divertor applications are the surfaces sources and the volume sources. The first is used for describing the recycling sources of neutrals (ions neutralised on the solid surfaces) and the second is used for describing the volume recombination. In both cases the primary sampled particle is an ion. One can also specify surface sources of neutrals to model gas puffing. The recycling sources are specified on the boundary of the B2 grid. It does not always reflect correctly physical location of the wall but the ion fluxes are available only on those surfaces.

The velocity distribution function of the background particles (ions) is taken to be a shifted Maxwellian. The velocity of ions incident on the surface is sampled from a trun-

cated shifted Maxwellian distribution:

$$f(\mathbf{v}) = Cv_n \exp\left[-\frac{m}{2T} \left(\mathbf{v} - \mathbf{V}_d\right)^2\right]$$
(1.44)

Here **v** is the velocity of the ion,  $v_n$  is the component of velocity normal to the surface,  $V_d$  and *T* are the drift velocity and the temperature of ions in front of the surface, *m* is the ion mass and *C* is the normalising constant. The cumulative distribution function for this probability density can not be expressed explicitly, therefore a special non-analog sampling procedure is applied, see [27] Section 1.5. For the target surfaces (surfaces intersected by magnetic field lines) the sheath acceleration (1.31) is added. After the sampling of velocity a surface interaction model is applied to the incident ion. The same surface model is used for the incident neutral particles.

EIRENE considers three kinds of surface processes: reflection of the fast particles, thermal desorption and sputtering. Several options are available for the fast particles reflection. The best option at the moment is to sample the probability of reflection, velocity and the scattering angle of the reflected particle using the pre-computed tables obtained by the TRIM code [61]. TRIM is a Monte-Carlo code for the solid-particle interaction. The data for the different pairs "target-projectile" (different chemical elements) can be found on <u>www.eirene.de</u>. If EIRENE can not find the data for a specific pair then it takes the available data with the closest reduced atomic mass of the target and projectile.

The particles which are not reflected as fast particles thermally desorb with Maxwellian velocity distribution at the wall temperature. The latter is usually set to 0.1 eV for target surfaces and to 0.04..0.07 eV for other surfaces. For particles with incident energy lower than a certain prescribed cut-off (usually 1 eV) the thermal desorption is considered as well. Hydrogen atoms are desorb as molecules. Only desorption (no fast reflection) is applied for molecules. A particle absorption coefficient (albedo) can be set for some surfaces to model pumping.

Two kinds of sputtering processes are considered: physical sputtering and chemical sputtering. The physical sputtering is described by the modified Roth-Bohdansky formula for the sputter yield, Thompson energy distribution and cosine angular distribution for emitted particles [62]. The necessary parameters are read from datafile SPUTER. As the physical sputtering by the hydrogen isotopes has a rather high energy threshold (e.g. 27 eV for D on graphite) it is not very important for divertor conditions. The chemical sputtering is switched on automatically for the carbon surfaces and hydrogenic ions or atoms. The sputtering coefficient can be calculated using the Roth formula [63] which includes a dependence on the particle flux. This option is not well tested and at the moment it is not suggested for use. In the actual calculations a constant sputtering yield was prescribed.

The volume processes can be divided into two groups: electron impact collisions and heavy particles collisions. The first group includes ionization, dissociation and recombination. The collision rates of the electron-impact processes are assumed to be independent of the test particle velocity (making use of the fast velocity of electrons). Their rates depend on the electron temperature and in some cases on the electron density (in the case of effective reaction rates - Collision-Radiative models). More details are given below in Sections 3.2 and 4.2.2.

The collisions of heavy particles are the elastic collisions and the charge-exchange collisions. The latter is in fact a special case of the elastic collisions (from numerical point of view). The collision rates for those processes depend on the plasma ion temperature and the velocity of the test particle, see Section 3.1. Elastic collisions may include the neutralneutral collisions, Chapter 2. The sampling of photons is described in Chapter 4.2.1.

The reaction rates are tabulated in the datafiles HYDHEL (old hydrogen-helium database taken from [64]) AMJUEL (new hydrogen-helium database described partly in Section 3.2) and METHANE (processes with carbon). The fitting formulas are described in Section 3.1.3.

For most of the output quantities (in EIRENE documentation they are called "talllies") the track-length estimator (1.41) is used. In particular for particle sources, densities, average kinetic energies, energy and momentum sources due to electron impact collisions. The standard option to calculate the momentum and energy sources due to heavy particle collisions uses the collision estimator (1.40). The corresponding track-length estimator was implemented in this work, Section 3.1.

The use of non-analog sampling in EIRENE is rather restricted. The Russian roulette is applied for inelastic collisions to choose the product to follow. This kind of treatment was also used for sputtering but it was replaced by analog sampling in order to improve the particle balance. In the EIRENE documentation this analog sampling is sometimes referred to as "splitting". The suppression of absorption by weight reduction is not used because it was found to be inefficient: it produces too long histories in the regions which are out of interest. The standard variance reduction techniques, such as splitting and Russian roulette on specified surfaces can be activated in EIRENE but the experience shows that the results must be analysed very carefully in this case. In particular, the standard deviation (1.43) may not give the true estimate of the statistical error [27], Section 1.3.1. The recycling source in EIRENE is usually splitted into several parts: the stratified sampling is used. The recycling sources from the different surfaces can have very different strength and the stratified sampling helps to distribute the primary sources of the test particles more uniformly.

## **1.3 ITER modelling**

The modelling shown in this work is dedicated mainly to the divertor plasma of ITER. ITER is an international project of the experimental fusion reactor. Its ultimate goal is to demonstrate the principle possibility of using the power of thermonuclear fusion as an industrial scale energy source. The partners in the project, - the ITER Parties, - are the European Union (represented by EURATOM), Japan, the Peoples Republic of China, India, the Republic of Korea, the Russian Federation and the USA. ITER will be constructed in Europe, at Cadarache in the South of France. The corresponding official decision was taken and approved by all the participating parties in 2006. The expected date of commissioning ("first plasma") is 2016. The up to date information about the project can be found on the official web-page www.iter.org.

ITER is a tokamak with a lower single-null divertor configuration. The major radius of the torus 6.2 m, minor radius of plasma 2 m. The linear dimensions are twice as large as those of the largest existing machines JET and JT-60. The superconducting coils allow to create an average toroidal magnetic field 5.3 Tesla. The expected plasma current is 15 MA. The reference mode is the long pulse operation with inductive current drive. The duration of one pulse is 400-600 sec (quasi steady-state operation). The power of auxiliary heating is 70 MW. The expected fusion power is 400-600 MW and the power amplification factor is  $\approx 10$ .

The fusion plasma has to be surrounded by the first wall integrated with the blanket structure beneath. The latter is to absorb most of the neutron flux produced by DT reaction. Currently in the reference design beryllium is chosen for the first wall coating due to its low Z. Most of the divertor is coated by tungsten because of its low sputtering yield and high thermo-mechanical properties (it is the metal with the highest melting temperature of 3.5 kK). The most severely loaded parts of divertor targets will be fabricated of Carbon-Fibber-Composite (CFC). All the structures are water cooled.

CFC is the only possible solution for ITER divertor targets which is currently foreseen. It is the only material able to receive expected thermal loads due to its high thermal conductivity ( $\approx 100 \text{ W/m} \cdot \text{K}$  for irradiated samples, [65]) combined with high sublimation point (5.5 kK, it does not melt). At the same time using carbon as a plasma facing material has a very strong limitation. Carbon forms stable chemical compounds with tritium which is beta-radioactive (with half-life 12.5 years). The migration of carbon due to its sputtering and re-deposition causes, therefore, the migration and retention of tritium inside the vacuum chamber which is very undesirable. A possibility to get rid of carbon as the plasma facing material and to switch to a full metal wall is being extensively studied at present. This will require to keep both the steady state and the transient loads relatively low.

The design of the ITER divertor is based on the experimental experience from the existing machines extrapolated with extensive use of numerical modelling. The experimental experience alone is not sufficient because the large dimensions and high densities expected in ITER can make significant the effects which are not well pronounced in the existing devices. Examples of such (non-linear) effects will be shown in particular in this Thesis. The main tool for the steady-state modelling of the ITER SOL plasma is the B2-EIRENE code.

The modelling allows at least two types of analysis. Some input parameters have a

high level of uncertainty: for example cross-field transport coefficients. It is impossible to specify those parameters precisely but it is possible at least to investigate the response of the solution to a variation of those parameters in some range, - i.e. to perform a sensitivity analysis. The second kind of analysis is the engineering analysis of possible consequences of the modification of design, for example the geometry of the divertor. The both kinds of analysis require that some range of the input parameters has to be investigated: no conclusions at all can be made from a single point.

It was found by extensive modelling [66, 67, 68, 69, 70] that the operational parameter space of the ITER divertor can be approximated by a set of scalings against a parameter which reflects the level of the neutral density in the divertor. In this work it is the average pressure of the neutrals at the edge of the Private Flux Region. The principal parameters which are important for the design of the machine may be called "the engineering output of the calculations".

The main purpose of the divertor is to pump the impurities. The parameters which are used to characterise the effectiveness of pumping are the average effective charge  $Z_{eff}$  and the helium concentration  $C_{He}$  at the separatrix. Helium is emphasised because it is the main core impurity in case of reactor operation (the product of fusion reaction). For ITER those parameters must not exceed 1.6 and 6 % respectively [67]. Since the target heat loads are the main concern for the divertor structure, the next important parameter is the maximal (peaking) steady-state target heat flux density  $q_{pk}$ . For ITER the constraint  $q_{pk} \leq 10 \ MW/m^2$  has to be fulfiled [67, 74].

One distinguishing feature of the ITER modelling is the way of density control. The simplest way to specify the level of density in the SOL is to fix a certain plasma density at the separatrix (more precisely: at Core-Edge Interface). However, in a real discharge the level of density is established due to the balance between plasma fuelling and pumping. This way of density control is mimiced in the numerical simulations presented in this work. Two types of fuelling are possible: gas puffing and pellet injection (core fuelling). The NBI heating brings a some small contribution to the core fuelling as well. The gas puffing is specified as a source in the neutral transport code. The pellet injection can be taken into account imposing a certain ion flux from the Core to the SOL region. The upstream density is, therefore, not fixed. For all the simulations shown below the core fuelling is zero. In this case the influx of ions to the SOL has to be equal to the flux of neutrals to the Core. For large devices this flux is very small (at least an order of magnitude smaller than the fuelling flux) and can be neglected. In practice a small flux is specified even in this case, for numerical stability. For the reference ITER design the maximum core fuelling rate is  $2.7 \cdot 10^{22}$  s<sup>-1</sup> and the maximum gas pumping rate is  $11 \cdot 10^{22}$  s<sup>-1</sup> (here: fluxes of nuclei). This latter imposes the limit on the total fuelling rate. The wall retention of hydrogen and outgasing are not taken into account in the simulations.

The implementation of the proper of density control required modification of the B2 code of ITER Team [66]. After a call of EIRENE the balance between the incident plasma fluxes and recycling fluxes of neutrals is sufficiently good. But as B2 starts relaxing its equations as described in Section 1.1.4 the incident plasma flux changes. If the neutral-related sources are not re-scaled accordingly, then the error in particle balance can reach  $10^{-2}$  of the recycling flux. The total recycling flux for ITER is  $\approx 10^{25} s^{-1}$ . This means that the error will be of the same order as the gas puffing (pumping) rate and the density control using the gas puffing is impossible. To solve this problem s rescaling is applied for the sources calculated by EIRENE on the B2 iterations [66]. This rescaling allows to reduce the error in particle balance by 3 orders of magnitude.

The ITER modelling set-up which was used for the calculations in this work was derived from the case ITER 828 obtained from Andrey Kukushkin, ITER International Team, Garching. The magnetic equilibrium configuration is shown in Figure 1.1a. The grid has 28 cells in the radial direction and 74 cells in the poloidal direction: 12 poloidal cells in each of the divertor legs, 8 rings in the core and PFR. The grid which combines the quasiorthogonal B2 grid with triangular grid for EIRENE is shown in Figure 1.1b. This figure also depicts some components of the divertor structure (dome, V-shapes, etc).

The dome is an extra structure which is used to retain (compress) neutrals near the entrance to the pumping duct. The dome support structures have windows distributed periodically in the toroidal direction. They are modelled by semi-transparent surfaces with the transparency coefficient of 0.56. The pumping duct is protected by a grill. It is



Figure 1.1: Magnetic equilibrium (a) and the grid with divertor structure (b)

modelled by specifying on this surface a non-zero absorption coefficient for the neutral particles: 0.7 % for the cases with Neutral-Neutral Collisions (NNC) and 1.15 % for the case without NNC. This ensures the pumping speed around 40  $m^3/s$  as expected for the ITER cryo-pumps. The fuelling of the discharge is performed by puffing the  $D_2$  through the slot on the top of the vacuum chamber, Figure 1.1a. The so called "V-shapes" were proposed in [66] to increase the neutral density in front of the targets.

The model plasma consists of 9 ion species:  $D^+$  and all charged states of He and C. D represents both D and T. The neutral species are D, He, C, D<sub>2</sub>. The perpendicular (anomalous) transport coefficients are taken to be constant: diffusivity  $D_{\perp} = 0.3 m^2/s$  and temperature diffusivity  $\chi_{\perp} = 1 m^2/s$ . Other parameters of the plasma transport are described in Section 1.1.2. The boundary conditions on the targets and wall surfaces are described in Section 1.1.3. The boundary conditions at the Core-Edge interface are the following. The total incoming power 100 MW is equally distributed between electrons and ions. A small incoming flux of  $D^+$  ( $9 \cdot 10^{20} s^{-1}$ ) is specified. The incoming flux of He<sup>++</sup> is calculated from the specified fusion power 600 MW. The influx of all other ions is set to 0. All particle and energy fluxes are distributed uniformly. The specified SOL input power is smaller than one fifth of the fusion power because it is assumed that some part of it is radiated directly from the Core. It has to be pointed out that the magnetic configuration of ITER in reality has also an upper null. Calculations made with double-null configuration [75] showed that its influence is negligible (only several percent of the total power will go in this direction) and it is therefore ignored in the modelling here.

All the plasma-facing components in the model are covered by carbon (including codeposited carbon). This assumption is based on the study which was made with the so called "realistic wall model" [71, 72]. The main idea of this model is to check the deposition and erosion rate of carbon for each part of the wall. If the erosion rate is higher, then the surface is assumed to be carbon free. In the opposite case (the deposition rate is higher) it is treated as been covered by carbon in further calculations. Several such iterations are made in a simulation. Applying this model to ITER conditions usually shows that most of the outer wall is covered by carbon. It was also found [72], that the operational scalings calculated with the "realistic wall model" are closer to those of the full carbon machine, rather than to the case with a full metallic wall. Therefore, the assumption of the full carbon wall can be considered as a good first approximation and was applied in this work. A constant chemical sputtering yield of carbon  $Y_{chem} = 1$  % was used for all surfaces. The released carbon atoms have constant energy 1 eV and cosine angular distribution. Complete sticking is assumed for all carbon atoms and ions. Other details of the wall interaction model can be found in Section 1.2.2. The choice of  $Y_{chem}$  ensures that roughly 60% of the power input from the core is radiated by carbon ions.

For the hydrogen atom charge-exchange and ionization are considered. The corresponding reaction rates are taken from databases HYDHEL (3.1.8) and AMJUEL (H.4 2.1.5). Ionization (HYDHEL H.2 2.3.9) and elastic collisions (AMJUEL 0.2T) are taken into account for helium. Only ionization is considered for carbon atoms (METHAN H.2 2.23). The model for the kinetics of  $H_2$  molecules is described in Section 3.2. Volume recombination (sum of radiative and three-body recombination) was taken into account only for hydrogen (AMJUEL H.4 2.1.8). The model for carbon (both erosion and volume processes) which is used at the moment is rather primitive and has to be revisited in future. In particular, it does not include hydrocarbon molecules as it was done in [73].

The old model for the neutral transport which was used for ITER modelling before 2004 (it will be referred to as "EIRENE 1996") did not include any kind of non-linear processes: neutral-neutral collisions and the opacity of line radiation. The main goal of the present work was to implement the upgraded model for ITER. The first step on this way was to couple the new EIRENE code with the B2.4 of ITER IT. Full backward compatibility was confirmed for the reference case ITER 828. The new version of the code successfully reproduced the results of the old version. In the benchmarks of EIRENE stand-alone the neutral density, particle and energy sources were compared (sums and maximum values in each divertor). To take into account statistical variance the relative difference of the results obtained with different number of histories N was followed and checked whether it reduces as  $1/\sqrt{N}$ . The B2-EIRENE runs were compared in terms of reproducing the time-tracings from the standard ITER set. As was said in the Introduction the model of EIRENE 1996 was updated in three steps which are described in the bulk of the thesis.

## **Chapter 2**

# **Neutral-neutral collisions**

## 2.1 Motivation

Neutral neutral collisions (NNC) can be almost safely ignored in divertor modelling of existing tokamaks and stellarators, because their related mean free path length is comparable or larger than other relevant spartial scales. NNC can however provide significant modification of divertor operation in large future devices, such as ITER, via the modification of the neutral gas flow near the divertor targets and in the plasma-free regions of the divertor volume. They can have especially strong influence on the efficiency of pumping. It is particularly important to take into account the effect of NNC to asses the elements of design which are used to control the neutral flow, like dome and V-shapes, see [51]. For the ITER divertor conditions the mean free path for NNC is typically several centimetres, thus the Knudsen number is 0.1..10 and one expects the flow to be in transition regime (transition between free molecular and hydrodynamic limit). Therefore, the modelling has to take into account kinetic effects.

In the current version of the EIRENE code the NNC are described using the so called BGK approximation [34, 35, 36, 37]. This option was implemented in EIRENE by Christoph May in the framework of his PhD thesis [38, 39] and tested with a fixed plasma back-ground. In the present work this extension of the code was incorporated into the self-consistent B2-EIRENE modelling which allows to take into account the effect of the neutral-neutral viscosity on the overall performance of divertor. The current Chapter shows a rigorous derivation of the BGK technique. Special attention is paid on deriving the relations between the BGK collision rates and the transport coefficients to clarify the physical meaning of the former. The derivation is based on the Chapman-Enskog method [58]. This issue was not completely clarified in May's work and was of concern in particular in [33]. The implementation of BGK in the EIRENE code is briefly described in Appendix A.3.

### **2.2 BGK approximation**

The Bhatnagar-Gross-Krook (BGK) approximation [34] represents the simplest example of the so called model equations: the approach which is widely used in rarefied gas dynamics to find approximate solutions of the Boltzmann equation [84]. The idea is to replace the Boltzmann collision integral with another relation which makes the problem easier to solve but which retains some (most important) features of the original equations.

Here the generalisation of the BGK method for a multi-species gas is used [35, 36]. The model equation for collision integral reads:

$$\mathbf{St}^{BGK}(f_i) = \sum_{j=1}^{N} \nu_{ij} \cdot \left[ f_{ij}^{M}(\mathbf{v}, \mathbf{r}; n_{ij}, T_{ij}, \mathbf{u}_{ij}) - f_i(\mathbf{v}, \mathbf{r}) \right] = \sum_{j=1}^{N} \mathbf{St}_{ij}^{BGK}(f_i)$$
(2.1)

Here  $f_i$  is the velocity distribution function of the species *i*;  $v_{ij}$  is the collision frequencies for collisions of the species *i* with the species *j*, *N* is the number of species. The collision rates  $v_{ij}$  are assumed to be independent of the relative velocity ("Maxwellian molecules").  $f_{ij}^M$  is the shifted Maxwellian distribution:

$$f_{ij}^{M}(\mathbf{r}, \mathbf{V}) = \frac{n_{ij}(\mathbf{r})\alpha_{ij}^{3/2}}{\pi^{3/2}(\mathbf{r})} \cdot \exp\left[-\alpha_{ij}(\mathbf{r})(\mathbf{V} - \mathbf{u}_{ij})^{2}\right], \quad \alpha_{ij} = \frac{m_{i}}{2kT_{ij}}$$
(2.2)

Here **r** is the spatial coordinate and **V** is the velocity of the test particle,  $m_i$  is the mass of the species *i*, *k* is the Boltzmann constant;  $n_{ij}$ ,  $u_{ij}$  and  $T_{ij}$  are parameters of the statistical model to be defined later.

The theory which is described below is built up for the case of elastic collisions (momentum and energy conservation in a collision event) for particles for which only the translatory energy changes in the collisions.

#### 2.2.1 Parameters of self collisions

For the self collisions (collisions of the particles of the same type)  $n_{ii}$ ,  $u_{ii}$  and  $T_{ii}$  can be found from particle, momentum and energy conservation:

$$\int \mathbf{St}_{ii}^{BGK}(f_i) d\mathbf{V} = 0; \quad \int \mathbf{V} \mathbf{St}_{ii}^{BGK}(f_i) d\mathbf{V} = 0; \quad \int V^2 \mathbf{St}_{ii}^{BGK}(f_i) d\mathbf{V} = 0$$
(2.3)

Here and below in this Section the integrals without limits denote an integral over the whole velocity space:

$$\int \cdots d\mathbf{V} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots dV_x dV_y dV_z$$

For  $v_{ii}$  which is independent of V this implies:

$$\int [f_{ii}^{M} - f_{i}] d\mathbf{V} = 0; \quad \int \mathbf{V} [f_{ii}^{M} - f_{i}] d\mathbf{V} = 0; \quad \int \frac{m_{i} V^{2}}{2} [f_{ii}^{M} - f_{i}] d\mathbf{V} = 0$$
(2.4)

For Maxwellian distribution (2.2):

$$\int f_{ii}^{M} d\mathbf{V} = n_{ii}; \quad \int \mathbf{V} f_{ii}^{M} d\mathbf{V} = \mathbf{u}_{ii}; \quad \int \frac{m_{i} V^{2}}{2} f_{ii}^{M} d\mathbf{V} = \frac{3}{2} k T_{ii} + \frac{m_{i} u_{ii}^{2}}{2}$$
(2.5)

one gets finally:

$$n_{ii} = \int f_i(\mathbf{V}) d\mathbf{V} = n_i; \quad \mathbf{u}_{ii} = \int \mathbf{V} f_i(\mathbf{V}) d\mathbf{V} = \mathbf{u}_i; \quad T_{ii} = \frac{m_i}{3k} \left( \int V^2 f_i(\mathbf{V}) d\mathbf{V} - u_i^2 \right) = T_i$$
(2.6)

The parameters (of the model) are simply the number density, average velocity and kinetic energy of the species *i*,  $v_{ii}$  is the remaining model parameter to be determined later in Chapter 2.3.1.

#### 2.2.2 Parameters of cross-collisions

For the cross collisions (collisions of the particles of different type) the condition of the particle conservation  $\int S t_{ii}^{BGK}(f_i) d\mathbf{V} = 0$  is valid as well as for the self collision, therefore  $n_{ij} = n_i$ . The determination of the parameters  $\mathbf{u}_{ii}$  and  $T_{ii}$  is less straightforward. They are calculated to have the correct rates of momentum and energy exchange in the case of so called "Maxwellian Molecules". These are the particles for which:

$$\sigma^{(1)}(v_r)v_r = 2\pi v_r \int_0^\infty \left[1 - \cos\chi(v_r, b)\right] b db = K_m = const$$
(2.7)

Here  $\sigma^{(1)}$  is the momentum transfer (diffusion) cross section,  $v_r$  is the magnitude of the relative velocity of colliding particles, *b* is the impact parameter,  $\chi$  is the scattering (deflection) angle in the centre-of-mass frame. This definition of  $\sigma^{(1)}$  can be found in [44];  $\sigma^{(1)}v_r$  corresponds to the value  $2\pi\phi_{12}^{(l)}$  from [58], Chapter 9. It should be pointed out that when using the term "Maxwellian Molecules" only the property (2.7) i meant but not the stronger assumption that the interaction potential is  $V(r) \sim \frac{1}{r^4}$  (where *r* is the intermolecular distance).

The momentum and energy transfer between two components with such kind of interaction does not depend on the shape of velocity distribution functions. To derive the corresponding equations it is convenient to use formulas from [10], Chapter 7. The momentum gained by particles of the type 1 due to their collisions with particles of the type 2 reads as:

$$\left(\frac{d\mathbf{p}}{dt}\right)_{21} = -m_r \int K_m(\mathbf{v}_1 - \mathbf{v}_2) f_2 d\mathbf{v}_2, \quad m_r = \frac{m_1 m_2}{m_1 + m_2}$$
(2.8)

and the kinetic energy gained by particles 1 due to their collisions with particles 2 is:

$$\left(\frac{de}{dt}\right)_{21} = -m_r \mathbf{v}_1 \int K_m \left(\mathbf{v}_1 - \mathbf{v}_2\right) f_2 d\mathbf{v}_2 + \frac{m_r^2}{m_1} \int K_m \left(\mathbf{v}_1 - \mathbf{v}_2\right)^2 f_2 d\mathbf{v}_2$$
(2.9)

In case of  $K_m$  = *const* the integration in (2.8) and (2.9) yields:

$$\left(\frac{d\mathbf{p}}{dt}\right)_{21}(\mathbf{v}_1) = m_r K_m n_2 \left(\mathbf{u}_1 - \mathbf{u}_2\right)$$
(2.10)

$$\left(\frac{de}{dt}\right)_{21}(\mathbf{v}_1) = m_r K_m n_2 \left[ (\mathbf{v}_1.\mathbf{u}_2) - v_1^2 + \frac{m_r}{m_1} \left( v_1^2 + \frac{\langle E_2 \rangle}{m_2} - 2(\mathbf{v}_1.\mathbf{u}_2) \right) \right] =$$
(2.11)  
$$\frac{2m_1 m_2}{m_2} K_m \left[ \left( E_1 \rangle - \frac{m_1 v_1^2}{m_1} + \frac{m_1 - m_2}{m_2} (\mathbf{v}_1 - \mathbf{v}_2) \right) \right] =$$

$$\frac{-m_1m_2}{m_0^2}K_m n_2 \left[ < E_2 > -\frac{1}{2} + \frac{m_1 - m_2}{2} (\mathbf{v}_1 \cdot \mathbf{u}_2) \right], \quad m_0 = m_1 + m_2$$

Here  $\langle E_i \rangle$  is the average kinetic energy of the particles  $i: \langle E_i \rangle = \int \frac{m_i v_i^2}{2} f_i d\mathbf{v}_i = \frac{3}{2} kT_i + \frac{m_i u_i^2}{2}$ The total rate of momentum and energy exchange between components 1 and 2 is calculated integrating (2.10) and (2.2.2) over the velocity space  $v_1$ :

$$\left(\frac{d\mathbf{P}}{dt}\right)_{21} = \int \left(\frac{d\mathbf{p}}{dt}\right)_{21} (\mathbf{v}_1) f_1 d\mathbf{v}_1 = m_r K_m n_1 n_2 (\mathbf{u}_2 - \mathbf{u}_1)$$
(2.12)

$$\left(\frac{dE}{dt}\right)_{21} = \int \left(\frac{de}{dt}\right)_{21} (\mathbf{v}_1) f_1 d\mathbf{v}_1 = \frac{2m_1m_2}{m_0^2} K_m n_1 n_2 \left(\langle E_2 \rangle - \langle E_1 \rangle + \frac{m_1 - m_2}{2} (\mathbf{u}_1 \cdot \mathbf{u}_2)\right)$$
(2.13)

To find  $\mathbf{u}_{12}$  one has to integrate the corresponding cross collision term in (2.1) over  $m_1$ **v**<sub>1</sub>d**v**<sub>1</sub> (momentum gained by particles 1) and equate it to (2.12):

$$\left(\frac{d\mathbf{P}}{dt}\right)_{21} = \int m_1 \mathbf{v}_1 \nu_{12} \left(f_{12}^M - f_1\right) d\mathbf{v}_1 = m_1 \nu_{12} n_1 \left(\mathbf{u}_{12} - \mathbf{u}_1\right) = K_m m_r n_2 n_1 \left(\mathbf{u}_2 - \mathbf{u}_1\right)$$

Therefore:

$$\mathbf{u}_{12} = \mathbf{u}_1 + \alpha \frac{m_2}{m_0} (\mathbf{u}_2 - \mathbf{u}_1), \quad \alpha = \frac{K_m n_2}{v_{12}}, \quad m_0 = m_1 + m_2$$
 (2.14)

With  $\alpha$  another free parameter.

Similarly for  $T_{12}$ : integrating the cross collision term over  $\frac{1}{2}m_1v_1^2dv_1$  and equating it to (2.13):

$$\left(\frac{dE}{dt}\right)_{21} = \int \frac{m_1 v_1^2}{2} v_{12} \left(f_{12}^M - f_1\right) d\mathbf{v}_1 = m_1 v_{12} n_1 \left(\frac{3}{2} k T_{12} + \frac{m_1 u_{12}^2}{2} - \frac{3}{2} k T_1 - \frac{m_1 u_1^2}{2}\right) = \frac{2m_1 m_2}{m_0^2} \left(\frac{3}{2} k T_2 + \frac{m_2 u_2^2}{2} - \frac{3}{2} k T_1 - \frac{m_1 u_1^2}{2}\right)$$
(2.15)

Substituting (2.14) and  $\mathbf{u} = \mathbf{u}_1 - \mathbf{u}_2$ :

$$T_{12} = T_1 + \frac{2\alpha m_1 m_2}{m_0^2} \left(T_2 - T_1\right) + \frac{m_1 m_2}{3km_0^2} \left(2m_2 u_2^2 - 2m_1 u_1^2 + 2(m_1 - m_2)(\mathbf{u}_1 \cdot \mathbf{u}) - \alpha m_2 u^2 - 2m_0(\mathbf{u}_1 \cdot \mathbf{u}_2)\right) =$$
  
$$= T_1 + \frac{2\alpha m_1 m_2}{m_0^2} \left(T_2 - T_1\right) + \frac{m_1 m_2}{3km_0^2} \alpha (2 - \alpha) u^2$$
(2.16)

Formulas for  $T_{21}$  and  $\mathbf{u}_{21}$  can be obtained from (2.14) and (2.16) by exchanging indices. This choice of the cross-collision parameters ensures that  $\left(\frac{d\mathbf{P}}{dt}\right)_{21} = -\left(\frac{d\mathbf{P}}{dt}\right)_{12}$  and  $\left(\frac{dE}{dt}\right)_{21} = -\left(\frac{dE}{dt}\right)_{12}$  and therefore the momentum and energy conservation is met automatically. The remaining free parameter  $v_{ii}$  (uniquely connected to *a*) will be determined below, Chapter 2.3.2. In the current implementation  $\alpha = 1$ , see Appendix A.3.

## **2.3 Effective collision rates**

#### 2.3.1 Self collisions

The choice of the self-collision rates  $v_{ii}$  can be done in such a way that the model gas will have the same viscosity as a real gas. For this the the Chapman-Enskog method is applied to the kinetic equation with collision term (2.1). The analysis below is based on the book of Chapman and Cowling [58], and the notation in this Section is kept close to this book.

The first approximation  $f^{(0)}$  in the Chapman-Enskog expansion is the Maxwellian distribution. In the considered case  $f^{(0)} = f^M$ . The equation for the correction of the second order approximation  $f^{(1)}$  ( $f = f^{(0)} + f^{(1)} + \cdots$ ) can be found expressing the transport operator D(f) (full time derivative of f) in terms of the peculiar velocity  $\mathbf{c} = \mathbf{v} - \mathbf{u}$  ([58], Equation 7.30.3):

$$\nu \left( f^{(0)} - (f^{(0)} + f^{(1)}) \right) = f^{(0)} \left[ \left( \frac{mc^2}{2kT} - \frac{5}{2} \right) \mathbf{c} \cdot \nabla \ln T + \frac{m}{kT} \mathbf{c} \mathbf{c} : \frac{\partial \mathbf{u}}{\partial \mathbf{r}} \right]$$
(2.17)

Note that here the notation of the kind cc denotes the so called dyadic but not the scalar product of two vectors which is denoted as c.c ([58], Chapter 1.3). To avoid misunderstanding, the notations for vector and tensor operators which are used in this chapter are explained in Appendix C.

Equation 2.17 yields:

$$f^{(1)} = -\frac{f^{(0)}}{\nu} \left[ \left( \frac{mc^2}{2kT} - \frac{5}{2} \right) \mathbf{c} \cdot \nabla \ln T + \frac{m}{kT} \mathbf{c} \mathbf{c} : \frac{\partial \mathbf{u}}{\partial \mathbf{r}} \right]$$
(2.18)

To find the viscosity coefficient in the BGK model the expression for the first order approximation of the stresses tensor is used ([58], Chapter 7.41):

$$\Pi^{(1)} = m \int f^{(1)} \mathbf{c} \mathbf{c} d\mathbf{c}$$
(2.19)

Substituting (2.18) into (2.19) and taking into account that the integrals over odd power of c are vanishing, yields:

$$\Pi^{(1)} = -\frac{m^2}{\nu kT} \int f^{(0)} \mathbf{c} \mathbf{c} \cdot \left( \mathbf{c}^{\mathbf{c}} : \frac{\partial \mathbf{u}}{\partial \mathbf{r}} \right) d\mathbf{c}$$

This relation can be transformed using the following integral theorem ([58], Chapter 1.421):

$$\int F(\mathbf{c})\mathbf{c}\mathbf{c}.(\mathbf{c}\mathbf{c}:\mathbf{w})d\mathbf{c} = \frac{2}{15}\frac{\mathbf{c}}{\mathbf{w}}\int F(\mathbf{c})c^4d\mathbf{c}$$

Here  $F(\mathbf{c})$  is any scalar function of  $\mathbf{c}$ . Therefore:

$$\Pi^{(1)} = -\frac{2m^2}{15\nu kT} \frac{\overline{\partial \mathbf{u}}}{\partial \mathbf{r}} \int f^{(0)} c^4 d\mathbf{c}$$

Using the definition of viscosity coefficient  $\mu$  ([58], Equation (7.41,2)):  $\Pi^{(1)} = -2\mu \overline{\frac{\partial u}{\partial r}}$  and substituting:

$$f^{(0)}d\mathbf{c} = 4\pi c^2 n \left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\alpha c^2} dc, \quad \alpha = \frac{m}{2kT}$$
(2.20)

yields:

$$\mu = \frac{4nm^2\alpha^{3/2}}{15\sqrt{(\pi)}vkT}\int_0^\infty c^6 e^{-\alpha c^2}dc$$

The integral can be calculated using the following formula ([58], Chapter 1.4):

$$\int_0^\infty c^r e^{-\alpha c^2} dc = \frac{1}{2} \alpha^{-(r+1)/2} \Gamma\left(\frac{r+1}{2}\right) = \frac{\sqrt{\pi}}{2} \frac{1}{2} \frac{3}{2} \frac{5}{2} \cdots \frac{r-1}{2} \alpha^{-(r+1)/2}$$
(2.21)

Therefore:

$$\mu = \frac{4nm^2\alpha^{3/2}}{15\sqrt{(\pi)}\nu kT} \cdot \alpha^{-7/2} \frac{\sqrt{\pi}}{2} \frac{1}{2} \frac{3}{2} \frac{5}{2} = \frac{nm^2}{4\nu kT\alpha^2} = \frac{kTn}{\nu}$$
(2.22)

If collision frequency  $\nu$  for the self collisions is calculated using Formula (2.22), then in the hydrodynamic limit the model will give the same viscosity as the real gas with viscosity coefficient  $\mu$ .

The thermal conductivity coefficient given by BGK model can be calculated in the similar way. The conductive heat flux is defined as ([58], Chapter 7.4):

$$q^{(1)} = -\frac{1}{2}m \int f^{(1)}c^2 \mathbf{c} d\mathbf{c}$$
 (2.23)

Substituting (2.18) into (2.23) and vanishing integrals over odd degree of c yields:

$$q^{(1)} = -\frac{m}{2\nu T} \int c^2 \left(\frac{mc^2}{2kT} - \frac{5}{2}\right) (\mathbf{c}.\nabla T) \, \mathbf{c} d\mathbf{c}$$

If **A** is any constant vector (independent of **c**), then the following formula is valid ([58], Equation (1.42.4)):

$$\int F(c) \left( \mathbf{A.c} \right) \mathbf{c} d\mathbf{c} = \frac{1}{3} \mathbf{A} \int F(c) c^2 d\mathbf{c}$$

In this case  $A = \nabla T$  and making use of the definition of thermal conductivity  $q^{(1)} = -\lambda \nabla T$  gives:

$$\lambda = \frac{m}{6\nu T} \int \left(\frac{mc^2}{2kT} - \frac{5}{2}\right) f^{(0)}(c)c^4 d\mathbf{c}$$

Substituting (2.20) and using (2.21) to calculate the integrals one arrives to:

$$\lambda = \frac{mn}{6vT} \int_0^\infty 4\pi \left(\frac{\alpha}{\pi}\right)^{3/2} \left(\alpha c^2 - \frac{5}{2}\right) c^6 e^{-\alpha c^2} dc = \frac{2mn\alpha^{3/2}}{3\sqrt{\pi}vT} \left[\alpha \int_0^\infty c^8 e^{-\alpha c^2} dc - \frac{5}{2} \int_0^\infty c^6 e^{-\alpha c^2} d\right] = \frac{2mn\alpha^{3/2}}{3\sqrt{\pi}vT} \cdot \alpha^{-7/2} \frac{\sqrt{\pi}}{2} \frac{1}{2} \frac{3}{2} \frac{5}{2} \left[\frac{7}{2} - \frac{5}{2}\right] = \frac{5k^2 Tn}{2mv}$$

The Prandtl number (Pr) can be calculated as:

$$a = \frac{\lambda}{C_p} = \frac{5k^2Tn/(2m\nu)}{\frac{5}{2}kn} = \frac{kT}{m\nu}, \quad \eta = \frac{\mu}{mn} = \frac{kTn/\nu}{mn} = \frac{kT}{m\nu}, \quad \Pr = \frac{a}{\eta} = 1$$

Here *a* is the temperature diffusivity and  $\eta$  is the kinetic viscosity.

Theoretical studies show that for all physically meaningful interaction laws the Pr number is close to 2/3, and this conclusion is confirmed experimentally (e.g. for air at normal conditions Pr=0.7) [85]. Therefore, the BGK model yields incorrect Pr number and thus leads to an overestimated (by 50%) thermal conductivity, if viscosity is matched. In other words, the simplest version of the BGK approximation does not allow matching both experimental viscosity and thermal conductivity and strictly valid only for isothermal flow.

#### 2.3.2 Cross-collisions

The BGK collision rates for the cross-collisions can be chosen in such a way to have the same energy exchange rate between two components as for the real gas. The expression for the energy exchange rate between two gases with Maxwellian velocity distribution and different temperatures  $T_1$ ,  $T_2$  and masses  $m_1$ ,  $m_2$  was found by Desloge [86] and Morse [87].

$$\left(\frac{dE}{dt}\right)_{21} = \frac{4\pi (m_1 m_2)^{7/2} (kT_2 - kT_1) n_1 n_2}{(2\pi)^{3/2} K^{5/2} (m_1 T_2 + m_2 T_1)} \int e^{-Kg^2} g^5 \sigma^{(1)}(g) d\mathbf{g} = \sqrt{\frac{2}{\pi}} \frac{m_1 m_2 n_1 n_2}{(m_1 + m_2)^2} (kT_2 - kT_1) K^{5/2} \frac{1}{K^3} \int_0^\infty x^5 \sigma^{(1)} \left(\frac{x}{\sqrt{K}}\right) e^{-x^2} dx = \frac{2}{\sqrt{\pi}} \frac{m_1 m_2 n_1 n_2}{(m_1 + m_2)^2} \sqrt{\frac{kT_{eff}}{m_r}} (kT_2 - kT_1) \Omega_{12}^{(1)} (T_{eff})$$
(2.24)

Here:

$$K = \left(\frac{2kT_1}{m_1} + \frac{2kT_2}{m_2}\right)^{-1} = \left(\frac{2kT_{eff}}{m_r}\right)^{-1}, \quad T_{eff} = \frac{m_2T_1 + m_1T_2}{m_1 + m_2}$$
(2.25)

The effective temperature  $T_{eff}$  corresponds to the average relative velocity between the particles of two components. The  $\Omega$ -integral is defined as ([58], Chapter 9.33):

$$\Omega_{12}^{(1)} = \sqrt{\frac{kT}{2\pi m_r}} \int_0^\infty x^5 \sigma^{(1)} \left( x \sqrt{\frac{2kT}{m_r}} \right) e^{-x^2} dx$$
(2.26)

Equation (2.24) gives the energy transferred from particles 2 to particles 1 per unit time per unit volume (W/m<sup>3</sup>). It is assumed that there is now macroscopic relative motion of two gases ( $\mathbf{u}_1 - \mathbf{u}_2 = 0$ ) or at least its velocity is much smaller than the thermal velocity:  $(\mathbf{u}_1 - \mathbf{u}_2)^2 << \min(\frac{2kT_i}{m_i})$ .

According to the Chapman-Enskog theory the integral (2.26) enters the first order approximation of the diffusion coefficient ([58], Chapter 9.81):

$$D_{12} = \frac{3kT}{16nm_r \Omega_{12}^{(1)}}$$

This diffusion coefficient defines the flux of the gas 1 in the gas 2 as  $\Gamma_{12} = -D_{12}\nabla n_1$ . For molecules with  $\sigma^{(1)}(v_r)v_r = const = K_m$ :

$$\Omega_{12}^{(1)} = \frac{1}{2\sqrt{\pi}} \int_0^\infty K_m x^4 e^{-x^2} dx = \frac{3}{16} K_m, \quad D_{12} = \frac{kT}{nm_r \nu}$$
(2.27)

The expression (2.21) was used to calculate the integral in 2.27.

If  $K_m$  is determined from Equation (2.27), then the gas with such collision frequency has the same  $\Omega_{12}^{(1)}(T)$  as the real gas with a diffusion coefficient  $D_{12}$ . At the same time, according to equation (2.24) it will have the same energy equipartition rate as the real gas. It was shown in the Section 2.2.2 that the BGK model yields exactly the same energy exchange rate as the given Maxwellian gas if  $v_{12} = K_m n_2/\alpha$ . Therefore, if the effective collision rate  $v_{12}$  is determined from the experimentally measured diffusion coefficient  $D_{12}$ using Equation (2.27) the model will give the same energy exchange rate between the two components with Maxwellian velocity distribution (and no macroscopic relative motion) as in the real gas.

### 2.4 Calculating the collision rates

In this section the calculation of the BGK collision rates using empirical data on viscosity and diffusivity will be shown. It repeats and cross-checks the calculations made by Christof May [38, 39].

The empirical formula for the diffusion coefficient  $D_{12}$  is [91, 92]:

$$D_{12} = \frac{10^{-2} T^{1.75} \sqrt{\frac{M_1 + M_2}{M_1 M_2}}}{P\left[ (\sum v_1)^{1/3} + (\sum v_2)^{1/3} \right]^2} = D_0 \frac{T^{0.75}}{n}$$
(2.28)

Here  $D_{12}$  is measured in m<sup>2</sup>/s, *P* is the total pressure (Pa), *n* is the total density (m<sup>-3</sup>),  $M_1$  and  $M_2$  are molecular masses of the components in kg/mol (not to be confused with the small *m* which denotes masses in kg), *T* is measured in K. ( $\sum v$ ) are the so called diffusion volumes which are found empirically. May used the diffusion volumes from [92]. The corresponding rate of the cross-collisions is calculated according to formula (2.27):

$$\langle \sigma v \rangle_{12} = s_0 T^{0.25}, \quad s_0 = \frac{k}{m_r D_0}$$
 (2.29)

For the self-collisions May used viscosity recalculated from the diffusion coefficient (2.28). In the notation of the book [93] the corresponding transport coefficients are:

$$\mu = \frac{5}{16} \frac{\sqrt{\pi MRT}}{\pi \sigma^2 \Omega_\nu} = \frac{5}{16} \frac{kT}{\sqrt{\frac{\pi kT}{m}} \sigma^2 \Omega_\nu}$$
(2.30)

$$D = \frac{3}{16} \left( 2\pi kT \frac{M_1 + M_2}{M_1 M_2} \right)^{1/2} \frac{1}{n\pi\sigma^2 \Omega_D} = \frac{3}{8} \frac{kT}{n\sqrt{\frac{\pi kT}{m}}\sigma^2 \Omega_D}$$
(2.31)

Here  $R = k/N_A = 8314$  J/(K·kmol) (gas constant),  $N_A$  is the Avogadro number. The formula for *D* was reduced to get the coefficient of self diffusion. Comparing the relations (2.30), (2.31) with corresponding formulas from [58], Chapter 9:

$$\mu = \frac{5}{8} \frac{kT}{\Omega_{12}^{(2)}(2)}, \quad D = \frac{3}{8} \frac{kT}{nm\Omega_{12}^{(1)}(1)}$$
(2.32)

one finds the connection between  $\Omega_{\nu}$  and  $\Omega_{D}$  and Chapman-Enskog  $\Omega$  integrals:

$$\Omega_{12}^{(2)}(2) = 2\sqrt{\frac{\pi kT}{m}}\sigma^2\Omega_{\nu}, \quad \Omega_{12}^{(1)}(1) = \sqrt{\frac{\pi kT}{m}}\sigma^2\Omega_D$$
(2.33)

The notation of [93] ensures that for the case of rigid spheres  $\Omega_{\nu} = \Omega_D = 1$ . Formulas (2.32) are only the first approximation of the decomposition into the Sonine polynomials [58]. But calculations of the higher order corrections made for some special cases show that they do not exceed 10 % for viscosity and diffusion coefficients [58, 94].

The connection between  $\mu$  and *D* can be found using relations (2.32):

$$\mu = \frac{5}{8} \frac{kT}{\Omega_{12}^{(2)}(2)} = \frac{5}{8} \frac{kT}{\Omega_{12}^{(2)}(2)} \frac{3nm\Omega_{12}^{(1)}(1)}{3nm\Omega_{12}^{(1)}(1)} = \frac{5}{3}Dnm\frac{\Omega_{12}^{(1)}(1)}{\Omega_{12}^{(2)}(1)} = \frac{5}{6}Dnm\frac{\Omega_D}{\Omega_V}$$
(2.34)

For most of the practical cases one can assume that  $\frac{\Omega_v}{\Omega_D} = 1.1$  [93], page. 551. Then, using expression (2.28) for the diffusion coefficient (reduced to self-diffusion) one obtains:

$$\mu = \frac{5}{6} \cdot \frac{1}{1.1} \frac{M}{R} \frac{10^{-2} T^{0.75} \sqrt{\frac{2}{M}}}{\left[2(\sum \nu)^{1/3}\right]^2} = 1.894 \cdot 10^{-3} \frac{\sqrt{2M} T^{0.75}}{R(\sum \nu)^{2/3}} = \mu_0 T^{0.75}$$
(2.35)

Here the temperature *T* is measured in K, the mass *M* in kg/kmol ( $\approx$ amu). The viscosity is calculated in Pa·s. This is exactly the formula which can be found in [38].

If the viscosity is known, then the collision rate is calculated using Formula (2.22):

$$<\sigma v >= s_0 T^{0.25}, \quad s_0 = k/\mu_0$$
 (2.36)

The results of calculating  $D_0$ ,  $\mu_0$  and  $s_0$  for some selected substances are shown in Table 2.1. The column "ln  $s_0$ " is the input data for EIRENE (where the temperature is translated from K to eV). The column  $L_0$  is the proportionality coefficient in the formula for the Mean Free Path (MFP, cm):

$$MFP = \frac{\sqrt{8kT}\pi m}{s_0 T^{0.25} n} = L_0 \frac{T^{0.25}, eV}{n, 10^{20} m^{-3}}$$
(2.37)

In other words  $L_0$  is the MFP of the test particle in the background gas with the temperature 1 eV and the density  $10^{20} m^{-3}$ .

To cross-check the May's data they were compared with the low-temperature diffusivity and viscosity data available in the engineering literature [95, 96]. The results are shown in Figures 2.1a, 2.1b. The maximum deviation is 26% for viscosity and 20% for diffusivity. The deviation tends to increase for higher temperatures. Figure 2.1c shows comparison with  $H_2$  viscosity calculated using Sutherland's formula:

$$\mu = \mu_0 \frac{0.555T_0 + C}{0.555T + C} \left(\frac{T}{T_0}\right)^{1.5}$$
(2.38)

Collision	$\mu_0$	$D_0$	<i>s</i> <sub>0</sub>	$\ln s_0$	$L_0$
D+D	2.6071e-07	-	5.2958e-11	-2.1322e+01	20.1
$D_2+D_2$	1.7881e-07	-	7.7217e-11	-2.0945e+01	9.75
D <sub>2</sub> +D	-	6.1275e+19	1.0177e-10	-2.0669e+01	D <sub>2</sub> : 7.40
	-				D: 10.5
He+D	-	8.6567e+19	7.2037e-11	-2.1014e+01	He: 10.5
	-				D: 14.8
He+D <sub>2</sub>	-	4.8060e+19	8.6505e-11	-2.0831e+01	8.70

Table 2.1: BGK collision rates (see notations in the text)



Figure 2.1: Comparison of the viscosity and diffusivity calculated by May [38] with the data from CRC Handbook [95] and Sutherland's approximation for  $H_2$  viscosity taken from [96] (Crane)

The constants  $\mu_0$ , *C* and  $T_0$  are taken from [96], the approximation is valid for temperatures below 800 K. For those low temperatures it matches the data from [95], Figure 2.1b. For high temperatures May's viscosity and formula (2.38) deviate significantly from each over. The deviation reaches a factor of 2.2 for T=2 eV, Figure 2.1c. This indicates at least that the relation of the form (2.28) with constant power is valid only for low temperatures. Indeed, the review [94] suggests that this power can vary from 1.5 to 2 for different temperature ranges.

Comparison of the extrapolation of empirical dependences for viscosity and diffusivity with the results of quantum-mechanical calculations was done in [33]. The quantum-calculations show that the temperature dependence of the transport coefficients saturates and begins to decrease starting from temperatures 0.5..1 eV, opposite to the formulas (2.28), (2.30), (2.38) which show constant increase. However, the calculated coefficients shown in [33] do not match the experimental values for low temperatures.

Everywhere in this work the May's collision rates are used, because the strong deviations between different approaches starts to be significant only for temperatures higher than 0.5 eV. But for such high temperatures the neutral-neutral collisions are not very important. The best solution would probably be to combine the low temperature empirical data with the results of the quantum calculations for high temperatures.

## 2.5 The effect of neutral-neutral collisions

The principal effects related to the neutral-neutral collisions (NNC) can be seen in the calculations with fixed plasma background. The calculations were made for the plasma background of the case ITER 828 with gas puffing rate  $5.7 \cdot 10^{22} \, s^{-1}$ , average neutral pressure in PFR 6 Pa, full carbon wall and input power to the SOL 100 MW. The model is described in Section 1.3. The distribution of the electron temperature and density in the divertor can be found in Section 3.3.1, Figures 3.18b, 3.19b.

The comparison of the neutral density and temperature without and with NNC is shown in Figures 2.2- 2.5. The "temperature" in the plots is the average kinetic energy multiplied by 2/3: it includes thus the energy of the drift motion. The shown figures are obtained after EIRENE runs with 700.000 histories. For BGK 15 iterations with approximately 20.000 and then 3 iterations with 700.000 histories were made. In this case the standard deviation for the density and average kinetic energy of neutrals in the region of interest does not exceed 5 %.

One can see a significant increase of the molecule density (the maximum increases by a factor of 3) in V-shapes and in the dome channel, Figure 2.3. The temperature of molecules increases by an order of magnitude. On the contrary, the density of atoms in those regions decreases, as well as their temperature. This behaviour will be explained below.

The main reason is the collisions of D atoms with  $D_2$  molecules. Directly in front of the targets near the strike points the density of atoms is high enough (>  $2 \cdot 10^{14} cm^{-3}$ , Figure 2.2)
to produce high D+D<sub>2</sub> collisionality, Figure 2.6. The shown Mean Free Path (MFP) was calculated directly by Monte-Carlo using the estimation:  $MFP = \sum_i \frac{V_i}{v_i} \cdot w_i \cdot t_i$ . Here *i* is the index of one free flight between two events (collision, changing the grid cell etc),  $t_i$  is the time between two events,  $w_i$  is the statistical weight,  $V_i$  is the current velocity of the test particle and  $v_i$  is the collision rate (for the collisions for which the MFP is calculated).

The D<sub>2</sub>+D collisions are responsible for the observed increase of D<sub>2</sub> temperature, Figure 2.5. The effect is so strong because in the absence of NNC there is no process (in the model of EIRENE 1996) which can increase the kinetic energy of molecules. In this case it is determined completely by the wall temperature. However, if the model includes elastic collisions of molecules with ions  $D_2+D^+$  (see Chapter 3), the heating due to NNC becomes unimportant. It's effect is studied here mostly because of its qualitative similarity to the effect of  $D_2+D^+$  collisions.

The resulting increase of the molecule density originates from their compression near the targets due to back-scattering. This effect is illustrated in Figure 2.7a which shows the incident flux of molecules to the inner and outer targets. When NNC are turned on the flux is a factor 3 higher. The increase of the return flux results in the increase of the molecule density in front of the targets, Figure 2.3. The increase of the molecular pressure in the vicinity of targets leads to the same grow in V-shapes and beneath the dome. This latter statement is based on the fact that the gas conductivity between those regions (target region - V-shape - dome channel, Figure 1.1b) is at least not decreased when NNC are switched on, thus the pressure gradient is not increased. This finally leads to a factor 3 higher pressure of the neutral gas in front of the pumping surface, Figure 2.7b.

The temperature of D atoms near the strike points does not experience significant modification because of permanent heating due to charge exchange with plasma ions. But in the "plasma-free" region their temperature reduces, Figure 2.4, because atoms transfer now a part of their kinetic energy to the molecules. The density of atoms in this region becomes smaller, almost vanishing in the middle of the dome channel, Figure 2.2. This happens because D+D<sub>2</sub> collisions increase the number of collisions of D atoms with the wall. According to the actual wall interaction model each such collision can lead to a transformation of the atom into a molecule (thermal desorption), thus decreasing the number of atoms and adding to the increase of the molecule density.

This vanishing of the density of atoms leads to a significant increase of the pumping speed, defined as the ratio of the pumping flux to the neutral pressure. Without NNC the atomic fraction constituted about 40 % of the total neutral pressure, Figure 2.7b. At the same time more than 90% of the entire particle flux incident on the pumping surface was associated with molecules, Figure 2.8a. The reason is that the incident flux scales as  $\frac{\text{Pressure}}{\sqrt{\text{Temperature}}}$  and the temperature of atoms without NNC is a factor 20 larger than

that of molecules. In other words, the pressure associated with atoms creates almost no pumped flux. The NNC remove this "useless" fraction, Figure 2.8a. Now the gas in the dome channel consists almost only of the cold (almost wall temperature) molecules. In order to have about the same particle throughput, the pumping speed at the duct entrance (absorption coefficient at the pumping surface) in all succeeding calculations was lowered by a factor of 1.6 compared to the old model (from 1.15 % to 0.7 %). This and previous effects of neutral-neutral collisions are described in the paper [50].

Figure 2.8b shows an example of the particle balance in the dome with and without NNC. Mostly atoms enter the dome channel and mostly molecules leave it. The net flux of nuclei is directed from the inner divertor to the outer one. One can see that this flux is an order of magnitude larger in the case with NNC. This can be partly explained by the increase of the molecule density, and partly by the increase of the channel conductivity as flow transits from the free-molecular to hydrodynamic regime: an effect, which is well known in the rarefied gas dynamics, see e.g. [97].

In the analysis above He atoms were not considered because their density is almost two orders of magnitude lower than that of D. Like D atoms, they experience cooling due to collisions with  $D_2$  molecules. The pumped flux of He increases by a factor of 2, Figure 2.8b.

Short mean free paths, Figure 2.6c suggest that the gas flow in V-shapes and in the dome channel should be close to hydrodynamics. The Velocity Distribution Function (VDF) in some selected spatial points was calculated directly for the case ITER 1055p1 (the case with photon transport and low density, see Section 4.3) in an EIRENE test run with



Figure 2.2: Density of D atoms

900.000 histories. Figure 2.9 shows the distribution function for the absolute magnitude of velocity of  $D_2$  molecules for two selected points. One point (point 10) lies in the middle of the dome channel, another one (point 14) lies in the inner V-shape. One can see a very good agreement with a Maxwellian, especially for the dome channel, as expected. Angular distribution of velocity (not shown) is also isotropic. However, whereas in the dome channel and V-shapes one finds molecular gas in quasi-equilibrium, at the entrance to the dome channel the MFP is larger than 5 cm, Figure 2.6c. This means a transition flow with Knudsen Number  $\approx 1$ .

The calculations shown above were made without elastic collisions of molecules and ions. To asses the effect of NNC for the model with up-to-date molecular kinetics, Chapter 3, the results with and without NNC were compared on the fixed plasm of case ITER 1055. The main difference is in the pressure distribution in the dome channel, Figure 2.10. The pressure "upstream", - at the bottom near the entrance to the channel, - is similar in both cases: 17..19 Pa on the inner side and 13..14 Pa on the outer side. But when NNC are switched on, the density in the middle of the dome channel increases from 5.3 to 8.5 Pa due to higher conductivity in the collisional case. The velocity pattern does not experience serious modification. The total hydrogenic fluxes to the dome and from the dome are changed by less than a factor of 1.5. NNC can also affect the efficiency of impurity pumping. Figure 2.11 shows relative thermal flux of He atoms  $\frac{(n\sqrt{T/m})_{He}}{(n\sqrt{T/m})_D + 2 \cdot (n\sqrt{T/m})_D}$ : the ratio of the one-side thermal flux of He and that of D nucleus. This quantity corresponds approximately to the fraction of He in the incident flux, thus in the pumped flux. He atoms enter the dome channel mainly from the inner side. NNC hinder their penetration further through the channel, increasing He concentration on the inboard side, and decreasing it on the outer side.



Figure 2.3: Density of  $D_2$  molecules



Figure 2.4: Temperature (average kinetic energy) of D atoms



Figure 2.5: Temperature (average kinetic energy) of D<sub>2</sub> molecules



Figure 2.6: Inverse average mean free path for  $D_2+D_2$  (a) and  $D_2+D$  (b,c) collisions. Red regions corresponds to MFP<1 cm for  $D_2+D_2$  and MFP<2 cm for  $D_2+D$  collisions



Figure 2.7: (a) The effect of back-scattering of molecules due to their collisions with atoms; (b) the increase of the neutral gas pressure in front of the pumping surface (see Figure 1.1b). "Distance from separatrix" is the distance along the target. Negative direction points towards PFR.



Figure 2.8: (a) The modification of the pumped flux; (b) the diagram of the neutral particle fluxes in the dome. Subfigure (a) shows the distribution along the pumping surface. "D" on the diagram stands for the number of nuclei ("D-at." is the flux of atomic D)



Figure 2.9: An example of the distribution function for the absolute magnitude of velocity for D<sub>2</sub> molecules for the point lying in the centre of the dome (a) and deep in the inner Vshape (b). The parameters of the gas in Point 10 and Point 14 are given in the table below. R and Z are the radial and vertical coordinates of the point, T is the temperature (average kinetic energy),  $V_{R,Z,\theta}$  are the radial, vertical and toroidal components of the average velocity.

Point	R, cm	Z, cm	T, eV	$V_R$ , cm/s	V <sub>Z</sub> , cm/s	$V_{\theta}$ , cm/s
10	485	-397	0.05	1.9e3	-5.4e2	-5.4e3
14	410	-382	0.10	-8.9e2	-2.4e3	-1.9e4



Figure 2.10: Pressure of  $D_2$  molecules with and without NNC on a fixed plasma (case ITER 1055)



Figure 2.11: Relative thermal flux of He atoms (estimate of the fraction of He in the incident flux) with and without NNC on a fixed plasma(case ITER 1055)

## **Chapter 3**

# **Molecular kinetics**

## **3.1 Elastic collisions**

#### **3.1.1 General definitions**

This section contains a detailed description of the current status of the model for elastic collisions in EIRENE. For completeness it contains the necessary theoretical background including some general terms and relations. In particular, a complete derivation of the momentum and energy transfer rates between test particles and a Maxwellian plasma background is shown, Section 3.1.4. These rates can be used to apply a Track Length Estimator instead of a Collision Estimator for the corresponding sources, which has been done in the present work. The Track Length Estimator can in some cases (low collisionality) increase the accuracy of calculations. This is a side-by result of this work because it was found almost irrelevant for the highly collisional ITER divertor conditions. However, using different estimators provides an independent consistency check of the implementation of elastic collisions, Section 3.1.8.

The term "collision" in this work is used to define an instant change of velocity and (or) the internal state of the test particle. The main physical assumption behind this model is that the forces acting between particles can be strong enough only for short distances. Only if the two particles approach each other to such short distance their velocities or state can be significantly perturbed. Such close approach is called "collision". It is assumed, therefore, that the distance of this approach is much smaller than the distance which particle travels between the two collisions ("strong perturbations"). Analogously, the time which is necessary to change the test particle's state (the time of one collision) is assumed to be much smaller than the time between two subsequent collisions. In the frame of this work only collisions between two particles are considered (with one exception: three-body recombination). The assumptions listed above are valid for a gas with relatively low density and short-range interaction potential between particles. They break down for high densities (e.g. pressures more than 10..100 bar for room temperature) or long range Coulomb-like interaction potentials.

Let a test particle with velocity  $\mathbf{v}_t$  moves in the background with a given velocity distribution  $f_p$ . Here and below the index *t* corresponds to the neutral ("test") particle and the index *p* corresponds to the background ion: "plasma" particle. The distribution  $f_p$  here is normalised to the particle density. The collision rate is the total number of collisions experienced by the test particle in a unit time interval. It is assumed that this number of collisions is large enough: either the time of observation is long, or an average over many test particles is calculated. The consideration below is based predominantly on the paper of Trubnikov [10]. The number of the test particles with velocities laying in the interval  $\{(v_x^p, v_x^p + dv_x^p), (v_y^p, v_z^p + dv_z^p)\}$  which cross the area  $bdbd\psi$ , Figure **??**, during a unit time interval is equal to:

$$\mathbf{v}_r n_p f(\mathbf{v}_p) b db d\psi dv_x^p dv_y^p dv_z^p, \quad \mathbf{v}_r = \mathbf{v}_t - \mathbf{v}_p \tag{3.1}$$

Here  $n_p$  is the number density of the background particles. The quantity *b* is called the impact parameter: it is the distance of closest approach of the two particles if no interaction

would exist, Figure **??**. To find the total number of collisions in a unit time interval  $R_t n_p$  this relation should be integrated over all possible values of b,  $\phi$  and  $\{v_x^p, v_y^p, v_z^p\}$ :

$$R_t n_p = n_p \int d\mathbf{v}_p \cdot v_r f(\mathbf{v}_p) \int_0^{2\pi} d\psi \int_0^{b_{max}} db \cdot b$$
(3.2)

The following common notation is used:



 $\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z = \int d\mathbf{v}$ 

The quantity:

$$\sigma^{t}(E_{r}) = \int_{0}^{2\pi} d\psi \int_{0}^{b_{max}} db \cdot b = 2\pi \int_{0}^{b_{max}} bdb$$
(3.3)

Figure 3.1: Towards definition of the collision rate and cross-section

is the total cross-section of the collision. The integration over the angle  $\psi$  is made assuming axial symmetry of the collision (*b* is independent of  $\psi$ ). Here  $\sigma^t$  is defined as a function of  $E_r$ :

$$E_r = \frac{m_r v_r^2}{2}, \quad \mathbf{v}_r = \mathbf{v}_t - \mathbf{v}_p, \quad m_r = \frac{m_p m_t}{m_p + m_t}$$

 $E_r$  is the kinetic energy of the relative motion,  $\mathbf{v}_r$  is the relative velocity,  $m_r$  is the reduced mass.

The parameter  $b_{max}$  in (3.7) is an artificial cut-off parameter which is introduced to avoid the disconvergence of the classical cross-section. The choice of this parameter depends in fact on the convention of what is called "collision". Collision which does not lead to the modification of internal state is a deflection near a centre of force. Formally a classical particle approaching to any distance to this centre of force will deflect to some (although probably very small) angle. This is the reason why the cross-section becomes formally infinite. Obviously, the collisions with too large impact parameters lead to a very weak deflection and do not have significant influence on the particle transport. The cut-off parameter serves therefore to eliminate the unimportant weak collisions. The choice of this parameter will be described later. The problem of the disconverges of the total crosssection can be rigorously solved only in quantum mechanics. For the classical treatment the choice of this cross section (equal to  $\pi b_{max}^2$ ) is not very important above some level, because it can only increase the amount of weak (low-angle) collisions.

Using definition (3.7) the integral (3.2) is expressed as:

$$R_t n_p = n_p \int \sigma^t (E_r) \cdot v_r f(\mathbf{v}_p) d\mathbf{v}_p$$
(3.4)

The calculation of the integral (3.4) for Maxwellian  $f(\mathbf{v}_p \text{ is considered in Section 3.1.2.}$ 

In this section only elastic collisions are considered i.e.: collisions which do not change the total kinetic energy. In case of classical interaction with spherically symmetric interaction potential V(r) the scattering angle  $\Theta$ , Figure **??** is calculated as (see e.g. [99], Chapter 4.18):

$$\Theta = \arccos(\cos\chi), \quad \chi(b, E_r) = \pi - 2b \int_{r^*}^{\infty} \frac{dr}{r^2 \sqrt{1 - V(r)/E_r - (b/r)^2}}$$
(3.5)

Here  $\chi$  is the deflection function,  $r^*$  is the distance of the closest approach, Figure **??**. In general  $\chi$  is different from the deflection angle  $\Theta$  because orbit-trajectories with  $\chi > \pi$  are possible [44]. The distance  $r^*$  can be found as the maximal root of the equation:

$$1 - V(r)/E_r - (b/r)^2 = 0$$
(3.6)

Using the deflection function  $\chi$  one can define the differential cross-section which depends on the scattering angle  $\Theta$  (see e.g. [44, 99]):

$$\sigma(\Theta, E_r) = \sum_i \frac{b_i}{\sin \chi} \left| \frac{db_i}{d\chi} \right|$$

In general *b* can be a multi-valued function of  $\chi$  and the sum over all the branches of *b* is calculated.

Using this definition, the total cross-section  $\sigma^t$  can be expressed as:

$$\sigma^{t}(E_{r}) = 2\pi \int_{0}^{\pi} \sigma(\Theta, E_{r}) \sin \Theta d\Theta$$
(3.7)

To describe momentum and energy exchange (see Section 3.1.4) the diffusion (momentum transfer) cross-section is introduced:

$$\sigma^{d}(E_{r}) = 2\pi \int_{0}^{\infty} (1 - \cos\Theta) \, b db = 2\pi \int_{0}^{\pi} (1 - \cos\Theta) \sin\Theta\sigma(\Theta, E_{r}) \, d\Theta \tag{3.8}$$

It is also common to define:

$$\sigma^{(0)}(E_r) = 2\pi \int_0^{b_{max}} bdb,$$
  

$$\sigma^{(l)}(E_r) = 2\pi \int_0^{\infty} \left(1 - \cos^{(l)}\Theta\right) bdb, \ l > 0$$
(3.9)

Then, taking into account that  $\cos \chi = \cos \Theta$  one gets (compare to (3.7) and (3.8)):  $\sigma^t = \sigma^{(0)}$ and  $\sigma^d = \sigma^{(1)}$ . In some places below  $\sigma^{(l)}$  is expressed as a function of  $v_r$  which is equivalent to  $\sigma^{(l)}(E_r)$  for given masses  $m_t$  and  $m_p$ .

The cross-sections  $\sigma^{(l)}$  for hydrogen-helium plasmas were calculated in [44] using prescribed potential V(r) (see Appendix B.2). In this paper the parameter  $b_{max}$  in the integral (3.7) was determined from a prescribed cut-off angle  $\chi_0$ . To find  $\chi_0$  the integral (3.8) (which always converges) was calculated using the same low angle cut-off and the result was compared to the calculation with the full integral. It was found that  $\chi_0 = 0.1$  gives a difference less than 1% for all relevant processes with hydrogen and helium.

In the next sections some major issues of implementing the sampling of the elastic collisions in a Monte-Carlo code are described. In section 3.1.2 the calculation of the collision rate for Maxwellian background is shown. Section 3.1.3 explains the treatment of the cross-section and collision rate data. For bookkeeping the the algorithm of sampling the velocity of the incident particle is described in Appendix B.1. The model for the interaction potential and the sampling of the scattering angle can be found in Appendix B.2. Derivation of the relations for momentum and energy transfer rates is given in Sections 3.1.4- 3.1.6. A numerical example is shown in Section 3.1.8.

#### 3.1.2 Collision rate for Maxwellian background

Everywhere in this work it is assumed that the background (plasma ions) has a shifted Maxwellian velocity distribution:

$$f_p(v_p^x, v_p^y, v_p^z)dv_p^x dv_p^y dv_p^z = \frac{\alpha^3 n_p}{\pi^{3/2}} v_p^2 \exp\left[-\alpha^2 \left((v_p^x - u_p^x)^2 + (v_p^y - u_p^y)^2 + (v_p^z - u_p^z)^2\right)\right] dv_p^x dv_p^y dv_p^z, \quad \alpha^2 = \frac{m_p}{2T}$$
(3.10)

Here  $m_p$ , T and  $\mathbf{u}_p$  are the mass, temperature (in energy units) and the average velocity of the background particles.

It is convenient to assume first the Maxwellian distribution without shift  $\mathbf{u} = 0$ :

$$f_p(v_p^x, v_p^y, v_p^z)dv_p^x dv_p^y dv_p^z = \frac{\alpha^3 n_p}{\pi^{3/2}} v_p^2 \exp\left(-\alpha^2 v_p^2\right) \sin\theta d\theta d\phi dv_p$$
(3.11)

Here  $\mathbf{v}_p$  is expressed in spherical coordinates with  $\theta$  being the angle between  $\mathbf{v}_t$  and  $\mathbf{v}_p$ , Figure 3.2.

Following the approach of Nakano and Baba [104] it is convenient to make a transformation from variables  $(v_p, \theta)$  to variables  $(v_p, v_r)$ . Taking into account that (see Figure 3.2):

$$v_r^2 = v_p^2 + v_t^2 - 2v_t v_p \cos\theta$$
(3.12)

the Jacobian of the transformation is:

$$\frac{\partial(v_p,\theta)}{\partial(v_p,v_r)} = \begin{vmatrix} \frac{\partial v_p}{\partial v_p} & \frac{\partial \theta}{\partial v_p} \\ \frac{\partial v_p}{\partial v_r} & \frac{\partial \theta}{\partial v_r} \end{vmatrix} = \left(\frac{\partial v_r}{\partial \theta}\right)^{-1} = \frac{v_r}{v_p v_t \sin \theta}$$
(3.13)



Figure 3.2: Towards integra-

Substituting (3.11) into (3.4), taking into account Jacobian (3.13) and integrating over angle  $\phi$  yields:

$$R_{t} = \frac{2\alpha^{3}}{\sqrt{\pi}v_{t}} \int_{0}^{\infty} dv_{r} \sigma^{(0)}(v_{r}) v_{r}^{2} \int_{v_{t}-v_{r}}^{v_{r}+v_{t}} dv_{p} v_{p} \exp\left(-\alpha^{2} v_{p}^{2}\right)$$
(3.14)

The integration limits for  $v_p$  can be found from the following geometrical considerations. Formula (3.12) shows that:

$$|v_t - v_p| < v_r < v_t + v_p$$

The corresponding region in the  $(v_p, v_r)$  plan is sketched in Figure 3.2. This region can also be defined by the inequality:

$$|v_t - v_r| < v_p < v_t + v_r$$

tion limits for  $v_p$  The limit  $|v_t - v_r|$  in the integral 3.14 is replaced by  $v_t - v_r$  because the integrand is anti-symmetric regarding zero. This means that if  $(v_t - v_r) < 0$  then:

$$\int_{v_t-v_r}^{|v_t-v_r|} \cdots dv_p = 0, \quad \text{therefore} \quad \int_{v_t-v_r}^{v_r+v_t} \cdots dv_p = \int_{|v_t-v_r|}^{v_r+v_t} \cdots dv_p$$

This rule works for any odd power of  $\nu$  which is in particular the case for all integrals considered below in Section 3.1.5.

It is convenient to introduce dimensionless velocities:

$$\xi = \alpha v_r, \quad v = \alpha v_p, \quad \delta = \alpha v_t \tag{3.15}$$

Note that  $\delta$  is a constant. The integral (3.14) then reduces to:

$$R_t = \frac{2\alpha^{-2}}{\sqrt{\pi}v_t} \int_0^\infty d\xi \cdot \xi^2 \sigma^{(0)}(\xi^2 T) \int_{\delta-\xi}^{\delta+\xi} d\nu \nu \exp\left(-\nu^2\right)$$
(3.16)

Here it is assumed that the cross-section  $\sigma^{(0)}$  is defined as a function of  $E_{lab} = \frac{m_p v_r^2}{2} \xi^2 T$ . Finally:

$$R_{t} = \frac{\alpha^{-2}}{\sqrt{\pi}v_{t}} \int_{0}^{\infty} d\xi \cdot \xi^{2} \sigma^{(0)}(\xi^{2}T) \left[ e^{-(\delta-\xi)^{2}} - e^{-(\delta+\xi)^{2}} \right] = \frac{\alpha^{-1}n_{p}}{\sqrt{\pi}v_{t}} \int_{0}^{\infty} dv_{r} \cdot v_{r}^{2} \sigma^{(0)}(v_{r}) \left[ e^{-\alpha^{2}(v_{t}-v_{p})^{2}} - e^{-\alpha^{2}(v_{t}+v_{p})^{2}} \right]$$
(3.17)

The Formula (3.17) can be found e.g. in [64]. It can be easily generalised for the case of a Maxwellian background with shift  $\mathbf{u}_p$  replacing  $v_t$  by the relative velocity of the test particle and the background  $|\mathbf{v}_t - \mathbf{u}_p|$ .

For the electron-impact processes, which will be considered in Section 3.2, the relation between the cross section  $\sigma(\mathbf{v}_r)$  and the collision rate *R* is simplified due to the fact that the thermal velocity of the electrons is much higher than that of the test particles. This allows one to assume  $\mathbf{v}_t = 0$  and  $\mathbf{v}_r = \mathbf{v}_t$  and Equation (3.17) is then reduced to:

$$R = \int \sigma^t \left( v_p \right) \cdot v_p f(\mathbf{v}_p) d\mathbf{v}_p = \frac{4\alpha^3 n_p}{\sqrt{\pi}} \int \sigma^t \left( v_p \right) \cdot v_p^3 \exp\left( -\alpha^2 v_p^2 \right) d\mathbf{v}_p$$
(3.18)

Thus, the collision rate (reaction rate) for the electron-impact collision is a function of electron temperature only. The average (macroscopic) velocity is neglected because for the electrons it has the same magnitude as for ions (due to ambipolarity), therefore it is much smaller than the electron thermal velocity.

#### **3.1.3 Cross sections and collision rates**

In this work the Janev-type polynomial approximation [64] is used for the atomic crosssections. The general form of this approximation as applied to elastic collisions is:

$$\begin{cases} E_{lab} \leq E_{min}, \quad \ln(\sigma) = \sum_{i=0}^{2} a_{li} \ln^{i}(E_{lab}) \\ E_{min} < E_{lab} < E_{max}, \quad \ln(\sigma) = \sum_{i=0}^{8} a_{i} \ln^{i}(E_{lab}) \\ E_{max} \geq E_{lab}, \quad \ln(\sigma) = \sum_{i=0}^{2} a_{ri} \ln^{i}(E_{lab}) \end{cases}$$
(3.19)

For convenience of calculating the rates (see Section 3.1.2) the energy of the relative motion  $E_r$  is replaced in the fittings by the energy of the plasma particle in moving frame  $E_{lab}$ :

$$E_{lab} = \frac{m_p v_r^2}{2} = \frac{m_p}{m_r} E_r$$
(3.20)

The whole energy range is divided into three parts by the following two energies:  $E_{min} = E_{lab\_c}$ ,  $E_{max} = E_{lab\_0}$ . The energy  $E_{lab\_c}$  is the parameter of the model used for the interaction potential, see Appendix B.2. The second characteristic energy  $E_{r0}$  appears due to the fact that the dependence  $\chi(b)$  is ambiguous: for  $E_r > E_{r0}$  one angle  $\chi$ , Equation (3.5), corresponds to 3 different values of the impact parameter *b*. The same data format (3.19) as for  $\sigma^{t}$  is used for the diffusion cross section, although for  $\sigma^{d}$  it is not necessary to separate the low and high energy branches.

To obtain the fitting approximations  $\sigma^{t}$  and  $\sigma^{d}$  were calculated for a number of energies  $E_{lab}$  using formulas (3.7) and (3.8) together with (3.5) and the model functions for V(r) [44]. The fitting coefficients were found by the Least Square method. The calculated fitting parameters  $a_{i}$ ,  $a_{li}$  and  $a_{ri}$  for  $0.01 \le E_{lab} \le 100 \ eV$  can be found in the database AMJUEL [106], Section H.1. The cross-sections  $\sigma^{t}$  and  $\sigma^{d}$  for  $H_{2} + H^{+}$  collisions are plotted in Figure 3.3a together with the cross section of the charge-exchange process  $H + H^{+}$  [64] for comparison. This latter is the effective cross-section comprising both charge-exchange and elastic collisions (which can be important for energies  $< 1 \ eV$ ). For energies  $E_{lab} < 10 \ eV$  the cross sections of both processes have similar magnitude. For  $E = T = 1 \ eV$  (where T is the background temperature) the collision rate for  $H_2 + H^+$  is  $10^{-8} \ cm^3/s$ . The average velocity of  $H_2$  molecule in this case is  $10^6 \ cm/s$ , therefore, the expected Mean Free Path for the plasma density  $10^{14} \ cm^{-3}$  is 1 cm. Note that despite similar collision rates one charge-exchange collision is "stronger" than one elastic collision: the former assumes a scattering to angle  $\pi$  (maximum possible scattering) whereas the latter is a deflection to some smaller angle.

Figure 3.3a shows also the diffusion cross-sections obtained by quantum-mechanical calculations by Krstić and Schultz [102]. The actual classical and quantum mechanical cross-section for  $H_2 + H^+$  collisions start to disconverge significantly (more than a factor 1.5) only for energies  $E_{lab}$  greater than 5 eV. Note that the comparison of the quantum calculations with the Bachmann-Reiter data in [102] shows too large discrepancy even for the low energies because the results of classical calculations were not rescaled from  $E_{lab}$  to  $E_r$ .

All cross-sections (and collision rates) which are used here are calculated for hydrogen. To apply them for its isotopes an appropriate mass rescaling should be used. The scaling relations for the hydrogen isotopes were studied by Krstić and Schultz [103] (see also [102]). They showed that for the case of H+H<sup>+</sup> collisions both total and momentum cross-sections scale as  $\sigma^{(l)}(v_r)$ . Taking into account that  $v_r = \sqrt{E_{lab}/m_p}$  the cross section  $\sigma_2^{(l)}$ for the mass  $m_{p2}$  can be calculated from known  $\sigma_1^{(l)}$  (for the mass  $m_{p1}$ ) as:

$$\sigma_2^{(l)}(E_{lab}) = \sigma^{(l)}\left(\frac{2E_{lab}}{m_{p2}}\right) = \sigma^{(l)}\left(\frac{2\frac{m_{p1}}{m_{p2}}E_{lab}}{m_{p1}}\right) = \sigma_1^{(l)}\left(\frac{m_{p1}}{m_{p2}}E_{lab}\right)$$

According to the same paper [103] the diffusion cross-section for H<sub>2</sub>+H<sup>+</sup> collisions scales as  $\sigma^{(1)}(E_r)$  where  $E_r = m_r/m_p E_{lab}$ . Therefore:

$$\sigma_2^{(d)}(E_{lab}) = \sigma^{(d)}\left(\frac{m_{r2}}{m_{p2}}E_{lab}\right) = \sigma^{(d)}\left(\frac{m_{r1}}{m_{p1}}\frac{m_{p1}m_{r2}}{m_{r1}m_{p2}}E_{lab}\right) = \sigma_1^{(d)}\left(\frac{m_{p1}m_{r2}}{m_{r1}m_{p2}}E_{lab}\right)$$
(3.21)

As it is shown in [103], for the H+H<sup>+</sup> collisions the rescaled total cross-section coincides with direct calculation within 1 % for energies greater than 1 eV (in this paragraph  $E_r$  is meant). For lower energies they start to diverge (because of increasing influence of elastic collisions). The deviation reaches 5 % for 0.5 eV and 25 % for 0.1 eV. The same behaviour is seen for the diffusion cross-section. For the collisions with H<sub>2</sub> molecules the diffusion cross-section is well scaled for energies below 2 eV, but for energies between 2 and 10 eV the deviation can reach a factor of 3 because of the influence of vibrationally excited states. For the total cross section for H<sub>2</sub>+H<sup>+</sup> Krstić and Schultz suggest the scaling  $\sigma^{(0)}(v_r)$ . But the increasing/decreasing the value of this cross section (in some range) is not very important because it will affect mainly the amount of the low angle deflections which are



Figure 3.3: (a) Total and diffusion cross-sections for elastic collisions  $H_2$ + $H^+$  (AMJUEL H.1 0.3T) and charge-exchange H+ $H^+$  (HYGHEL H.1 3.1.8 [64]). (b) total collision rates for the same processes for selected values of background temperature T (AMJUEL H.3 0.3T and HYDHEL H.3 3.1.8 respectively). "Krstić-Schultz" is the diffusion cross-section taken from [102]

of low importance for transport, see Section 3.1.1. From the classical point of view all cross-sections must be functions of  $E_r$  only, see Formulas (3.5), (3.6).

For a Maxwellian background the collision frequency  $R_t$  (integral (3.4)) is expressed as a two-parametric dependence  $R_t(E,T)$ , Formula (3.17). Here *T* is the temperature of the background ions and  $E = \frac{1}{2}m_p|\mathbf{v}_t - \mathbf{u}_p|^2$  (the kinetic energy of the relative motion of the test particle and the background). This function of two variables is approximated by the Janevtype two parametric fitting [64] using similar least-square fitting as for cross-sections but in two dimensions:

$$\ln [R_t(E,T)] = \sum_{i=0}^{8} \sum_{j=0}^{8} a_{ij} \ln^i(E) \ln^j(T)$$
(3.22)

The fitting coefficients can be found in database AMJUEL [106], Section H.3. The relative error of the fitting does not exceed 4 %. The mass-rescaling for the collision rates is discussed in Appendix A.4.2. The dependence  $R_t(E, T)$  for H<sub>2</sub>+H<sup>+</sup> together with that for charge-exchange H+H<sup>+</sup> [64] is shown in Figure 3.3b.

#### **3.1.4** General relations for the transfer rates

In this and the next sections a rigorous way of calculating the momentum and energy transfer rates (further: transfer rates) is presented. These rates define the total amount of momentum and kinetic energy transferred by the test particles to the background during a unit time interval. They are applied is the Track Length Estimator, see Section 1.2.1, for the corresponding momentum and energy sources for plasma due to its friction with neutrals. The calculations are based on based on the work of Trubnikov [10], Chapter 7.

The velocity of a test particle  $\mathbf{v}_t$  involved in a collision event can be expressed in terms of the relative velocity  $\mathbf{v}_r$  and the centre-of mass velocity  $\mathbf{v}_c$ :

$$\mathbf{v}_c = \frac{m_p \mathbf{v}_p + m_t \mathbf{v}_t}{m_p + m_t} = \frac{m_p (\mathbf{v}_t - \mathbf{v}_r) + m_t \mathbf{v}_t}{m_p + m_t} = \mathbf{v}_t - \frac{m_p}{m_p + m_t} \mathbf{v}_r$$
(3.23)

Because of momentum conservation the centre of mass velocity remains constant during the collision event, hence the increment of the test particle velocity  $\Delta \mathbf{v}_t = \mathbf{v}'_t - \mathbf{v}_t$  is equal to:

$$\Delta \mathbf{v}_t = \frac{m_p}{m_p + m_t} \Delta \mathbf{v}_r = \frac{m_r}{m_t} \Delta \mathbf{v}_r \tag{3.24}$$

Here and below in this Chapter all quantities with prime ' are those after collision.

The momentum and energy gained by the test particle in the collision (and, respectively, lost by the background):

$$\Delta \mathbf{p}_t = \mathbf{p}'_t - \mathbf{p}_t = m_t \Delta \mathbf{v}_t = m_r \Delta \mathbf{v}_r \tag{3.25}$$

$$\Delta E_t = E'_t - E_t = \frac{m_t}{2} \left( \mathbf{v}_t + \Delta \mathbf{v}_t \right)^2 - \frac{m_t}{2} \mathbf{v}_t^2 = \frac{m_t}{2} \left( \Delta \mathbf{v}_t^2 + 2(\Delta \mathbf{v}_t \cdot \mathbf{v}_t) \right) = m_r \left( \frac{m_r}{2m_t} \Delta \mathbf{v}_r^2 + (\mathbf{v}_t \cdot \Delta \mathbf{v}_r) \right)$$
(3.26)

Here  $\Delta v_t$  was expressed using Formula (3.24). Up to this point the conservation of kinetic energy in the collision was not used. Expressions (3.25), (3.26) make use only of the momentum conservation (3.24). For an elastic collision  $v_r$  does not change it's magnitude but only the direction, therefore:

$$(\mathbf{v}_r + \Delta \mathbf{v}_r)^2 - \mathbf{v}_r^2 = 2(\mathbf{v}_r \cdot \Delta \mathbf{v}_r) + (\Delta \mathbf{v}_r)^2 = 0, \quad (\Delta \mathbf{v}_r)^2 = -2(\mathbf{v}_r \cdot \Delta \mathbf{v}_r)$$

Substituting this relation into (3.26) yields:

$$\Delta E_t = m_r \left( \frac{m_r}{2m_t} \Delta \mathbf{v}_r^2 + (\mathbf{v}_t . \Delta \mathbf{v}_r) \right) = m_r \left( \mathbf{v}_t . \Delta \mathbf{v}_r \right) - \frac{m_r^2}{m_t} \left( \mathbf{v}_r . \Delta \mathbf{v}_r \right)$$
(3.27)

To find the total momentum  $R_p n_p$  and energy  $R_E n_p$  transfer rates the increments  $\Delta \mathbf{p}_t$  and  $\Delta E_t$  should be multiplied by the differential (3.1) and integrated over the whole velocity space:

$$\mathbf{R}_{p} = -m_{r} \int d\mathbf{v}_{p} \cdot v_{r} f(\mathbf{v}_{p}) \int_{0}^{2\pi} d\phi \int_{0}^{\infty} db \cdot b\Delta \mathbf{v}_{r}$$

$$R_{E} = \left(\mathbf{v}_{t} \cdot \mathbf{R}_{p}\right) + \frac{m_{r}^{2}}{m_{t}} \int d\mathbf{v}_{p} \cdot v_{r}^{2} f(\mathbf{v}_{p}) \int_{0}^{2\pi} d\phi \int_{0}^{\infty} db \cdot b\Delta \mathbf{v}_{r}$$
(3.28)

Here the sign was changed to get the loss for the test particle (the gain for the background).

To simplify the integrals (3.28)  $\mathbf{v}_r$  is expressed in spherical coordinates  $v_r, \psi, \Theta$ , Figure **??**. Then  $\Delta \mathbf{v}_r = \mathbf{v}'_r - \mathbf{v}_r$  is equal to:

$$\Delta v_r^z = v_r \cos \Theta - v_r$$
$$\Delta v_r^x = v_r \cos \psi \sin \Theta - 0$$
$$\Delta v_r^y = v_r \sin \psi \sin \Theta - 0$$

Thus:

$$\int_{0}^{2\pi} d\psi \int_{0}^{\infty} db \cdot b\Delta \mathbf{v}_{r} = \begin{cases} -v_{r} \int_{0}^{2\pi} d\psi \int_{0}^{\infty} (1 - \cos\Theta) bdb = -v_{r} \sigma^{(1)}(v_{r}) \\ v_{r} \int_{0}^{2\pi} d\psi \cos\psi d\phi \int_{0}^{\infty} \sin\Theta bdb = 0 \\ v_{r} \int_{0}^{2\pi} d\psi \sin\psi d\phi \int_{0}^{\infty} \sin\Theta bdb = 0 \end{cases} = -\mathbf{v}_{r} \sigma^{(1)}(v_{r})$$
(3.29)

Here it was assumed that *b* is independent of  $\psi$  (axial symmetry) and the definition (3.9) is used. Substituting (3.29) into (3.28) yields:

$$\mathbf{R}_{p} = m_{r} \int \sigma^{(1)}(v_{r})v_{r}\mathbf{v}_{r}f(\mathbf{v}_{p})d\mathbf{v}_{p}$$

$$R_{E} = \left(\mathbf{v}_{t}.\mathbf{R}_{p}\right) - \frac{m_{r}^{2}}{m_{t}} \int \sigma^{(1)}(v_{r})v_{r}^{3}f(\mathbf{v}_{p})d\mathbf{v}_{p}$$
(3.30)

These formulas were obtained by Trubnikov, [10], Equation (7.29).

Instead of vector quantity  $\mathbf{R}_p$  it can be convenient to use its projection on the direction of  $\mathbf{v}_t$ . This projection  $R_{pt}$  can be calculated using the following relation:

$$(\mathbf{v}_r.\mathbf{v}_t) = (\mathbf{v}_t - \mathbf{v}_p.\mathbf{v}_t) = v_t^2 + (\mathbf{v}_p.\mathbf{v}_t)$$
  

$$(\mathbf{v}_r.\mathbf{v}_r) = v_r^2 = v_p^2 + v_t^2 - 2(\mathbf{v}_p.\mathbf{v}_t)$$
(3.31)

Therefore:

$$(\mathbf{v}_r.\mathbf{v}_t) = \frac{1}{2} \left( 2v_t^2 - v_p^2 - v_t^2 + v_r^2 \right) = \frac{1}{2} \left( v_t^2 - v_p^2 + v_r^2 \right)$$
(3.32)

This yields:

$$R_{pt} = \frac{1}{v_t} \left( \mathbf{R}_p \cdot \mathbf{v}_t \right) = \frac{m_r}{v_t} \int \sigma^{(1)}(v_r) v_r \left( \mathbf{v}_r \cdot \mathbf{v}_t \right) f(\mathbf{v}_p) d\mathbf{v}_p = \frac{m_r}{2v_t} \int \sigma^{(1)}(v_r) v_r \left( v_t^2 - v_p^2 + v_r^2 \right) f(\mathbf{v}_p) d\mathbf{v}_p$$

$$R_E = v_t R_{pt} - \frac{m_r^2}{m_t} \int \sigma^{(1)}(v_r) v_r^3 f(\mathbf{v}_p) d\mathbf{v}_p \tag{3.33}$$

In the next sections it will be shown how to transform integrals (3.33) for the special case of Maxwellian distribution  $f(\mathbf{v}_p)$ .

#### 3.1.5 Transfer rates for Maxwellian background

If  $f(\mathbf{v}_p)$  is the Maxwellian distribution without shift (3.11), then integrals (3.33) can be calculated in completely the same way as the integral (3.4), Section 3.1.2. This results in the following relations:

$$R_{pt} = \frac{2\alpha^3 m_r}{2\sqrt{\pi}v_t^2} \int_0^\infty dv_r \sigma^{(1)}(E_{lab}) v_r \int_{v_t - v_r}^{v_r + v_t} dv_p \cdot \left(v_t^2 - v_p^2 + v_r^2\right) \cdot v_p e^{-\alpha^2 v_p^2} = \frac{\alpha^{-4}}{\sqrt{\pi}v_t^2} \int_0^\infty d\xi \sigma^{(1)}(T\xi^2) \xi \int_{\delta - \xi}^{\delta + \xi} dv \cdot \left(\delta^2 - v^2 + \xi^2\right) v e^{-v^2}$$
(3.34)

$$v_{t}R_{pt} - R_{E} = \frac{m_{r}^{2}}{m_{t}} \frac{2\alpha^{3}}{\sqrt{\pi}v_{t}} \int_{0}^{\infty} dv_{r}\sigma^{(1)}(E_{lab})v_{r}^{3} \int_{v_{t}-v_{r}}^{v_{r}+v_{t}} dv_{p}v_{p}e^{-\alpha^{2}v_{p}^{2}}$$
$$= \frac{m_{r}^{2}}{m_{t}} \frac{2\alpha^{-4}}{\sqrt{\pi}v_{t}} \int_{0}^{\infty} d\xi \sigma^{(1)}(T\xi^{2})\xi^{3} \int_{\delta-\xi}^{\delta+\xi} dv \cdot ve^{-v^{2}}$$
(3.35)

One can express  $R_{pt}$  and  $R_E$  in terms of I-integrals which were introduced in [44]:

$$I^{(l,n)}(E,T) = \frac{\alpha^{-2}}{\sqrt{\pi}\nu_t} \int_0^\infty d\xi \xi^{2+n} \sigma^{(l)} \left(T\xi^2\right) \left[e^{-(\xi-\delta)^2} - (-1)^n e^{-(\xi+\delta)^2}\right]$$
(3.36)

The following relations will be used below:

$$\int_{\delta-\xi}^{\delta+\xi} dv \cdot v \exp\left(-v^2\right) = \frac{1}{2} \left[ e^{-(\delta-\xi)^2} - e^{-(\delta+\xi)^2} \right]$$
(3.37)

and (using partial integration):

$$\int_{\delta-\xi}^{\delta+\xi} dv \cdot v^3 \exp\left(-v^2\right) = \frac{1}{2} \left(1 + \delta^2 + \xi^2\right) \cdot \left[e^{-(\delta-\xi)^2} - e^{-(\delta+\xi)^2}\right] - 2\delta\xi \cdot \left[e^{-(\delta-\xi)^2} + e^{-(\delta+\xi)^2}\right]$$
(3.38)

Applying integrals (3.37) and (3.38) to (3.34) yields:

$$R_{pt} = \frac{\alpha^{-4}m_r}{\sqrt{\pi}v_t^2} \int_0^\infty \sigma^{(1)}(T\xi^2)\xi^2 d\xi \left\{ \left( \delta^2 + \xi^2 - 1 - \delta^2 - \xi^2 \right) \cdot \left[ e^{-(\delta - \xi)^2} - e^{-(\delta + \xi)^2} \right] + 2\delta\xi \left[ e^{-(\delta - \xi)^2} + e^{-(\delta + \xi)^2} \right] \right\} = \frac{m_r \alpha^{-2}}{2v_t} \left[ 2\delta I^{(1,1)} - I^{(1,0)} \right] = m_r \alpha^{-1} \left[ I^{(1,1)} - \frac{1}{2\delta} I^{(1,0)} \right] = m_r \sqrt{\frac{2T}{m_p}} \left[ I^{(1,1)} - \frac{1}{2} \sqrt{\frac{m_t T}{m_p E}} I^{(1,0)} \right]$$
(3.39)

Here the a variable *E* was introduced:  $v_t = \sqrt{\frac{2E}{m_t}}$ , thus  $\delta = v_t \alpha = \sqrt{\frac{m_t T}{m_p E}}$ . For the energy transfer rate (3.35) and (3.37) yield:

$$R_{E} = v_{t}R_{pt} - \frac{m_{r}^{2}}{m_{t}}\frac{\alpha^{-4}}{\sqrt{\pi}v_{t}}\int_{0}^{\infty}\sigma^{(1)}(T\xi^{2})\xi^{3}\left[e^{-(\delta-\xi)^{2}} - e^{-(\delta+\xi)^{2}}\right]d\xi = v_{t}R_{pt} - \frac{m_{r}^{2}}{m_{t}}\alpha^{-2}I^{(1,2)} = v_{t}R_{pt} - \frac{2m_{r}^{2}}{m_{t}m_{p}}TI^{(1,2)}$$
(3.40)

Formulas similar to (3.39) and (3.40) were obtained in [44]. Note that the paper [44] contains a mistake in the formula for  $R_E$ . The integrals  $R_p$  and  $I^{(1,2)}$  calculated for H<sub>2</sub>+H+ and H+H+ collisions are shown below in Section 3.1.7, Figures 3.4. The rescaling of those integrals to another isotope masses (see Section 3.1.3) is shown in Appendix A.4.2.

#### 3.1.6 Transformation to background with shift

The rates (3.39) and (3.40) were calculated for the case of the background without average macroscopic velocity (drift velocity). The frame of reference having this property will be called below the "rest-frame" or R-frame. The results can be generalised for the frame of reference where the background has a drift velocity  $\mathbf{u}_p$ : the laboratory frame, L-frame. This can be done by calculating  $R_{pt}$  and  $R_E$  in R-frame and then transforming them into L-frame. The following notation will be used below:

$$\langle X \rangle = \int d\mathbf{v}_p \cdot v_r f(\mathbf{v}_p) \int_0^{2\pi} d\psi \int_0^\infty db \cdot b \cdot X$$

Here *X* is any function of  $v_r$  and *b*. The connection between velocity in the L-frame and in the R-frame is:

$$\mathbf{v}^L = \mathbf{v}^R + \mathbf{u}_p$$

Here and below superscript L denotes the variables calculated in L-frame and R stays for R-frame. One can write the momentum lost by the test particle as:

$$\mathbf{R}_{p}^{L} = -m_{p} \left\langle \Delta \left( \mathbf{v}_{p}^{L} \right) \right\rangle = -m_{p} \left\langle \Delta \left( \mathbf{v}_{p}^{R} + \mathbf{u}_{p} \right) \right\rangle = -m_{p} \left\langle \Delta \left( \mathbf{v}_{p}^{R} \right) \right\rangle = \mathbf{R}_{p}^{R} = R_{pt}^{R} \frac{\mathbf{v}^{R}_{t}}{v_{t}^{R}}$$

Here the operator  $\Delta$  denotes the velocity after collision minus velocity before collision.  $\Delta(\mathbf{u}_p) = 0$  because this velocity does not change. The momentum source in the R-frame is directed along the velocity  $\mathbf{v}_t^{\mathbf{R}}$  because it is the only special direction in case of isotropic background. The independence of the momentum source on the frame of reference is a direct consequence of the fact that the acceleration and therefore the force is invariant regarding the choice of inertial frame of reference.

The projection of the momentum sources on the direction of the magnetic field (the parallel momentum source) is of particular interest for B2-EIRENE applications:

$$R_{p||} = R_{pt}^{R} \frac{\left(\mathbf{v}_{t}^{L} \cdot \hat{\mathbf{B}}\right)}{v_{t}^{L}} = \frac{R_{pt}(E^{R}, T)}{v_{r}^{R}} \left[ \left(\mathbf{v}_{p}^{L} \cdot \hat{\mathbf{B}}\right) - \left(\mathbf{u}_{p} \cdot \hat{\mathbf{B}}\right) \right]$$
(3.41)

Here  $\hat{\mathbf{B}}$  is the unit vector of magnetic field,  $R_{pt}(E^R, T)$  is calculated using equation (3.39) and the test particle kinetic energy in R-frame  $E^R$ .

For the energy lost by the test particles:

$$R_{E}^{L} = -\frac{m_{t}}{2}\left\langle \left(\mathbf{v}_{t}^{L}\right)^{2} \right\rangle = -\frac{m_{t}}{2}\left\langle \left(\mathbf{v}_{t}^{R} + \mathbf{u}_{p}\right)^{2} \right\rangle = -\frac{m_{t}}{2}\left\langle \left(v_{t}^{R}\right)^{2} \right\rangle - m_{t}\left(\mathbf{u}_{p}, \left\langle \mathbf{v}_{t}^{R} \right\rangle \right) = R_{E}^{R} + \left(\mathbf{u}_{p}, \mathbf{R}_{p}^{R}\right) = R_{E}^{R} + \left(\mathbf{u}_{p}, \mathbf{v}_{t}^{R}\right) \frac{R_{pt}^{R}}{v_{t}^{R}}$$

Therefore, equation (3.40):

$$R_E^L = R_{pt}(E^R, T) \left[ v_t + \frac{\left( \mathbf{u} \cdot \mathbf{v}_t^R \right)}{v_t^R} \right] - \frac{2m_r^2}{m_t m_p} T I^{(1,2)}(E^R, T)$$
(3.42)

Here  $R_{pt}$  and  $I^{(1,2)}$  are calculated again using the R-frame energy  $E^{R}$ .

#### 3.1.7 Simplified approach

Assuming  $\sigma^{(1)}v_r = const$ , the integrals (3.30) can be easily calculated and one gets formulas (2.12) and (2.13) from Section 2.2.2. They can be used as a first approximation for the integrals (3.30) with realistic dependence of  $\sigma^{(1)}(v_r)$  by substituting  $I^{(1,0)}$  in place of the constant  $K_m$ :

$$\mathbf{R}_{\mathbf{p}} \approx m_r I^{(1,0)}(E,T) \left( \mathbf{u}_t - \mathbf{u}_p \right)$$

$$R_E \approx \frac{2m_r^2}{m_p m_t} I^{(1,0)}(E,T) \left[ E - \left( \frac{3}{2}T + \frac{m_p u_p^2}{2} \right) + \frac{m_t - m_p}{2} (\mathbf{v}_p \cdot \mathbf{u}_t) \right]$$
(3.43)

(3.43)

Here the test particle kinetic energy E is calculated in the rest frame (see Section 3.1.6. The relation for  $R_p$  which corresponds to this approximate treatment is:

$$R_p \approx m_r I^{(1,0)}(E,T) v_t = m_r I^{(1,0)}(E,T) \sqrt{\frac{2E}{m_t}}$$
 (3.44)

To find the corresponding relation for  $I^{(1,2)}$  on should equate the formula (3.40) with the relation for  $R_E$  (3.43) for the case  $\mathbf{u}_p = 0$ . This yields:

$$\frac{2m_r^2}{m_p m_t} I^{(1,0)} \left[ E - \frac{3}{2}T \right] = R_p v_t - \frac{2m_r^2}{m_p m_t} T I^{(1,2)}$$

Substituting (3.44) yields finally:

$$I^{(1,2)} \approx I^{(1,0)} \left( \frac{m_p}{m_t} E + \frac{3}{2} T \right)$$
(3.45)

The comparison of the full integrals  $R_p$  and  $I^{(1,2)}$  with those calculated applying relations (3.44) and (3.45) is shown in Figures 3.4. Figures 3.4a, 3.4c present the result for the charge-exchange H+H<sup>+</sup> (CX) (the cross-section from [64]) and Figures 3.4a, 3.4c show the result for elastic collisions H<sub>2</sub>+H<sup>+</sup>. For CX the difference between full and simplified approach does not exceed 25 % for both  $R_p$  and  $I^{(1,2)}$ . For elastic collisions the difference for  $R_p$  is a factor of 2 and more. This estimate shows that the simplified approach can be applied with reasonable accuracy to the hydrogen charge-exchange, whereas elastic collisions of molecules with ions need full treatment.

For CX collisions one can use an assumption  $\Theta = \pi$ . This yields:

$$\sigma^{(1)} = 2\pi \int_0^\infty \left(1 - \cos\Theta\right) b db = 4\pi \int_0^\infty b db = 2\sigma^{(0)}$$

Therefore  $I^{(1,0)} = 2I^{(0,0)}$ . Assuming in addition  $m_p = m_t = m$ , Formulas (3.43) can be reduced to the following simple relations:

$$\mathbf{R}_{p} = mI^{(0,0)}(\mathbf{v}_{t} - \mathbf{u}), \quad \frac{R_{E}}{R_{t}} = I^{(0,0)} \left[ E - \left(\frac{3}{2}T + \frac{mu_{p}^{2}}{2}\right) \right]$$
(3.46)

The relations (3.46) correspond to the complete exchange of the momentum and energy in each collision. They are used in EIRENE as a built-in default option for CX.

#### 3.1.8 A numerical test

The momentum and energy transfer rates calculated in the previous sections were used to replace the Collisional Estimator (CL) for the corresponding sources with the Track Length Estimator (TL). Technical aspects of the implementation of this option in the code are described in Appendix A.4.1. To test the correctness of the implementation and to study the influence on the level of statistical noise the plasma parallel momentum and energy sources calculated with TL and CL were compared to each other. Note that for correct comparison the rejection sampling must be enforced for CL (NFLAG>3 in subroutine VELOEL). This benchmark can be considered also as a consistency check of the whole treatment of elastic collisions in the code. The calculations were performed on the fixed plasma background of ITER 1055 case, see Section 3.3. Because of technical reasons the compared values include both contribution from elastic collision, ionization and ion conversion. They are called thus "sources due to D<sub>2</sub>+plasma collisions". The contribution of elastic collisions near the targets is thought to be dominant. The results of the benchmarking are shown in Table 3.1 and Figures 3.5, 3.6.

Table 3.1 contains the following quantities: maximum values of the sources (per unit volume) in the inner and outer divertor regions (MAX) and their sum over the whole inner and outer divertor (TOTAL).  $\Delta$  is the relative difference between CL and TL:

$$\Delta X = \frac{|X_{TL} - X_{CL}|}{X_{TL}} \cdot 100 \ \%$$



Figure 3.4: Momentum transfer rate  $R_{pt}$  (a),(b) and integral  $I^{(1,2)}$  (c),(d) for charge-exchange H+H<sup>+</sup> and elastic collisions H<sub>2</sub>+H<sup>+</sup> for selected background temperatures. The blue dashed curves show the results of the approximate approach, Section 3.1.7

Here  $X_{TL}$  and  $X_{CL}$  are estimations of the variable *X* with the corresponding estimator. N is the number of histories per target. The total number of histories is 5N. The maximum  $S_{max}$  and average  $S_{avr}$  standard deviations of a variable *X* are calculated as following:

$$S_{max} = \frac{\max |\sigma_i X_i V_i|}{|X_I V_I|}, \quad S_{avr} = \frac{\sqrt{\sum_i (\sigma_i X_i V_i)^2}}{\sum_i X_i V_i}$$

Here *i* is the index of the grid cell, *I* is the index of cell for which max  $|\sigma_i X_i V_i|$  is reached, *V* is the cell volume,  $\sigma$  is the relative standard deviation of the estimation *X*, see Section 1.2.1. The operations max and  $\Sigma$  are taken over all cells of the computational grid in the specified domains: within 12 poloidal cells near the inner and outer targets. In other words,  $S_{max}$  is the maximum relative standard deviation and  $S_{avr}$  is the mean relative standard deviation.

Both momentum and energy sources are strongly localised near the target surfaces: in fact within few first poloidal cells (1-3 cm away from the target) of the computational grid. The profiles of the radial distributions (distributions along the targets) of these quantities in the first two poloidal cells of the grid are shown in Figures 3.5, 3.6. The comparison of TL and CL shows a good agreement: for N=10000 the difference for the total momentum source <3% and for the total energy sources <1.3%. The same is true for the maximum rates: 4 % (for momentum) and 1 % (for energy). This difference does not decrease as N increases because of systematic errors of fitting for  $R_{pt}$  and  $I^{(1,2)}$  which can reach 3%.

The figures shown in Table 3.1 do not give any evidence that TL yields lower level of statistical errors than CL. On may expect that in this case TL will give a better statistics because some averaging was done "exactly" (without using Monte Carlo). From the other hand, it is well known that in some cases CL can outperform TL for high collisionality. In addition, looking at the shown standard deviations one can conclude that the statistical error is larger than the sources themselves. Large variance of the momentum sources was a particular concern in [33]. However, using standard deviation for this quantity may be misleading. One can see in Figures 3.7a, 3.7b that the result obtained with N=10<sup>5</sup> is relatively well reproduced by the calculations with N=10<sup>3</sup>, whereas the standard deviation is very large (100% and more!) in both cases, Figures 3.7c, 3.7d. It is possible, that the standard deviation which was used to estimate the statistical error fails to serve as a reliable diagnostic in this case. The issue of the proper way of calculating the momentum sources are not estimating its statistical error needs further investigation.

	Energy source (W, W/cm <sup>3</sup> )				Momentum source (N, N/cm <sup>3</sup> )			
	$N=10^{3}$		N=10 <sup>4</sup>		$N=10^{3}$		N=10 <sup>4</sup>	
	CL	TL	CL	TL	CL	TL	CL	TL
	Inner Target							
TOTAL	2.93e6	2.94e6	2.91e6	2.87e6	307	299	302	294
$\Delta$ , %	0.28		1.2		2.7		2.8	
MAX	68.0	69.1	64.6	64.3	1.03e-2	9.10e-3	9.30e-3	9.00e-3
$\Delta$ , %	1.6		0.47		13		3.6	
$S_{max}, \%$	23	26	8.6	9.2	7.6e3	1.1e4	3.0e3	2.9e3
S <sub>avr</sub> , %	5.8	5.0	1.8	1.6	131	114	69	68
	Outer Target							
TOTAL	2.69e6	2.75e6	2.93e6	2.94e6	258	243	280	276
$\Delta$ , %	2.3		0.60		5.9		1.2	
MAX	91.8	101	114	115	1.03e-2	9.89e-3	1.25e-2	1.22e-3
$\Delta$ , %	8.7		0.81		3.4		2.3	
$S_{max}, \%$	24	24	7.6	8.1	1.14e3	1.125e3	164	164
S <sub>avr</sub> , %	7.1	6.2	2.2	2.0	227	214	43.7	42.5

Table 3.1: Comparing the Collisional (CL) and Track Length (TL) estimators



Figure 3.5: Distribution of the parallel momentum sources due to  $D_2$ +plasma collisions along the targets for the first two poloidal cells (i<sub>x</sub>). Plasma background of the case ITER 1055,  $10^4$  histories per target.



Figure 3.6: Distribution of the energy sources due to  $D_2$ +plasma collisions along the targets for the first two poloidal cells ( $i_x$ ). Plasma background of the case ITER 1055, 10<sup>4</sup> histories per target.



Figure 3.7: Comparison of the total (due to atoms and molecules) parallel momentum sources for the first two poloidal cells  $(i_x)$  calculated with  $10^3$  and  $10^5$  histories. Plasma background of the case ITER 1055. Track Length Estimator. MOL=contribution of molecules only

## **3.2 Hydrogen molecular chemistry**

#### 3.2.1 Introduction

In this work the description of the hydrogen reaction kinetics is based on the Collision Radiative Model (CRM) of Sawada and Fujimoto [40, 41] updated by Reiter and Greenland [42, 43]. The general ideas of the CRM-approach are sketched in the next paragraphs.

In the most general form the kinetics of one species (different excited states of atoms and molecules can be treated as separate species) is described by a differential equation:

$$\frac{dn}{dt} = \frac{\partial n}{\partial t} + div\left(\Gamma_n\right) = \text{Sources} - \text{Sinks}$$
(3.47)

Here *n* is the density of the species in question and  $\Gamma_n$  is its flux density. The righthand side of this equation is an algebraic expression without differential operators. For each species one considers two basic time-scales. The time-scale of transport  $\tau_{tr}$  and the characteristic time of formation and decay of the species  $\tau$  (referred below as "lifetime"). The transport time scale  $\tau_{tr}$  is the time which the particle needs to cover the distance comparable to the spatial non-uniformity of the background parameters (or the distance to a solid surface). In case of numerical solution it is determined by the size of the computational grid.

In case of  $\tau < \tau_{tr}$  one can neglect the transport in Equation (3.47) and for a steady-state case it reduces to pure algebraic equation. For the species for which  $\tau > \tau_{tr}$  one has to consider the transport explicitly. The following notation is often used: species with  $\tau < \tau_{tr}$  are called "species of class Q" and species with  $\tau > \tau_{tr}$  are the "species of class P" (see e.g. [105]).

For the conditions of ITER divertor plasma the characteristic transport time is of the order  $10^{-6}.10^{-5}$  sec: thermal velocity  $\approx 10^6 \text{ cm/s}$  and a spatial scale  $\approx 1 \text{ cm}$ . An example of a direct Monte-Carlo estimation of this time is shown in Section 3.3.2, Figure 3.27. The typical life time of the electronically excited states is  $10^{-8}..10^{-7}$  sec. It is is determined by the spontaneous radiative transitions and electron-impact processes. In the current model no transport is assumed for all electronically excited states. Only the transport of the ground state species is treated explicitly. Therefore, the P-space is  $P = [H(1s), H_2(X^1\Sigma_g^+), H_2^+(X^2\Sigma_g^+)]$ . Negative ions  $H^-$  and molecular ions  $H_3^+$  are not taken into account. In fact the molecular ion  $H_2^+$  belongs to Q-class as well because in the current version of the code its motion is not considered and it is assumed to decompose at the same place where it emerges. The possibility to treat its motion is reserved for the future.

For the considered problem of H<sub>2</sub> chemistry Equations (3.47) without transport and time-dependence form a set of linear equations for the densities of the excited states. Most of the coefficients of this set of equations are the collision rates of the electron impact processes multiplied by  $n_e$ . The rates themselves are the functions of  $T_e$ , Formula 3.18, Section 3.1.2. The densities of the ground states H(1s),  $H_2(X^1\Sigma_g^+)$  and  $H_2^+(X^2\Sigma_g^+)$  will be denoted as  $n_H$ ,  $n_{H_2}$  and  $n_{H_2^+}^+$  respectively. They enter those equations linearly as parameters. Therefore, the solution can be expressed as a linear combination of  $n_H$ ,  $n_{H_2}$ ,  $n_{H_2^+}^+$  and this yields the following balance equations:

$$\frac{dn_{H_2}}{dt} = -(D_{H_2} + S_{H_2} + I_{H_2})n_e n_{H_2}$$

$$\frac{dn_{H_2^+}}{dt} = S_{H_2}n_e n_{H_2} - (R_{H_2^+} + D_{H_2^+} + S_{H_2^+})n_e n_{H_2^+}$$

$$\frac{dn_H}{dt} = (2D_{H_2} + I_{H_2^+})n_e n_{H_2} + (2R_{H_2^+} + D_{H_2^+})n_e n_{H_2^+} - I_H n_e n_H + R_H n_e n_{H_1^+}$$

$$\frac{dn_{H^+}}{dt} = I_{H_2}n_e n_{H_2} + (D_{H_2^+} + 2S_{H_2^+})n_e n_{H_2^+} + I_H n_e n_H - R_H n_e n_{H_1^+}$$
(3.48)

The coefficients in the Equations (3.48) (they are functions of  $T_e$  and  $n_e$ ) are called "effective reaction rates". The corresponding effective processes are listed in Table 3.2. The effective reaction rates are tabulated in the datafile AMJUEL [106], card H.4. The rates calculated for Hydrogen are applied for all its isotopes, including the cases with vibrational kinetics, see below.

Note that CRM does not include collisions with heavy particles: charge-exchange, elastic collisions. This indirectly involves the assumption that the life time of the excited states is smaller than the characteristic time of such collisions.

The new model for molecular chemistry was compared to the old one used in EIRENE 1996. This latter is based on the reaction rates from the monograph of Janev et. al [64] which are stored in database HYDHEL. In addition to the new reaction rates the production of molecular ions due to the ion conversion process was added. This later, if followed by dissociative recombination of  $H_2^+$  can give rise to the so called Molecular Assisted Recombination (MAR) [109].

A special comment should be made on vibrationaly excited states. In the current model they are taken into account only in reactions AMJUEL H.4 2.1.5g, AMJUEL H.2 3.2.3 and indirectly in the rates for  $H_2^+$  (see Section 3.2.3). In both cases vibrational states are treated as Q-species: vibrational equilibrium is assumed (Quasi Steady-State, QSS approximation). Estimations show that for the conditions relevant for a divertor plasma the time of establishing the vibrational equilibrium is of the order  $10^{-6}$ .. $10^{-5}$  sec [107, 108] which is the same order of magnitude as for  $\tau_{tr}$ . This means that in principle one has to consider the transport of excited states explicitly (to treat them as P species). This was done earlier in the simulations for ASDEX-Upgrade [43] but no serious difference compared to QSS-approximation was found. The EIRENE calculations made in [108] for ITER for the fixed plasma showed only moderate modification (within 10..30 %) of the principal particle sources. This estimation backed the application of the QSS-approximation in this work. However, this approach can be considered as only a first approximation and has to be revisited in future. Particular concern is the possible energy transport in vibrational states [111]. Note also that the rotational energy is not taken into account in any of the atomic physics models at all.

The next two sections describe in more detail the constituents of the effective reaction rates for  $H_2$  and  $H_2^+$ . Section 3.2.3 addresses the issue of MAR as well.

Effective Process	Notation	Name	Database Entry	
	in text		HYDHEL	AMJUEL
$H_2 + e \rightarrow 2H + 2e$	$D_{H_2}$	Dissociation	H.2 2.2.5	H.4 2.1.5g
$H_2 + e \rightarrow H_2^+ + 2e$	$S_{H_2}$	Ionization	H.2 2.2.9	H.4 2.1.9
$H_2 + e \rightarrow H + H^+ + 2e$	$I_{H_2}$	Dissociative	H.2 2.2.11	H.4 2.1.10
		Ionization		
$H_2^+ + e \rightarrow H + H + 2e$	$R_{H_{2}^{+}}$	Dissociative	H.2 2.2.14	H.4 2.2.14
-	2	Recombination		
$H_2^+ + e \to H + H^+ + 2e$	$D_{H_2^+}$	Dissociation	H.2 2.2.12	H.4 2.2.12
$H_2^+ + e \to 2H^+ + 2e$	$S_{H_{2}^{+}}$	Dissociative	H.2 2.2.11	H.4 2.2.11
	2	Ionization		
$H_2(\nu) + H^+ \rightarrow H_2^+ + H$	-	Ion	-	H.2 3.2.3
_		Conversion		

Table 3.2: Effective reactions for molecular chemistry model in EIRENE

#### 3.2.2 Molecules

The following set of equations describes the kinetics of molecules:

$$\sum_{q < p} C_{H_2}(q, p) n_e n_{H_2}(q) - \left[ \left( \sum_{q < p} F_{H_2}(p, q) + \sum_{q > p} C_{H_2}(p, q) + S_{H_2}(p) \right) n_e \right] + \sum_{q < p} A_{H_2}(p, q) n_{H_2}(p) + \sum_{q > p} \left[ F_{H_2}(q, p) n_e + A_{H_2}(q, p) \right] n_{H_2}(q) = 0$$

(3.49)

Here q and p are the indices of excited states; C and F are the rate coefficients for the electron impact excitation and de-excitation, A is the spontaneous transition probability and *S* is the ionization rate. The Equations (3.49) as they are shown here do not contain recombination of molecular ions  $H_2^+$  into molecules. The ion-impact processes are neglected as well.

To describe the multi-step processes involving the excited atoms Equation (3.49) has to be coupled to the corresponding model for kinetics of atoms. For further use it is convenient to introduce the notation:

$$M(p)\{n_{H}(p')\} = \left( \left| \sum_{q'>p'} C_{H}(p',q') + \sum_{q'p'} F_{H}(q',p')n_{e}n_{H}(q') - \sum_{q'>p'} A_{H}(q',p')n_{H}(q') \right)$$

$$(3.50)$$

Here M(p) is an operator which acts on the vector  $n_H(p')$ . The meaning of all the coefficients is the same as in Equation (3.49). Using this notation the balance equation for atomic excited state H(p') can be written as:

$$M(p')\{n_H(p')\} = E_{H_2}(p')n_e n_{H_2}$$
(3.51)

Here  $E_{H_2}(p')$  is the rate of producing the atomic state H(p') due to dissociative excitation of molecules (see below). The prime ' is used for atomic excited states to distinguish them from those for molecules. In addition in some places below the electronically excited atoms will be denoted as H(n) or H(m) and vibrationally excited molecules will be denoted as  $H_2(v)$ 

For the excited level n = 2 (where *n* is the principal quantum number) three different singlet and triplet states are considered. Level  $b^{3}\Sigma_{u}^{+}$  is a repulsive state. It is assumed that all transitions from the stable states into this state result in dissociation. The transitions from the stable states to other repulsive states are assumed to auto-ionize and are included in  $S_{H_{2}}(p)$ . For levels with n > 2 only one singlet and one triplet state is considered. The levels up to n = 28 are taken into account. The details of the used atomic data can be found in [40, 41].

The solution of the set of linear algebraic Equations (3.49), (3.51) can be presented in the form:

$$n_{H_2}(p) = R_{2H}^{H_2}(p, n_e, T_e)n_{H_2}, \quad n_H(p') = R_H^{H_2}(p', n_e, T_e)n_{H_2}$$
(3.52)

Here  $R_{2H}^{H_2}(p, n_e, T_e)$  and  $R_{H}^{H_2}(p', n_e, T_e)$  are the population factors.

The following paths contribute to effective dissociation of molecules.

1. Direct excitation from the ground state  $X^1\Sigma_g^+$  to the repulsive level  $b^3\Sigma_u^+$  by electron impact:

$$H_2(X^1\Sigma_g^+) + e \to H_2(b^3\Sigma_u^+) + e$$

$$H_2(b^3\Sigma_u^+) \to H(1s) + H(1s)$$
(3.53)

2. Dissociative excitation, which produces excited hydrogen atom H(n). This excited atom can be further excited or de-excited finally reaching the ground state:

$$H_2\left(X^1\Sigma_g^+\right) + e \to H(1s) + H(n) + e \tag{3.54}$$
$$H(n) \to H(1s)$$

Here and below  $\rightarrow \rightarrow$  denotes a chain of processes.

3. Excitation of the ground-state molecule to a stable excited molecule  $H_2^*$  by electron impact. This excited molecule  $H_2^*$  is further excited or de-excited to other stable state by collisional and radiative processes reaching finally the repulsive state  $b^3 \Sigma_u^+$ :

$$H_{2}\left(X^{1}\Sigma_{g}^{+}\right) + e \to H_{2}^{*} + e$$

$$H_{2}^{*} \to H_{2}\left(b^{3}\Sigma_{u}^{+}\right)$$

$$H_{2}\left(b^{3}\Sigma_{u}^{+}\right) \to H(1s) + H(1s)$$
(3.55)

The effective dissociation rate is:

$$D_{H_2} = C_{H_2} \left( X^1 \Sigma_g^+, b^3 \Sigma_u^+ \right) + \sum_{p'>1} \left[ A_H(p', 1)/n_e + F_H(p', 1) \right] R_H^{H_2}(p') + \sum_{p>1} \left[ A_{H_2} \left( p', b^3 \Sigma_u^+ \right) / n_e + F_{H_2} \left( p', b^3 \Sigma_u^+ \right) \right] R_{H_2}^{2H}(p)$$
(3.56)

The first, second and third terms of this formula represent the contributions from the paths (3.53), (3.54) and (3.55) respectively. The corresponding reaction rate from [64], HY-DHEL 2.2.5, includes only the direct electron-impact excitation to repulsive level  $b^3\Sigma_u^+$  (3.53) and electron impact excitation to level  $a^3\Sigma_g^+$  or  $c^3\Pi_u$  with successive radiative decay to level  $b^3\Sigma_u^+$ .

The effective ionization of molecules (formation of molecular ion) includes the following paths.

1. Direct ionization by electron impact:

$$H_2\left(X^1\Sigma_g^+\right) + e \to H_2^+\left(X^2\Sigma_g^+\right) + 2e \tag{3.57}$$

2. Excitation of the ground-state of the molecule by electron impact. The produced excited molecule  $H_2^*$  is further excited and finally ionized into molecular ion:

$$H_{2}\left(X^{1}\Sigma_{g}^{+}\right) + e \rightarrow H_{2}^{*} + e$$

$$H_{2}^{*} + e \rightarrow H_{2}^{**} + e$$

$$H_{2}^{**} + e \rightarrow H_{2}^{+}\left(X^{2}\Sigma_{g}^{+}\right) + 2e$$
(3.58)

The effective ionization rate is:

$$S_{H_2} = S_{H_2} \left( X^1 \Sigma_g^+ \right) + \sum_{p>1} S_{H_2}(p) R_{2H}^{H_2}(p)$$

The first and second terms are the contributions from path (3.57) and path (3.58) respectively. The reaction rate from the old model HYDHEL 2.2.9 includes only the process (3.57).

The dissociative ionization can result from the following paths.

1. Ionization through the unstable molecular ion  $H_2^+(X^2\Sigma_g^+ \text{ or } \Sigma_u^+)$ :

$$H_2\left(X^1\Sigma_g^+\right) + e \to H_2^+\left(X^2\Sigma_g^+ \text{ or } \Sigma_u^+\right)$$

$$H_2^+\left(X^2\Sigma_g^+ \text{ or } \Sigma_u^+\right) \to H(1s) + H^+ + 2e$$
(3.59)

2. Ionization via excited hydrogen atom H(n) originating from dissociative excitation (3.54):

$$H_2(X^1\Sigma_g^+) + e \to H(1s) + H(n) + e$$

$$H(n) \to H(m)$$

$$H(m) + e \to H^+$$
(3.60)

The effective rate of dissociative ionization is:

$$I_{H_2} = S(H_2^+ \left( X^2 \Sigma_g^+ \text{ or } \Sigma_u^+ \right)) + \sum_{p'>1} S_H(p) R_H^{H_2}(p')$$

The first and second terms are the contributions from path (3.59) and path (3.60) respectively. The old reaction rate from [64], HYDHEL 2.2.10, takes into account only the process (3.59).

In the model described above it was always assumed that the initial state in any of the transition is the ground vibrational-rotational state. Vibrational states are taken into account in the effective dissociation rate AMJUEL H.4 2.2.5g. The model which is used

to calculate the population of vibrational states includes only the excitation by electron impact [41, 43]:

$$H_2(v) + e \rightarrow H_2^- \rightarrow H_2(w) + e$$

Here v and w are the indices of the vibrational levels. The population of excited states is calculated on the assumption of a vibrational equilibrium (QSS-approximation) using the excitation and de-excitation rates tabulated in the database H2VIBR [42, 112]. The current model considers only the electronic ground states. Vibrational population from the radiative decay of the electronically excited states:

$$H_2(\nu = 0) + e \rightarrow H_2\left(B^1\Sigma_u^+, C^1\Pi_u\right) \rightarrow H_2(w) + e + h\nu$$

is not taken into account. The issue of applicability of QSS was briefly discussed in Section 3.2.1.

The treatment of the energy balance for the processes in question is the same as it was for the old model and described in [110]. For the dissociation  $H_2 \rightarrow 2H$  it is assumed that the both resulting atoms have kinetic energy 3 eV [64]. Here and below the kinetic energy of heavy particles in the centre-of-mass frame is meant. Together with the potential energy of the molecule 4.48 eV this yields the electron energy loss 10.5 eV per one (effective) collision. For the ionization  $H_2 \rightarrow H_2^+$  the electron energy loss is 15.4 eV per one collision. For dissociative ionization  $H_2 \rightarrow H + H^+$  it is assumed that the kinetic energy of the both products (ion and atom) is 5 eV. Together with potential energy 4.5 eV and ionization energy of the atom 13.6 eV it yields 28 eV of the electron energy loss per one effective collision. The current treatment of the energy balance is to large extent approximate and has to be revisited in future.

The calculated effective rates are shown in Figure 3.8 for the range of  $n_e$  and  $T_e$  relevant for divertor plasma. For comparison, the old rates from HYDHEL are shown in the same figure. In the temperature range in question CRM without vibrational states yields the same rate of dissociation  $H_2 \rightarrow 2H$  as HYDHEL. Including the vibrational states leads to a somewhat higher rate but the maximum difference is only a factor  $\approx 2$ . The difference between AMJUEL and HYDHEL for the ionization rate  $(H_2 \rightarrow H_2^+)$  is higher, reaching an order of magnitude for temperatures below 2 eV. The new effective rate of the dissociative ionization  $H_2 \rightarrow H + H^+$  is an order of magnitude higher than that from HYDHEL. But for the temperatures less than 30 eV this process is always unimportant compared to the previous two.



Figure 3.8: Effective reaction rates for molecules  $H_2$  calculated using CRM [41] (AMJUEL, see Table 3.2) confronted to the old data from [64] (HYDHEL). Thin black line is the reaction rate for dissociation calculated without vibrational states (AMJUEL H.4 2.2.5)

#### **3.2.3 Molecular Ion**



In addition to ionization (3.57), (3.58) another possible channel of producing the molecular ion is the Ion Conversion:

$$H_2(\nu) + H^+ \to H_2^+ + H$$
 (3.61)

This process takes place for vibrationaly excited molecules starting to be effective from level v = 4. In the current model it is described (approximately) as a charge-exchange like reaction with a temperature dependend rate. This effective rate was calculated by means of the QSS-distribution of vibrational states, the same as for dissociation of molecules, see Section 3.2.2. It was also assumed that  $T_e = T_i$ , and the kinetic energy of  $H_2$  is 0.1 eV. As in the case of

Figure 3.9: Rate of Ion Conversion

molecules the QSS can be considered as a first approximation, see the comment in Section 3.2.1.

Three kinds of processes are included in the effective rates for  $H_2^+$ .

1. Dissociative recombination:

$$H_2^+\left(X^2\Sigma_g^+\right) + e \to H(1s) + H(n) \tag{3.62}$$

2. Dissociative excitation:

$$H_2^+\left(X^2\Sigma_g^+\right) + e \to H^+ + H(n) + e \tag{3.63}$$

3. Ionization:

$$H_2^+\left(X^2\Sigma_g^+\right) + e \to 2H^+ + 2e \tag{3.64}$$

Only electronic ground state  $X^2\Sigma_g^+$  is considered but the rates are averaged over the vibrational distribution, see below.

The further evolution of the excited atom H(n) produced in the processes (3.62) and (3.63) is described in the same way as in the case of molecules, Section 3.2.2. Using the notation (3.50) the balance equations for excited atoms and their formal solution can be written as:

$$M(p')\{n_H(p')\} = \left[ E_{H_2^+}(p')n_e + \alpha(p')n_e \right] n_{H_2^+}$$
$$n_H(p') = \left[ R_{2H}^{H_2^+}(p', n_e, T_e) + R_H^{H_2^+}(p', n_e, T_e) \right] n_{H_2^+}$$

Here  $E_{H_2^+}(p')$  is the rate of dissociative excitation in which excited atom H(p') is produced,  $\alpha(p')$  is the same but for dissociative recombination,  $R_{2H}^{H_2^+}$  and  $R_{H}^{H_2^+}$  are the population factors for atoms originating due to the processes (3.62) and (3.63) respectively.

The effective dissociative recombination results from the process (3.62) followed by the decay of H(n) to the ground state:

$$H_2^+ + e \to H^+ + H(n) \tag{3.65}$$
$$H(n) \to \to H(1s)$$

The effective rate is:

$$R_{H_{2}^{+}} = \sum_{p'>1} \left[ A_{H}(p',1)/n_{e} + F_{H}(p',1) \right] R_{2H}^{H_{2}^{+}}(p') = \sum_{p'>1} \left[ \alpha(p') - S(p')R_{2H}^{H_{2}^{+}}(p') \right]$$
(3.66)

The effective dissociation of  $H_2^+$  can result from the following paths.

1. Dissociative excitation followed by further excitation and final ionization of the excited atom H(n):

$$\begin{aligned} H_2^+ + e &\to H + H(n) \\ H(n) &\to \to H(m) \\ H(m) + e &\to H^+ + 2e \end{aligned}$$
 (3.67)

2. Dissociation followed by the decay of H(n) to the ground state:

$$H_2^+ + e \to H^+ + H(n) + e \tag{3.68}$$
$$H(n) \to H(1s)$$

The effective rate is:

$$D_{H_2^+} = \sum_{p'>1} \left\{ E_{H_2^+}(p') R_{2H}^{H_2^+}(p') + \left[ A_H(p',1)/n_e + F_H(p',1) \right] R_H^{H_2^+}(p') \right\}$$
(3.69)

The effective ionization  $H_2^+ \rightarrow 2H^+$  results from the dissociation followed by multi-step ionization of the excited atom H(n):

$$H_{2}^{+} + e \rightarrow H^{+} + H(n) + e \qquad (3.70)$$
$$H(n) \rightarrow H(m)$$
$$H(m) + e \rightarrow H^{+} + 2e$$

as well as direct ionization (3.64). The effective rate is:

$$S^{H_2^+} = S^{H_2^+} \left( X^2 \Sigma_g^+ \right) + \sum_{p'>1} \left[ S_H(p') \mathcal{R}_H^{H_2^+}(p') \right]$$
(3.71)

Here  $S^{H_2^+}(X^2\Sigma_g^+)$  is the rate of the process (3.64).

The reaction rates for the processes (3.62)-(3.64) are taken from [64]. For dissociative recombination (3.62) it is the process 2.2.14, for dissociation: 2.2.12 (the product is H(1s)) and 2.2.13 (the product is H(n = 2)), and for dissociative ionization (3.64) the process 2.2.11. Note that in the book [64] the rate 2.2.13 is a factor 10 overestimated because of a misprinting. Vibrationally excited levels of  $H_2^+$  are not taken into account explicitly, but the rate coefficients are averaged over the vibrational distribution of the products of the ionization  $H_2 \rightarrow H_2^+$  (see [64], reaction 2.2.9). In the old model of EIRENE 1996 the rates HYDHEL 2.2.11, 2.2.12., 2.2.14 from [64] were applied directly without taking into account the kinetics of the resulting atom. It was thus assumed that all produced excited atoms reach the ground state.

As in the case of molecules the energy balance is treated in the same way as in the old model [110] with one exception. For dissociative recombination  $H_2^+ \rightarrow 2H$  the effective electron energy loss rate AMJUEL H.8 2.2.14 calculated by CRM is used. This rate can be roughly estimated as  $0.88 \cdot T_e$  per effective collision (old model). The estimation of the kinetic energy of the products and the electron energy loss for other reactions is based on [64]. For  $H_2^+ \rightarrow 2H$  the kinetic energy of the both products is taken to be 0.5 eV, for  $H_2^+ \rightarrow H + H^+$  it is 4.3 eV and for  $H_2^+ \rightarrow 2H^+$  0.25 eV. Again, it is the kinetic energy in the centre-of-mass frame. The electron energy loss per one collision for  $H_2^+ \rightarrow H + H^+$  is 10.5 eV and for  $H_2^+ \rightarrow 2H^+$  15.5 eV. As in the case of molecules this simplified treatment has to be revised in future.

The comparison of the rates from HYDHEL with those calculated applying CRM [41] for the range of  $n_e$  and  $T_e$  relevant for divertor plasma is shown in Figure 3.10. For higher density the effective rate of recombination  $H^+ \rightarrow 2H$  is lower than that from HYDHEL. The reason is that the excited atoms produced by dissociative recombination (3.62) can be further ionized instead of decaying to the ground state. In this case this is a contribution to the effective dissociation  $H_2^+ \rightarrow H + H^+$  rather than to effective recombination, see Equations (3.66) and (3.69). This effect causes a strong increase of the effective dissociation compared to HYDHEL, especially for temperatures below 2 eV. One can also see that for the temperatures less than 20 eV the effective ionization  $H_2^+ \rightarrow 2H^+$  is unimportant compared to the two previous processes, despite it becomes an order of magnitude higher than that from HYDHEL.

From Figure 3.10 one can see that the rate of decomposition of  $H_2^+$  either by recombination or by dissociation is always greater than  $10^{-8} \text{ cm}^3/\text{s}$ . Therefore for the electron density larger than  $10^{14} \text{ cm}^{-3}$  the life-time of  $H_2^+$  is always shorter than  $10^{-6} \text{ s}$ , thus shorter than the transport time-scale. This estimation justifies the approach in which no transport of molecular ion is considered.

Ion conversion (3.61) followed by the dissociative recombination (3.62) can lead to effective recombination of  $H^+$ :

$$H_2(\nu) + H^+ \to H_2^+ + H \tag{3.72}$$
$$H_2^+ + e \to 2H$$

This channel of recombination is called Molecular Assisted Recombination (MAR). It was first proposed by S. Krasheninnikov et al. [109]. Another possible way of this kind of recombination is via the negative ion  $H^-$  [109]:

$$H_2(\nu) + e \to H^- + H \tag{3.73}$$
$$H^- + H \to 2H$$

Estimates made in [42, 109] show that for the conditions of a divertor plasma this channel is of smaller importance than the previous one because of the small production rate of  $H^-$ .

First calculations made with reaction rates from [64] showed that MAR may outperform conventional 3-body recombination by a factor of  $\approx 30$  for temperatures around 1 eV because the recombination channel  $H_2^+ \rightarrow 2H$  is stronger than dissociation for temperatures lower than 1.3 eV. But if the CRM is applied, then for the densities greater than  $10^{14} \text{ cm}^{-3}$  this temperature is shifted to 0.4.0.5 eV. In this temperature domain the conventional 3-body recombination is already strong enough. As a result, in the calculations for ITER plasma the effective recombination through the channel (3.2.3) constitutes only  $\approx 20$  % of the total recombination, see below in Section 3.3. A similar result was obtained in [98] (DEGAS-2 simulations for DIII-D plasma conditions). Note also that using the QSS-approximation for calculating the rate of the ion conversion (3.61) more likely tends to overestimate the effect rather than to underestimate it.

The ion conversion process (3.61) implemented with the old reaction rates from HYDHEL can cause numerical instability producing particles with very large statistical weight. The reason is the following. For inelastic collisions EIRENE uses Russian Roulette to decide which of the reaction products to follow. This can lead to the following chain of collisions with increasing statistical weight *W*:

$$D_2(W=1) \to (D_2 + D^+ \to D_2^+ + D) \to D_2^+(W=2) \to$$

$$\to (D_2^+ + e \to 2D) \to D(W=4) \to (D + wall) \to D_2(W=2)$$
(3.74)

In a wall-collision the atom is re-emitted as a thermal molecule. The weight of the molecule at the end of this chain is two times larger than the initial weight. As a result, some of the test particles can gain very high statistical weight, which spoils the Monte-Carlo statistics. It happens if the absorption processes for  $D_2$  are not strong enough to stop the weightbreading chain (3.2.3) before it becomes destructive. This numerical instability results in the fatal violation of the particle balances because of too strong statistical variations which is diagnosed by the code.

## **3.3** The effect of molecular kinetics

#### **3.3.1** Comparison of the full B2-EIRENE runs

To compare the results of B2-EIRENE calculations made with the old and the new neutral transport model a series of runs was made for the reference ITER case with 100 MW SOL input power and full carbon wall. The model set-up is described in Section 1.3.

The comparison of the following models will be shown:

- ITER 828 is the model with EIRENE 1996. No neutral-neutral collisions. The reaction rates for the electron-impact processes with  $D_2$  and  $D_2^+$  are taken from database HYDHEL. No elastic collisions  $D_2+D^+$  and ion conversion.
- ITER 1048. The model of ITER 828 with added NNC of D, D<sub>2</sub> and He with each over (all possible combinations)
- ITER 1055. The model of ITER 1048 with added elastic collisions  $D_2+D^+$  and ion conversion. The reaction rates for the electron-impact processes with  $D_2$  and  $D_2^+$  are taken from database AMJUEL.



Figure 3.10: Effective reaction rates for molecular ion  $H_2^+$  calculated using CRM [41] (AMJUEL, see Table 3.2) compared to the old data from [64] (HYDHEL)

The basic parameters of the modelling cases are shown in Table 3.3. In this table  $p_{PFR}$  is the average neutral pressure at the edge of the Private Flux Region,  $S_{puff}$  is the gas puffing rate. The initial idea was to choose the cases with similar conditions near the inner target as the region of the strongest expected difference. For this purpose the cases with matched profiles of the incident heat flux to the inner target were chosen, see Figure 3.15a below. The neutral pressure  $p_{PFR}$  is the key parameter which determines the conditions in the divertor, see Section 1.3. The cases ITER 1048 and ITER 1055 are significantly different in  $p_{PFR}$ . Nevertheless, to demonstrate the effects which will be considered below this kind of comparison is justified. Already from Table 3.3 one can see that for the updated model similar divertor conditions are reached with significantly higher  $p_{PFR}$ .

	828	1048	1055
$p_{PFR}$ , $Pa$	7.0	8.5	10.6
$S_{puff}, s^{-1}$	$5.7 \cdot 10^{22}$	$8.9 \cdot 10^{22}$	$15.3 \cdot 10^{22}$

Table 3.3: Parameters of the modelling cases

The plasma parameters in front of the targets for the three modelling cases are shown in Figures 3.11-3.14. One can see that including NNC and then the updated Molecular Kinetics (MK) decreases the density in front of the inner target, Figure 3.11a. But a few centimetres away from the target the maximum of the density gets a factor 1.5 higher, Figure 3.11c. Note that the density does not increase monotonically towards the targets any more, showing a "detachment-like" behaviour with a density peak away from the target. The temperature near the inner target falls down and does not exceed 3 eV for the new model, Figure 3.12a. At the outer target the maximum of the temperature does not change but it shifts downwards towards the separatrix, Figure 3.12b. The ion temperature in front of the targets is almost the same as that of electrons.

The effect can be to large extent explained by the compression of molecules described in Section 2.5. For elastic collisions  $D_2+D^+$  (EL) it works in the same way as for NNC: the density of molecules near the targets increases due to backscattering, see Figure 3.13. Similar increase is seen for the atoms due to secondary particles produced by dissociation, Figure 3.14. This effect "presses" the neutrals towards the targets, "pushing" the plasma in the opposite direction.

This is illustrated once more in Figure 3.17 which shows the contour plots of some parameters in the inner divertor (in this region the effect is stronger). For the cases when NNC and MK were switched on a strong concentration of molecules near the strike point can be seen, Figure 3.17a. At the same time their density in the high temperature region above the separatrix increases because hotter particles can penetrate deeper into the plasma. The modification of the molecule density is followed by the atom density, Figure 3.17b. As a result of this modification of the neutral gas parameters, the "tongue" of the hot plasma approaches the target closer near the strike point but steps back in the upper hot region, Figure 3.17c.

One can say that NNC and EL shrink the recycling zone in the poloidal direction. Here both NNC and EL are referred to as the reason of this effect. But EL alone can cause it even in the absence of NNC. This is an important note since: i) This effect is likely to occur even in the devices much smaller and having lower density than ITER; ii) the lack of very reliable NNC collisionality data discussed in Appendix 2.4 does not affect this conclusion.

The modification of the incident heat flux profile is shown in Figure 3.15. The inner target heat flux profile is the same because it was intentionally matched for those modelling cases, , Figure 3.15a. The outer target loads become somewhat higher, Figure 3.15b indicating the increase of the asymmetry between the inner and outer divertors. The reason may be that the effects related to the compression of molecules are stronger near the inner target. As expected, the incident heat flux due to neutrals is somewhat higher for the new model, Figure 3.16. The incident heat flux transferred to the inner targets by plasma (kinetic and potential energy of ions) is significantly reduced with the new model, Figure 3.15a, dashed lines. This is partly because of the increased heat flux related to neutrals, partly due to the shift of the peak of the radiation heat loads downwards. This decrease of the plasma heat flux is consistent with the observed decrease of the temperature and density, because the former scales as ~  $nT^{1.5}$ .



Figure 3.11: Electron density in front of the targets for three modelling cases

The comparison of the 2D distribution of the plasma parameters for EIRENE 1996 and the current ITER version are shown in Figures 3.18-3.21. One can see that the new model shows a well pronounced pressure drop near the inner target, Figure 3.20. Such kind of behaviour is typical for detached conditions. The detachment-like behaviour can be also seen for the electron particle sources, Figure 3.21 as well as for the electron density profiles, Figures 3.11a, 3.11c.

The reason for the higher pressure gradient is the strong parallel momentum sink due to collisions with molecules, Figure 3.22b. For the new model this channel of momentum removal becomes dominant (see below in Section 3.3.2). Comparing this sink with the corresponding sink due to charge-exchange in the old model, Figure 3.22a, one can see that the latter is a factor 3 smaller, but distributed more uniformly in space (to large extent due to secondary atoms produced from dissociating molecules). The fact that the momentum sink due to collisions with molecules can be at least not smaller than that due to atoms was noticed already back in the past in the paper [44].

#### 3.3.2 Analysis for the fixed plasma background

The analysis of the individual contributions of the different model features was made by applying different models for molecular kinetics on a fixed plasma background. In this case it was the background of ITER 1055. In addition to the model with full molecular kinetics (ITER 1055 itself) the two reduced cases were considered. ITER 1055m1, with the old model for molecular kinetics (but with NNC), and ITER 1055m2 with the old model for molecular chemistry, but with elastic collisions  $D_2+D^+$ . The effect of NNC on a fixed plasma background was shown in Section 2.5. The distributions of the neutral parameters shown below were obtained with test runs of EIRENE with  $10^6$  histories. The statistical error for the neutral density is less than 5% for the domain of interest. The relative error in the particle balance is smaller than 0.5 %.

The molecule density in front of the targets for the three models is shown in Figure 3.23.



Figure 3.12: Electron temperature in front of the targets for three modelling cases



Figure 3.13: The density of  $D_2$  molecules in front of the targets for three modelling cases



Figure 3.14: The density of D atoms in front of the targets for three modelling cases



Figure 3.15: The total incident target heat flux for three modelling cases. Dashed line: the incident heat flux due to plasma only



Figure 3.16: The neutral incident target heat flux for three modelling cases



Figure 3.17: Comparison of the spatial distributions of the neutral and plasma parameters near the inner target. Red: ITER 828, Green: ITER1048, Blue: ITER 1055



Figure 3.18: Electron density for the model of EIRENE 1996 (ITER 828) and the current ITER model (ITER 1055)



Figure 3.19: Electron temperature for the model of EIRENE 1996 (ITER 828) and the current ITER model (ITER 1055)



Figure 3.20: Plasma pressure for the model of EIRENE 1996 (ITER 828) and the current ITER model (ITER 1055)



Figure 3.21: Electron particle source for the model of EIRENE 1996 (ITER 828) and the current ITER model (ITER 1055)


Figure 3.22: Dominant Parallel Momentum Sinks for the old and new models

Case	Inner Target			Outer Target		
	D+	D	$D_2$	D+	D	$D_2$
ITER 1055	1.03	3.38	6.04	1.73	3.08	4.11
ITER 1055m2	1.03	1.62	4.58	1.73	1.95	3.43
ITER 1055m1	1.03	1.83	1.56	1.73	1.90	7.93
ITER 828	1.83	3.59	0.686	2.32	3.63	0.808

Table 3.4: Fluxes incident on the targets,  $10^{24} s^{-1}$ 

Elastic collisions increase the density near the inner target in  $\approx 2$  times. Note, that the compression due to elastic collisions is additional to that due to NNC, see Section 2.5. The contribution of the modified molecular chemistry is small, especially for the outer target. The effect of "compression" is related to the increase of the "back-scattered" flux of molecules due to elastic collisions. This is illustrated in Table 3.4 which shows the total incident fluxes on the targets. The total flux of molecules for the case ITER 1055 is an order of magnitude larger compared to ITER 828 despite lower ion flux.

Including the new molecular chemistry (MC) into the model yields a small difference. The 2D plots of the parameters related to MC can be found in Appendix D. The strongest observed effect of MC is the increase of the molecular ion density due to the ion conversion, Figures D.1.

Table 3.5 shows the constituents of the particle balance for the hydrogenic particles in the inner and outer divertor for the case ITER 1055: the total sinks of atoms and molecules due to different processes. "Inner" and "Outer divertor" stands for the regions within 12 poloidal cells near the corresponding targets. The column "Global" are the integrals over the whole computational domain. The row "Surface,  $D_2$ " shows the sources of molecules due to thermal desorption from the wall originated by the incident atoms.

The main primary source of the neutral particles is the target recycling. Volume recombination is in total a factor of 2 lower, but in the inner divertor alone it is almost equal to the recycling sources, compare Table 3.5 rows  $\text{RECYC}_D$ ,  $\text{RECYC}_D$  and  $\text{RCMB}_D$ .

The amount of recycled particles leaving the target as atoms and as molecules is roughly the same, Table 3.5, rows  $\text{RECYC}_D$  and  $\text{RECYC}_{D_2}$ . Most of the molecules dissociate: the amount of ionized molecules is almost a factor 4 smaller, Table 3.5 rows  $\text{DISS}_{D_2}$ ,  $\text{IONIZ}_{D_2}$  and Figure D.2.

The main channel of producing  $D_2^+$  is the ion conversion: it is an order of magnitude stronger than the ionization, Table 3.5, rows IONIZ<sub>D<sub>2</sub></sub>, IC<sub>D<sub>2</sub></sub> and Figures D.2a, D.3a. The



Figure 3.23: Density of  $D_2$  molecules in front of the targets for three different models on a fixed plasma background. ITER 1055 is the full model, ITER 1055m1 is the old model for molecular kinetics (but with NNC), ITER 1055m2 is the old model for molecular chemistry but with elastic collisions of molecules and ions

Notation	Process	Inner Divertor	Outer Divertor	Global
$\operatorname{RECYC}_D$	Recycling, D	4.38e+23	6.75e+23	1.14e+24
$\operatorname{RECYC}_{D_2}$	Recycling, D <sub>2</sub>	2.95e+23	5.29e+23	8.38e+23
$\text{RCMB}_D$	Recombination, D	8.04e+23	5.68e+23	1.39E+24
$\text{SRF}_{D_2}$	Surface, D <sub>2</sub>	1.15e+24	9.50e+23	3.31e+24
IONIZ <sub>D</sub>	Ionization, D	1.68e+24	2.16e+24	4.03E+24
$\mathrm{DISS}_{D_2}$	Dissociation, D <sub>2</sub>	5.24e+23	6.77e+23	1.28E+24
$IONIZ_{D_2}$	Ionization, D <sub>2</sub>	9.10e+22	2.42e+23	3.79E+23
$\mathrm{DI}_{D_2}$	Dissociative			
	Ionization, D <sub>2</sub>	4.81e+21	1.26e+22	1.80e+22
$IC_{D_2}$	Ion Conversion	1.29e+24	1.15e+24	2.47E+24
$\mathrm{DISS}_{D_2^+}$	Dissociation, $D_2^+$	1.24e+24	1.26e+24	2.57E+24
$\text{RCMB}_{D_2^+}$	Recombination, $D_2^+$	1.37e+23	1.22e+23	2.67E+23
$\mathrm{DI}_{D_2^+}$	Dissociative			
~	Ionization, $D_2^+$	3.3097e+21	7.6868e+21	1.1813e+22

Table 3.5: Particle balance for the case ITER 1055,  $s^{-1}$ 

Notation	Type of Energy	Inner Target	Outer Target	Total
$P^i_{kin}$	Ions Kinetic	1.0	9.1	11.6
$P^i_{pot}$	Ions Potential	2.5	4.1	6.9
$P_{kin}^n$	Neutrals Kinetic	2.2	2.5	7.0
$P^n_{diss}$	Neutrals Diss.	1.0	1.1	3.0
$P_{tot}^p$	Total in Particles	6.7	16.8	28.5
P <sub>rad</sub>	Radiation	11.5	17.6	70.5
P <sub>tot</sub>	Total	18.2	34.4	99.0
		Radiatio	on in the volume	
		Inner Divertor	Outer Divertor	Total
$P_{rad}^n$	Neutrals	4.1	3.7	8.1
$P^i_{rad}$	Ions	25.0	30.1	62.4

Table 3.6: Power balance for the case ITER 1055, MW

strength of the dissociative recombination of  $D_2^+$  is an order of magnitude smaller than that of the dissociation: Table 3.5, rows  $\text{DISS}_{D_2^+}$ ,  $\text{RCMB}_{D_2^+}$  and Figures D.3b, D.3c. The local rate of MAR can be estimated as:

$$n_{D_2^+} \frac{R_{IC}}{R_{IC} + R_I} R_{DR} \approx n_{D_2^+} R_{DR}$$

Here  $R_{IC}$ ,  $R_I$  and  $R_{DR}$  are the rates of the ion conversion, ionization of molecules and dissociative recombination of molecular ions. Assuming that  $R_{IC} > R_I$  one can approximate the rate of MAR by the rate of dissociative recombination (this yields an overestimation!). The total rate of MAR estimated in this way constitutes only 20 % of the "common" recombination: Table 3.5, rows RCMB<sub>D</sub>, RCMB<sub>D</sub>, and Figures D.3c, D.3d, Appendix D.

Evaluating the particle balance for individual species is one of the primary "fast" diagnostics in the EIRENE code. For illustrative purposes a numerical example for the case ITER 1055 is shown below (see also Table 3.5). All the sources below are expressed in  $s^{-1}$ .

The balance for *D* atoms is:

$$\begin{split} SOURCE &= RECYC_D + RCMB_D + 2 \cdot DISS_{D_2} + DI_{D_2} + DISS_{D_2^+} + \\ & 2 \cdot RCMB_{D_2^+} + IC_{D_2} = 1.1441 \cdot 10^{24} + 1.3880 \cdot 10^{24} + 2 \cdot 1.2764 \cdot 10^{24} \\ & + 1.8025 \cdot 10^{22} + 2.5673 \cdot 10^{24} + 2 \cdot 2.6703 \cdot 10^{23} + 2.4684 \cdot 10^{24} = 1.0673 \cdot 10^{25} \\ SINK &= IONIZ_D + 2 \cdot SRF_{D_2} + S_{pump}^D = 4.0287 \cdot 10^{24} + 2 \cdot 3.3048 \cdot 10^{24} + 5.0128 \cdot 10^{20} = 1.0639 \cdot 10^{25} \end{split}$$

Here  $S_{pump}^{D}$  is the pumped flux.

The same for  $D_2$  molecules:

$$SOURCE = IRECYC_{D_2} + SURF_{D_2} + S_{puff} =$$

$$= 8.3772 \cdot 10^{23} + 3.3048 \cdot 10^{24} + 7.6500 \cdot 10^{22} = 4.2190 \cdot 10^{24}$$

$$SINK = DISS_{D_2} + IONIZ_{D_2} + DI_{D_2} + IC_{D_2} + S_{pump}^{D_2} =$$

$$1.2764 \cdot 10^{24} + 3.7885 \cdot 10^{23} + 1.8025 \cdot 10^{22} + 2.4684 \cdot 10^{24} + 7.6395 \cdot 10^{22} = 4.2180 \cdot 10^{24}$$

Here  $S_{puff}$  and  $S_{pump}^{D_2}$  are gas puffing and pumping rates. The pumped flux of nuclei  $S_{pump}^D + 0.5S_{pump}^{D_2} = 1.538 \cdot 10^{23} s^{-1}$  is equal with a good accuracy (< 0.2 %) to the specified input flux  $1.53 \cdot 10^{23} s^{-1}$ 

For the molecular ion  $D_2^+$ :

$$SOURCE = IC_{D_2} + IONIZ_{D_2} = 2.4684 \cdot 10^{24} + 3.7885 \cdot 10^{23} = 2.8472 \cdot 10^{24}$$
$$SINK = DISS_{D_2^+} + RCMB_{D_2^+} + DI_{D_2^+} = 2.5673 \cdot 10^{24} + 2.6703 \cdot 10^{23} + 1.1813 \cdot 10^{22} = 2.8461 \cdot 10^{24}$$

The power losses due to particle fluxes to the wall and radiation are shown in Table 3.6. In this table the row "Ions Kinetic" shows the energy flux related to the kinetic energy

Notation	Sinks	Inner	Outer	Total	
		For e	electrons due	to	
$SEE_a$	Atoms	6.53e+06	7.44e+06	1.48e+07	
$SEE_m$	Molecules	1.13e+06	1.79e+06	3.17e+06	
$SEE_i$	Molecular Ion	2.23e+06	2.30e+06	4.68e+06	
SEE <sub>tot</sub>	Total Sink	9.89e+06	1.15e+07	2.27e+07	
$SEE_{rcmb}$	Recombination	-3.03e+05	-2.05e+05	-5.08e+05	
		For ions due to			
$SEI_a$	Atoms	-1.51e+06	-1.77e+06	-2.00e+06	
$S E I_m$	Molecules	2.78e+06	2.53e+06	5.40e+06	
$SEI_i$	Molecular Ion	-1.17e+06	-1.16e+06	-2.40e+06	
SEI <sub>tot</sub>	Total Sink	9.97e+04	-4.03e+05	-3.03e+05	
SEI <sub>rcmb</sub>	Recombination	3.83e+05	2.71e+05	6.75e+05	

Table 3.7: Power losses due to neutrals, W

of the incident ions ("Neutrals Kinetic" is the same for neutrals), "Ions Potential" is the ion flux multiplied by the ionization energy (for all ion species) and "Neutrals Diss." is the flux of molecules produced on the targets times the release of potential energy in recombinations of atoms (4.48 eV). For neutral particles the net flux is shown: kinetic energy of the incident particles minus kinetic energy of the emitted particles. All the numbers for neutrals in Table 3.6 are taken directly from EIRENE and the numbers for plasma are taken from B2PLOT.

About 70 % of the input power is radiated. The rest is deposited mainly by the incident ion flux. For the inner target the power deposited due to neutrals is the same as due to plasma but for the outer target it is a factor 4 smaller. The bulk of the total radiation comes from impurities. The radiation of neutrals constitutes only  $\approx 10$  % of the radiated power. The main radiator is Carbon: for the case in question the total radiation from Helium is only 0.45 MW and the bremsstrahlung radiation is only 0.1 MW.

Table 3.7 shows the distribution of the plasma energy losses due to neutrals between different channels (this means that the sign "minus" stands for the energy gained by plasma). The electrons loose energy for ionization and dissociation of neutrals but can gain it from recombination. The ions loose energy in charge-exchange and elastic collisions as well as due to ion conversion and recombination and gain it from ionization. The ion energy loss due to neutrals is an order of magnitude smaller than that for electrons.

Tables 3.6 and Table 3.7 represent the energy balance from two points of view. If one considers the plasma and the neutral gas as one system, then the total loss of power is:

$$P_{SOL} = P_{kin}^{i} + P_{pot}^{i} + P_{kin}^{n} + P_{diss}^{n} + P_{rad}^{n} + P_{rad}^{i} = 11.6 + 6.9 + 7.0 + 3.0 + 8.1 + 62.4 = 99 MW$$
(3.75)

 $P_{kin}^{n}$  includes also the kinetic energy of neutrals penetrating into the core (0.4 MW, the atom flux to the core is  $3 \cdot 10^{21} s^{-1}$ ). Another point of view on the energy balance is to consider only the plasma (only charged particles) and to take into account its energy exchange with the neutral gas. In this case the total loss of power is:

$$P_{SOL} = P_{kin}^{t} + P_{rad}^{t} + SEE_{tot} + SEE_{rcmb} + SEI_{tot} + SEI_{rcmb} = 11.6 + 62.4 + 22.7 - 0.51 - 0.3 + 0.68 = 96.57 MW$$
(3.76)

The term  $P_{rad}^n$  does not enter this sum because it is included into  $SEE_{tot}$ . Formula (3.76) does not include a small term which takes into account the recombination energy of the pumped atoms. The power loss calculated according to relations (3.75) and (3.76) is within 5 % of the specified input power 100 MW which is a normal accuracy of the energy balance in B2-EIRENE for ITER modelling. The difference between balances (3.75) and (3.76) is due to some inconsistencies in the coupled code (linearisation and rescaling of the sources). In EIRENE alone a small error in the energy balance appears because of using the tracklength estimators for both particle and energy sources.

The total momentum losses in the inner and outer divertors are shown in Table 3.8. The quantities there are the integrals of the parallel momentum sources over the corresponding volumes (within 12 poloidal cells in on the inner and outer side): i.e. the total forces parallel to magnetic field. The term "loss" is related to a force directed away from the

	ITER	1055	ITER 828		
	Inner	Outer	Inner	Outer	
Total	2.24e+02	2.36e+02	1.06e+02	4.35e+01	
Atoms	8.37e+00	1.01e+01	6.38e+01	1.42e+01	
Molecules	2.44e+02	2.50e+02	0	0	
Test Ions	-5.35e+01	-4.14e+01	8.32e-02	-1.37e-01	
Recombination	2.51e+01	1.65e+01	4.23e+01	2.95e+01	

Table 3.8: Momentum losses due to neutrals, N

target. The dominant mechanism of the plasma momentum loss in divertor for the new model (ITER 1055) is the collisions with molecules. It includes both elastic collisions and ion conversion. The contribution of atoms is an order of magnitude smaller. This is partly because the atomic contribution includes ionization which can be a net source of momentum. In addition, a molecule transfers on average more momentum to the wall than an atom.

The reason for this is that on the wall an atom can turn into a molecule (thermal reabsorption) but not vice versa. As a result the amount of collisions with the wall which a molecule can experience is limited only by its lifetime in plasma. Whereas for atoms the probability of the next collision depends on the number of the previous ones. One can see that the incident flux of molecules is larger than that of atoms, Table 3.4, despite higher primary sources of the former Table 3.5 (RECYC<sub>D</sub> and RECYC<sub>D</sub>).

For comparison, the momentum losses for the old model (ITER 828) are shown in the same Table 3.8. The momentum losses due to atoms are higher than for ITER 1055, because of different plasma background (larger region with lower temperature, Figures 3.12 and 3.17c). Nonetheless are still a factor 2-3 lower than the loss due to molecules for the new model. The observed drop in the plasma pressure near the inner target, Figure 3.20, corresponds to the momentum sink due to elastic collisions  $D_2+D^+$ . The momentum source due to molecules for the ITER 828 case is very small because it is only due to dissociative ionization  $D_2 \rightarrow D + D^+$ . The sources related to  $D_2^+$  become two order of magnitude higher because the density of  $D_2^+$  drastically increases due to ion conversion, Figure D.1, Appendix D. The momentum sink due to recombination is similar in both cases.

As it was shown in Chapter 3.1.3 the expected Mean Free Path (MFP) for elastic collisions  $D_2+D^+$  can be less than 1 cm. This fact is illustrated in Figure 3.24a which shows the inverse Mean Free Path estimated in the same way as in Section 2.5. In the most of the region of interest in the inner and outer divertors it is really shorter than 1 cm, sometimes reaching 1 mm. The plasma density there is up to  $10^{21} m^{-3}$  and even higher, Figure 3.18b. The MFP for  $D_2+D^+$  collisions can be even smaller than that for charge-exchange, Figure 3.24b, because the molecules are slower.

For such a high collisionality one would expect totally hydrodynamic behaviour of the neutral particles, but it is not exactly the case: kinetic effects can be also important. As it was already mentioned above, the momentum transfer is largely determined by the particles which hit the wall several times before being ionized (dissociated). To study the deviation from the quasi-equilibrium, the Velocity Distribution Function (VDF) was calculated directly for a number of grid cells for the plasma background of the case ITER 1055p1 (see below in Section 4.3). The examples of VDF for each component of velocity are shown in Figures 3.25 and 3.26 for atoms and molecules respectively. The "Point 1" lies in the inner divertor in the first cell after the target between the separatrix and the location of the maximum heat flux density. "Point 5" has the similar location but for the outer target, see Table 3.9. This table also shows the macroscopic parameters of the neutrals and ions for the selected cells. R and Z are the radial and vertical coordinates and  $\theta$  is the toroidal coordinate, T stands for the temperature and V for the average (drift) velocity. In both cells in question the electron density  $n_e >\approx 10^{21} m^{-3}$ .

In addition to the calculated VDF Figures 3.25 and 3.26 show the Maxwellian distribution with the same macroscopic parameters as well as VDF of ions. As expected (fast thermalization due to charge-exchange), VDF of atoms is almost Maxwellian and very close to that of ions, Figure 3.25. For the molecules, however, one can see a strong anisotropy of VDF, Figure 3.26, although their temperature is almost the same as the ion temper-



Figure 3.24: Inverse Mean Free Path of elastic collisions  $D_2+D^+$  and charge-exchange  $D+D^+$ 

Point	R, cm	Z, cm	Specie	T, eV	$V_R$ , cm/s	$V_Z$ , cm/s	$V_{\theta}$ , cm/s
1	413.6	-374.8	$D^+$	0.59	-2.3e4	-1.1e4	-3.7e5
	$n_e = 9.7$	$\cdot 10^{20} m^{-3}$	D	0.55	-4.8e4	-1.1e4	-3.8e5
			D <sub>2</sub>	0.6	7.6e3	-4.1e4	-3.5e5
5	555.2	-439.6	$D^+$	0.84	2.7e4	-6.5e4	7.2e5
	$n_e = 1.6$	$\cdot 10^{21} m^{-3}$	D	0.79	4.6e4	-8.3e4	7.0e5
			D <sub>2</sub>	0.77	-5.5e4	-5.3e4	5.9e5

Table 3.9: Parameters of the diagnostic points in Figures 3.25, 3.26

ature. The observed effect may be related to the presence of wall and to the fact that in each collision the molecule tends to deflect to relatively small angle, quite opposite to the charge-exchange of atoms. In the next cell away from the target both atoms and molecules have almost equilibrium Maxwellian distribution with the same temperature and drift velocity as ions. This example shows that the kinetic description of molecules can be important in the region close to the wall, in particular for the correct description of the momentum transfer which may be sensitive to the anisotropy of VDF.

The approximate residence time of atoms and molecules was mentioned before to justify the application of the QSS-approximation for molecular chemistry. The Monte-Carlo sampling allows getting a more sound estimation of this quantity. For this purpose the following estimator was defined:

$$\tau_r = \frac{\sum_i (t_i \cdot w_i t_i)}{\sum_i w_i t_i)} \tag{3.77}$$

Here  $t_i$  is the time interval between two "interrupting events",  $w_i$  is the statistical weight of the test particle. The sum over i is taken over the all "interrupting events" in the control volume (the grid cell). The "interrupting events" are: i) the test particle enters or leaves the control volume; ii) the test particle changes its state (ionization, dissociation, thermal re-absorption). The time  $\tau_r$  is the time between "interrupting events" averaged other the velocity distribution. The denominator of this formula is proportional to the number density. This estimation takes into account that the particles with smaller residence time have smaller contribution to the density. Note that a more obvious estimation for the residence time as  $\tau_r = L/V$  where V is the average (drift) velocity and L is the characteristic size would be misleading because it does not take into account that particles move in different directions. Consider for example two counter beams with equal density and velocity u. Then  $\tau_r = L/V$  yields infinity because the average velocity is 0. Whereas the estimation (3.77) will give the correct value  $\tau_r = L/u$  in this case.



Figure 3.25: Velocity distribution function of D atoms near the target. Point 1 is located in front of the inner target and Point 5 in front of the outer target, see Table 3.9



Figure 3.26: Velocity distribution function of  $D_2$  molecules near the target. Point 1 is located in front of the inner target and Point 5 in front of the outer target, see Table 3.9



Figure 3.27: Estimated residence time for D atoms and  $D_2$  molecules. Solid line is the first poloidal cell after the target and dashed line is the next poloidal cell

The estimation of  $\tau_r$  made for the plasma background of the case ITER 1055p1 (see in Section 4.3 below) is shown in Figures 3.27. This figure shows the residence time of D<sub>2</sub> molecules and D atoms in the first two poloidal cells of the computational grid in front of each target. As expected, the characteristic time-scale is  $10^{-6}$  s and for molecules the time is somewhat larger (a factor of 2) than for atoms. For this particular grid the first cell extends approximately one centimeter from the target surface. If the steep gradients in front of the target were resolved better, the estimated  $\tau_r$  could be even smaller.

## **Chapter 4**

# **Radiation opacity**

## 4.1 Introduction

All simulations shown in the previous chapters were made on the assumption that the neutral gas is transparent for the hydrogen line radiation. Simple estimates (see e.g. [113]) show, however, that for neutral densities typical for the divertor region ( $10^{13} \text{ cm}^{-3}$  and larger) the hydrogen  $Ly_{\alpha}$  and  $Ly_{\beta}$  lines are likely to be opaque. This evaluation is backed by experimental measurements. The investigation of the  $D_{\gamma}/D_{\alpha}$  and  $D_{\beta}/D_{\alpha}$  line ratios in Alcator C-Mod [114] and JET [115] tokamaks show evidence of such re-absorption. The absorption of the line radiation can increase the effective ionization rate of a hydrogen atom due to ionization of the photo-excited states. The effect can reach 1-2 orders of magnitude, see e.g. [113]. This extra channel of ionization can change the whole ionization-recombination balance in the divertor and, therefore, has to be taken into account in the modelling.

A feasibility study of implementing the radiation transport in the EIRENE code was done by Sven Wiesen in the framework of his PhD thesis and by Betra Börner for her diploma work. This work included in particular an experimental benchmarking for automotive lighting industry applications (HID-lamps) [48, 116]. The calculations have been carred out for ITER [45, 46] and Alcator C-mod [90, 117] tokamaks as well. In those EIRENE calculations, self-consistency is achieved between the radiation field (photon gas) and neutral gas, but was restricted to fixed plasma background. The calculations for the ITER divertor plasma showed a factor  $\approx$  reduction of the neutral density due to extra ionization from the photo-excited states, with unclear consequences for the divertor plasma itself. A qualitatively similar effect (a factor  $\approx 2$  reduction of the neutral density) was observed in the calculations for Alcator C-Mod tokamak. In this latter case EIRENE was applied to model the transport of neutrals and photons in a fixed plasma background reconstructed from experimental measurements [90]. A self-consistent modelling of the neutral kinetics including photon trapping effects using the CRETINE code [118] together with a 1D model of plasma transport based on fluid equations was done recently in [119, 120]. These calculations showed that the plasma reacts to the higher ionization by increasing its density and decreasing temperature near the target.

The model which is used in this work is different from the original model of S. Wiesen [45, 46]. The current model comprises the Monte-Carlo line radiation transport coupled with a Collision Radiative Model for the short living hydrogen excited states and a Monte Carlo kinetic model for the ground state. It was first applied for Alcator C-Mod calculations [90]. In the present work this model is incorporated into self-consistent 2D B2-EIRENE modeling of the divertor plasma. The material of this Chapter can be found partly in the paper [121].

## 4.2 The model

#### **4.2.1** Transport of photons

Photon transport is implemented in EIRENE in the same way as the transport of neutral particles. Photons are represented in the code as a particular neutral species, emitted

by the corresponding volume sources (from excited states) similar to those for volume recombination of atoms (from ions). The probability of spontaneous radiative decay  $A_{nm}$  (first Einstein Coefficient) plays the role of the recombination rate. Induced radiation ("Laser" effect) is not taken into account because the expected density of the radiation field is not so high. Currently only *Ly*-series photons are considered. Natural and Doppler broadening and Zeeman splitting are taken into account in the calculation of the line absorption and emission profiles. The natural broadening results from the finite life-time of the excited level. Doppler broadening appears due to non-zero velocity of the emitters: atoms in thermal motion. Zeeman splitting is the splitting of the atom energy levels in the magnetic field.

Estimations of the line broadening due to the various mechanisms are shown in Table 4.1. The numerical formulas are given for Deuterium atom. The numbers are calculated for the reference point T = 1 eV,  $n_e = 10^{15} cm^{-3}$ , B = 6 T which represent typical parameters near the strike points in ITER. A simple formula from [53] was used for the Doppler broadening. Zeeman splitting was estimated according to Formula (4.1) below. Stark broadening results from the microscopic electric fieled of the charged particles surrounding the atom. Formulas 7.3.33-36 from [124] were used for the electron impact broadening, and Equation 7.3.15 from the same book for the width of the Holtsmark profile (ion impact broadening). This latter estimate is based on the Holtsmark theory and does not take into account Debye shielding and the ion motion which can reduce the effect [124, chapt. 7.3.2].

Table 4.1 shows that Doppler broadening is the dominant expected mechanism and the natural broadening is negligible for the conditions in question. The value of the Zeeman splitting can be of the same order as the Doppler shift. This estimate also shows that the ion micro-field Stark broadening, which is not included in the model so far, can be also important even for the  $Ly_{\alpha}$  line. The figures in Table 4.1 and the test calculations made with electron Stark broadening [116] show that this effect is of minor importance for the divertor conditions. The broadening due to reduction of the life time of the excited level which takes place besides the spontaneous radiative decay: electronic de-excitations, ionization etc., is not taken into account in the current model as well.

Mechanism	Formula for $\frac{\Delta E}{E_0}$	$Ly_{\alpha}, \frac{\Delta E}{E_0}^2$	$Ly_{\beta}, \frac{\Delta E}{E_0}^2$
Natural	$4.8 \cdot 10^{-17} A_{nm}$	$2.3 \cdot 10^{-8}$	$2.7 \cdot 10^{-9}$
Doppler	$5.5 \cdot 10^{-5} \sqrt{T}$	$5.5 \cdot 10^{-5}$	$5.5 \cdot 10^{-5}$
Electron Stark	$1.6 \cdot 10^{-22} n^4 n_e / \sqrt{T_e}$	$2.6 \cdot 10^{-6}$	$1.2 \cdot 10^{-5}$
Ion Stark	$6 \cdot 10^{-16} (n^2 - m^2) n_e^{2/3}$	$1.8 \cdot 10^{-5}$	$4.8 \cdot 10^{-5}$
Zeeman	$4.3 \cdot 10^{-6}B$	$2.6 \cdot 10^{-5}$	$2.6 \cdot 10^{-5}$

Table 4.1: Comparison of the different line broadening mechanisms

The energy of the emitted photon is sampled in the following way. First, the photon velocity vector  $\mathbf{v}_{ph}$  is sampled isotropically (its magnitude is of course the speed of light). The initial photon energy is set to the centre-line energy  $E_c$  (energy of transition). This energy is corrected to take into account the Zeeman splitting (Zeeman-Lorentz triplet) [128]:

$$E_z = E_c + k \cdot \mu_B B, \quad P(k) = \frac{1}{4} \begin{cases} 1 + \cos^2 \theta, k = \pm 1; \\ 2\sin^2 \theta, k = 0 \end{cases}, \quad \cos \theta = \frac{(\mathbf{v_{ph}}.\mathbf{B})}{cB} \end{cases}$$
(4.1)

Here P(k) is the discrete probability density for k, **B** is the magnetic induction,  $E_z$  is the corrected energy of transition and  $\mu_B$  is the Bohr magneton:

$$\mu_B = \frac{e\hbar}{2m_e} = 5.7884 \cdot 10^{-5} \frac{eV}{Tesla}$$

Where  $\hbar = h/2\pi$  is the Planck constant,  $m_e$  is the electron mass. After that, the energy of emitted photon *E* is sampled from the Lorentz profile to take into account the natural broadening:

$$I(E) = \frac{1}{\pi} \frac{\gamma}{(E - E_z)^2 + \gamma^2}, \quad \gamma = \frac{A_{nm}h}{4\pi}$$
(4.2)

Finally, the Doppler shift is added:

$$E_d = E \cdot \left( 1 + \frac{(\mathbf{v_{ph}}, \mathbf{v_n})}{c^2} \right)$$
(4.3)

 $E_d$  is the final energy of the emitted photon,  $\mathbf{v}_n$  is the velocity of the emitter. To sample the velocity  $\mathbf{v}_n$  the Velocity Distribution Function (VDF) of atoms needs to be known.

In order to define this VDF, the excited atoms are split into two groups: atoms produced due to recombination of ions and atoms produced due to excitation of the ground state. The corresponding populations are calculated with a Collision-Radiative model, see below in Section 4.2.2. It is assumed that the particles of each group have a shifted Maxwellian velocity distribution. The temperature and the drift velocity of the first group are taken to be the same as those of ions, and for the second group the parameters of atoms are used. This model does not take into account the heavy particle collisions for excited states. The validity of this assumption will be addressed below in Section 4.2.2. For the conditions of the ITER divertor this is not very important because the VDF of atoms is almost the same as of ions, see Section 3.3.2.

This model also does not include the radiation from excited levels produced due to dissociative recombination of  $D_2^+$ , see Section 3.2.3, process (3.62) and (3.63). This channel is not very important for ITER conditions, see below in Section 4.3, but can be important for lower densities, e.g. for linear devices [126]

The same assumption of the shifted Maxwellian VDF is applied for calculating the crosssection of the photon absorption  $\sigma_a(E)$ . If the absorber moves, then the absorption crosssection of the photon with energy *E* in case of natural broadening is [124], Section 7.1.5:

$$\sigma_a(E) = \frac{B_{mn}E_c}{c} \frac{\gamma h}{(E - E_c [1 + v/c])^2 + \gamma^2}$$
(4.4)

Here  $E_c$  is the line-centre energy,  $B_{mn}$  is the second Einstein coefficient for induced transition from level *m* to level *n*, *v* is the projection of the velocity of absorber **v** to the velocity of the photon:

$$v = \frac{\left(\mathbf{v} \cdot \mathbf{v}_{ph}\right)}{c} \tag{4.5}$$

Factor [1 + v/c] describes the Doppler shift. This cross-section has to be averaged over the velocity distribution of the absorber. In case of shifted Maxwellian distribution this yields the integral, see [124], Section 7.1.6:

$$\sigma_{a}(E) = \frac{B_{mn}E_{c}h}{c} \int_{-\infty}^{\infty} \frac{\gamma}{\left(E - E_{c}\left[1 + v/c\right]\right)^{2} + \gamma^{2}} \frac{1}{\sqrt{\pi}v_{T}^{2}} \exp\left(-\frac{\left(v - u\right)^{2}}{v_{T}^{2}}\right) dv =$$

$$= \left|\xi = \frac{v - u}{v_{T}}\right| = \frac{B_{mn}E_{c}h}{\sqrt{\pi}c} \int_{-\infty}^{\infty} \frac{\gamma \exp\left(-\xi^{2}\right)}{\left(E - E_{c}\left[1 + v_{t}\xi/c + u/c\right]\right)^{2} + \gamma^{2}} d\xi =$$

$$\frac{B_{mn}E_{c}h}{\sqrt{\pi}c\Delta_{D}} \int_{-\infty}^{\infty} \frac{\frac{\gamma}{\Delta_{D}}\exp\left(-\xi^{2}\right)}{\left(\frac{E - E_{c}\left[1 + u/c\right]}{\Delta_{D}} + \xi\right)^{2} + \left(\frac{\gamma}{\Delta_{D}}\right)^{2}} d\xi = \frac{B_{mn}E_{c}h}{\sqrt{\pi}c\Delta_{D}} \left[W\left(\frac{E - E_{d}}{\Delta_{D}}, \frac{\gamma}{\Delta_{D}}\right)\right]$$

$$(4.6)$$

Here  $v_T$  and  $\Delta_D$  are the thermal velocity and the Doppler width:

$$v_T = \sqrt{\frac{2kT}{M}}, \qquad \Delta_D = \frac{E_m}{c} v_T$$
 (4.7)

*T* is the temperature of atoms, *M* is the mass of atom. *u* is is the projection of the (average) drift velocity of absorber **u** on the velocity of photon (formula (4.5)).  $E_d$  is the line-centre energy corrected for the Doppler shift:

$$E_d = E_c \left[ 1 + \frac{u}{c} \right] = E_c \left[ 1 + \frac{(\mathbf{v}_{ph}, \mathbf{u})}{c^2} \right]$$
(4.8)

The integral (4.6) is expressed in terms of the complex error function (Faddeeva function) W(x, y), see e.g. [127], Chapter 7:

$$W(x,y) = W(z = ix - y) = e^{z^2} \cdot \left[1 - \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt\right] = e^{z^2} \cdot [1 - \operatorname{Erf}(z)]$$
(4.9)

Line	$Ly_{\alpha}$	$Ly_{\beta}$	$Ly_{\gamma}$	$H_{\alpha}$	$H_{\beta}$
Transition	$1 \rightarrow 2$	$1 \rightarrow 3$	$1 \rightarrow 4$	$2 \rightarrow 3$	$2 \rightarrow 4$
$b_{mn}, 10^{-15} cm^2 \sqrt{\frac{eV}{amu}}$	54.7	8.76	3.05	454	328

Table 4.2: Coefficients of the approximate formula (4.12)

As was already mentioned, for the condition of a large divertor plasma the Lorentzian part is negligible. This general formula is used in the code to keep the possibility to extend the treatment for the case where the Lorentzian and Doppler parts are equally important. For the case in question one can take into account only the Doppler broadening for the central part of the line, but at the wings the Lorentzian part has to be taken into account anyway, see [124], Chapter 7.1.6.

To take into account the Zeeman splitting the sum over the line centre energies defined by relations (4.1) with corresponding weights P(m) has to be calculated. Each term in this sum is calculated for the centre energy corrected for both Doppler shift (4.8) and Zeeman splitting (4.1). The final result is:

$$\sigma_a(E) = \frac{B_{mn}E_ch}{\sqrt{\pi}c\Delta_D} \sum_{k=-1,0,1} \left( Re\left[ W\left(\frac{E-E_{zd}}{\Delta_D}; \frac{\gamma}{\Delta_D}\right) \right] \cdot P(k) \right)$$
(4.10)

$$E_{zd} = E_c \left( 1 + \frac{\left( \mathbf{v}_{ph} \cdot \mathbf{u} \right)}{c^2} \right) + k \cdot \mu_B B$$
(4.11)

Here  $E_c$  is the initial ("unperturbed") energy of transition.

There is no model for photon-wall interaction in the code at the moment: it is assumed that all incident photons are absorbed.

Comparison of the absorption profile obtained using Formula (4.11) with the sampled emission profile serves as a numerical test of the implementation: for uniform conditions the emission and absorption profiles must be the same. Some other tests which were used for the photon transport model are described in [47]: reproducing the Plank profile for thermodynamical equilibrium and escape factors in cylinder geometry.

The computational experience shows that the self-consistent solution for plasma parameters is insensitive to the details of the radiation transport treatment because of the high opacity (a similar conclusion was made in [119]). More accurate treatment of emission and absorption profiles can be important for devices with lower opacity than ITER and for the analysis of diagnostic signals.

If  $\mathbf{B} = 0$  and  $\mathbf{u} = 0$  (neither magnetic field, nor drift) then from the Equation (4.11) one can get a simple estimate of the absorption cross-section at the line centre (maximum cross-section):

$$\sigma_a^{max}(E) = \frac{B_{mn}E_ch}{\sqrt{\pi}c\Delta_D} = \frac{c^3h^3}{8\pi\sqrt{2\pi}}\frac{g_n}{g_m}\frac{A_{nm}}{E_c^3}\sqrt{\frac{M}{T}} = 3.091 \cdot 10^{-20}\frac{g_n}{g_m}\frac{A_{nm}}{E_c^3}\sqrt{\frac{M}{T}} = b_{mn}\sqrt{\frac{M}{T}}$$
(4.12)

To get the final relation it was taken into account that for the line centre W(0, y) = 1 (assuming  $y \ll 1$ , thus neglecting the natural broadening),  $\Delta_D$  was substituted from (4.8), and  $B_{mn}$  was expressed through  $A_{nm}$  using Einstein relation:

$$B_{mn} = \frac{g_n}{g_m} \frac{c^3 h^2}{8\pi E_m^3} A_{nm}$$

where  $g_m$ ,  $g_n$  are statistical weights of the initial and final states respectively. In the formula (4.12) with numerical coefficient *T* is in eV, *M* is in amu and the cross-section is calculated in cm<sup>2</sup>. The constants  $b_{mn}$  for some lines are shown in Table 4.2. The numerical value of  $b_{mn}$  corresponds to the maximal absorption cross-section for hydrogen (M = 1) for T = 1 eV.

Table 4.2 shows that already for an atom density  $10^{13} cm^{-3}$  the Mean Free Path (MPF) for  $Ly_{\alpha}$  is only 2 cm. The absorption cross-section for  $Ly_{\beta}$  is only 6 times smaller. For the ITER divertor conditions: densities  $10^{14} cm^{-3}$  and larger on a characteristic special scale 1 cm, both those lines are expected to be opaque. For  $H_{\alpha}$  and  $H_{\beta}$  lines  $b_{mn}$  is more than an



Figure 4.1: Profiles of the photon absorption cross-section for two lines of Deuterium in a gas without drift velocity and with temperature 1 eV, magnetic field 6 Tesla. Two curves correspond to the photons which incident along  $(\mathbf{v}_{ph} || \mathbf{B}_{ph})$  and perpendicular  $(\mathbf{v}_{ph} \perp \mathbf{B}_{ph})$  to the magnetic field. Abscissa is the photon energy shifted by the line-centre energy  $E - E_c$ 

order of magnitude larger than for the Lyman lines. Therefore, it is possible that the lines of the Balmer series are effectively re-absorbed as well, because the relative population of the n = 2 level for the conditions in question is  $10^{-4} .. 10^{-3}$ , see below in Figure 4.4. The absorption of Balmer lines is not taken into account in the current model.

The figures shown in Table 4.2 are the maximal absorption cross section at the line centre. At the wings of the line the absorption probability rapidly decreases. An example of  $\sigma_a(E)$  profile for  $Ly_{\alpha}$  and  $Ly_{\beta}$  lines of Deuterium is shown in Figures 4.1. The profiles are calculated for a gas without drift, with temperature of 1 eV and magnetic field 6 Tesla using Formula (4.11). The two curves correspond to different directions of the photon velocity: photons which incident along ( $\cos \theta = 1$  in Equations (4.1)) and perpendicular (( $\cos \theta = 0$ ) to magnetic field. The Zeeman effect results in a profile with two maxima. As expected, Table 4.1, the splitting due to Zeeman effect is roughly half of the Doppler width.

#### 4.2.2 Photo-induced ionization

The ionization from the photo-excited states is taken into account through a correction to the effective ionization rate. This extra effective ionization is called here the "photo-induced" ionization. In the model described below it will be assumed that the transport of the excited states is negligible and that they do not experience any kinds of heavy particle collisions, - the assumptions commonly made for Collision Radiative Models (CRM).

The characteristic transport time-scale of recycled atoms is  $10^{-6} s$  (see e.g. the direct estimation in Section 3.3.2). It can be easily shown that the life time of the electronically excited levels of a hydrogen atom is much shorter. Indeed, the rate of radiative decay of the n = 2 level yields a maximum life time  $1/A_{21} = 2 \cdot 10^{-9} s$ , for level n = 3 it is  $2 \cdot 10^{-8} s$  and for level n = 4 it is  $10^{-7} s$ . But already in the case n = 3 the ionization rate for  $T_e = 1 \ eV$  is  $4 \cdot 10^{-7} \ cm^3/s$ . That means that even for  $n_e = 10^{14} \ cm^{-3}$  the life time regarding this process is  $2.5 \cdot 10^{-8} s$  (the numbers for the estimates are taken from [64]). Therefore, the life-time of the excited states, limited either by the spontaneous radiative decay or by ionization is by two orders of magnitude shorter than the transport time scale. In this way the assumption of neglecting the transport of excited states is justified.

Neglecting the heavy-particle collisions is a somewhat stronger assumption. In Section 3.1.3 it was shown that the collision rate of the charge-exchange for temperatures around 1 eV is approximately  $10^{-8} \ cm^3/s$ . For densities ~  $10^{15} \ cm^{-3}$  which can be found in front of the targets, this implies collision time ~  $10^{-7} \ s$ . The rate of charge-exchange of the excited states can be much higher than that of the ground state: it scales as  $n^4$  with the principal quantum number [122]. That means that the charge-exchange of excited states may have the same time-scale as their life time.

The derivation of a CRM which takes into account charge-exchange collisions (assuming velocity independent collision rates) was shown by Krasheninnikov et al. in [123]. In the presented work all kinds of heavy particle collisions for excited states were neglected.

However, the approach of paper [123] will be used to show the rigorous way of deriving a CRM from kinetic equation.

Taking into account the assumptions made, the kinetic equation for one excited state reads:

$$\left(\left|\sum_{q>p} C_{pq} + \sum_{qp} F_{qp} n_e f_q - \sum_{q>p} A_{qp} n_q = R_p n_e f^+ + \left(C_{1p} n_e + B_{1p} n_{ph}^{1p}\right) f_1$$
(4.13)

Here  $f_p(\mathbf{v})$  is the velocity distribution function of the atomic excited state,  $f^+(\mathbf{v})$  is that for ions,  $n_e$  is the electron density, *C* is the rate of electron-impact excitation, *F* is the electronic de-excitation, *A* is the spontaneous radiative decay, *S* is the ionization, *R* is the recombination, *B* is the photo-excitation. The subscript pq denotes transition from level pto level q, p alone denotes transition to (from) continuum, 1 stands for the ground state;  $n_{nb}^{1p}$  is the number density of photons corresponding to transition  $1 \rightarrow p$ .

The velocity distribution of excited states, produced either due to excitation from the ground state, or due to recombination, is not perturbed by any collisions. Therefore, the distribution function  $f_p$  can only be a linear combination of  $f_p$  and  $f^+$ :

$$f_p(\mathbf{v}) = n_p^1 \hat{f}_p(\mathbf{v}) + n_p^+ \hat{f}^+(\mathbf{v}) = r_p^1 n_1 \hat{f}_p(\mathbf{v}) + r_p^+ n^+ \hat{f}^+(\mathbf{v})$$
(4.14)

Here  $\hat{f}$  denotes the distribution normalized to the corresponding density,  $r_p^1$  and  $r_p^+$  are the population factors. Further they will be called "the population coupled to ground state" and "the population coupled to continuum" respectively. Substituting (4.14) into (4.13) yields two sets of linear algebraic equations for  $r_p^1$  and  $r_p^+$ :

$$M\{r_p^1\} = C_{1p}n_e + B_{1p}n_{ph}^{1p}, \quad M\{r_p^+\} = R_pn_e$$
(4.15)

Here the following matrix operator is introduced (in this definition  $r_p$  is a vector):

$$M\{r_{p}\} = \left( \left[ \sum_{q > p} C_{pq} + \sum_{q < p} F_{pq} + S_{p} \right] n_{e} + \sum_{q < p} A_{pq} \right) r_{p} - \sum_{1 < q < p} C_{qp} n_{e} r_{q} - \sum_{q > p} F_{qp} n_{e} r_{q} - \sum_{q > p} A_{qp} r_{q}$$
(4.16)

The kinetic equation for the ground state reads:

$$\frac{df_1}{dt} = -\left[S_1 + \sum_{p>1} \left(C_{1p} + B_{1p} n_{ph}^{1p}\right)\right] n_e f_1 + \sum_{p>1} \left(F_{p1} n_e + A_{p1}\right) f_p + R_1 n_e f^+ = \\ = -\left\{\left[S_1 + \sum_{p>1} \left(C_{1p} + B_{1p} n_{ph}^{1p}\right)\right] - \sum_{p>1} \left(F_{p1} + \frac{A_{p1}}{n_e} + \right) r_p^1\right\} n_e f_1 + \left\{\sum_{p>1} \left(F_{p1} n_e + A_{p1}\right) r_p^+ + R_1\right\} f^+ \quad (4.17)$$

Here  $\frac{df_1}{dt}$  denotes the transport and all processes which are not related to electron-impact collisions: heavy particle collisions, collisions with wall etc. From the form of Equation (4.17) it can be readily seen that:

$$S(T_e, n_e) = \left[ S_1 + \sum_{p>1} \left( C_{1p} + B_{1p} n_{ph}^{1p} \right) \right] - \sum_{p>1} \left( F_{p1} + \frac{A_{p1}}{n_e} \right) r_p^1$$
(4.18)

is the effective ionization rate, and:

$$R(T_e, n_e) = \sum_{p>1} \left( F_{p1} n_e + A_{p1} \right) r_p^+ + R_1$$
(4.19)

is the effective recombination rate. Population factors are found from the solution of algebraic equations (4.15). Therefore, *S* and *R* are functions of  $n_e$  and  $T_e$ .

The rates  $S(T_e, n_e)$  and  $R(T_e, n_e)$  can be also obtained considering the kinetic equation for ions:

$$\frac{df^{+}}{dt} = S_1 n_e f_1 + \sum_{p>1} S_p n_e f_p - \left(\sum_p R_p\right) n_e f^{+} = \left[S_1 + \sum_{p>1} S_p r_p^1\right] n_e f_1 - \left[\sum_p R_p - \sum_{p>1} S_p r_p^+\right] n_e f^{+} \quad (4.20)$$

This yields:

$$S(T_e, n_e) = S_1 + \sum_{p>1} S_p r_p^1, \quad R(T_e, n_e) = \sum_p R_p - \sum_{p>1} S_p r_p^+$$
(4.21)

The reaction rates obtained using Formulas (4.18), (4.19) and Formulas (4.21) must be equal. This fact provides a numerical test of the calculated effective rates S and R.

The Collision-Radiative Model which is expressed by Equations (4.15), (4.18), (4.19). In this work CRM of Sawada and Fujimoto was applied [41] to calculate the effective rates (extended to include the photo-excitation). It is the same model and the same code as in Section 3.2.

The population coupled to ground state can be split into two parts  $r_p^1 = r_p^e + r_p^{ph}$ .

$$M\{r_p^e\} = C_{1p}n_e, \quad M\{r_p^{ph}\} = B_{1p}n_{ph}^{1p}$$
(4.22)

The part  $r_p^e$  may be called "the population due to the electron impact excitation" and  $r_p^{ph}$  is "the population due to the photon-impact excitation". The effective ionization rate can be split accordingly:

$$S = S^{e} + S^{ph}$$

$$S^{e} = \left[S_{1} + \sum_{p>1} C_{1p}\right] - \sum_{p>1} \left(F_{p1} + \frac{A_{p1}}{n_{e}}\right) r_{p}^{e} = S_{1} + \sum_{p>1} S_{p} r_{p}^{e}$$

$$S^{ph} = \sum_{p>1} B_{1p} n_{ph}^{1p} - \sum_{p>1} \left(F_{p1} + \frac{A_{p1}}{n_{e}}\right) r_{p}^{ph} = \sum_{p>1} S_{p} r_{p}^{ph}$$
(4.23)

Here  $S^e$  is the "ordinary" optically thin ionization and  $S^{ph}$  is the additional effective ionization rate due to absorption of radiation. It is called here "the photo-induced" ionization.

Another approach is often used to take into account the influence of absorption of line radiation on the ionization-recombination balance, see e.g. [113, 119, 125]. If one considers the sum of the balance equations (4.15) and transfers the photon absorption rates  $B_{pq}n_{ph}^{pq}$  to the left hand side, then one can introduce the so called radiation escape probability factor  $P_{esc}^{p}$ :

$$A_{pq}r_p - B_{pq}n_{ph}^{pq} = A_{pq}r_p \left(1 - \frac{B_{pq}n_{ph}^{pq}}{A_{pq}r_p}\right) = A_{pq}r_p P_{esc}^p, \quad P_{esc}^p = 1 - \frac{B_{pq}n_{ph}^{pq}}{A_{pq}r_p}$$
(4.24)

The coefficient  $P_{esc}^p$  is thus the fraction of the radiation which is not re-absorbed. This transformation yields to a set of linear equations, similar to (4.15), without photo-excitation term but with a modified matrix M. This matrix defines now the so-called kinetics with suppressed radiative transition. The equation can be split into ionization and recombination parts:

$$M\{r_r^{(1,op)}\} = C_{1p}n_e, \quad M\{r_p^{(+,op)}\} = R_pn_e$$
(4.25)

Population factors  $r_p^{(1,op)}$  and  $r_p^{(+,op)}$  obtained by solving this set of equations can be substituted then into Formulas (4.18), (4.19) or (4.21). The resulting effective ionization and recombination rates  $S^{op}$  and  $R^{op}$  will be called here "the opaque rates". The "opaque rates" for hydrogen atom calculated on assumption of total opacity ( $P_{esc}^p = 0$ ) are shown in Figure 4.2a. For comparison, the corresponding "optically thin" rates are shown in Figure 4.2b. The recombination rate  $R^{op}$  is more than an order of magnitude lower than in the optically thin case.

The opaque rates are different from the rates *S* and *R* calculated before. The relation between these rates can be found from the condition that both approaches must yield the same net particle source in the continuity equation, and therefore:

$$Rn^{+} - Sn_{1} = R^{op}n_{+} - S^{op}n_{1}, \quad S = S^{op} + (R - R^{op})\frac{n^{+}}{n_{1}}$$
(4.26)

Here  $n^+$  and  $n_1$  are the ion and atom (ground state) density. Two special cases of this relation are shown in Figure 4.3. In case of zero recombination  $S = S^{op}$ . And if the "opaque" ionization is completely balanced by the "opaque" recombination, then:

$$R^{op}n_{+} = S^{op}n_{1}, \quad S = S^{op}\frac{R}{R^{op}}$$
(4.27)



Figure 4.2: "Opaque" (a) and "optically thin" (b) rates for hydrogen atom calculated with CRM [41]. Numbers in the legends are the electron densityes in cm<sup>-3</sup>. For "opaque" rates total suppression of the radiative transitions was assumed ( $P_{esc}^{p} = 0$ )

The rates shown in Figure 4.3 are calculated on assumption of the complete opacity. The optically thin ionization is shown in the same figure for comparison. For temperatures below 5 eV the "equilibrium rate" (4.27) is more than an order of magnitude higher than the optically thin rate. It is the same effect as shown in Figures 4.2. The difference is smaller for higher densities where the electron-impact excitation becomes stronger. Note also that the "optically thick" rates are much less sensitive to the electron density.



Figure 4.3: The "equilibrium" effective ionization rate, Formula (4.27), the "opaque" ionization rate and the optically thin ionization rate

The approaches of using "the photo-induced ionization rate" or "the opaque rates" are completely equivalent only in terms of the continuity equation. In terms of the kinetic equation they are equivalent only if velocity distribution functions of ions and atoms are equal. The reason is that "opaque" rates assume in fact that recombining atoms have the same VDF as ions. This assumption is correct in general only if the time scale of the excitation of ground state is shorter than that for the transport and the elastic collisions. The approach of photo-induced ionization is more general. As it was shown before, it is strictly correct in terms of the kinetic equation within the assumptions taken for CRM. However, for the conditions of an ITER-like divertor plasma this difference is not important because the ions and atoms have almost the same velocity distribution as it is shown in Section 3.3.2.

Figures 4.4 show the comparison of the relative population of two excited levels (n = 2 and n = 3) calculated either with assumption of an optically thin system, or using the model with a full suppression of radiative transitions. In both cases (optically thin and completely opaque) the population of the n = 2 level coupled to ground state reaches  $10^{-3}..10^{-2}$  for temperature around 10 eV and the population coupled to continuum can be  $10^{-4}..10^{-3}$  for the temperature below 1 eV. For the n = 3 level these figures are roughly an order of magnitude lower. Like for the ionization rate, the effect of the radiation opacity is weaker for a higher density.

The extra electron energy loss due to photo-induced ionization  $S_{E}^{ph}$  can be calculated



Figure 4.4: Relative population of the levels n = 2 and n = 3 coupled to ground state (in red) and to continuum (in blue) calculated on assumption of an optically thin system and for the case of total opacity.



Figure 4.5: The electron energy loss per one ionization event for the optically thin case (blue) and extra energy loss for the effective ionization due to absorption of  $Ly_{\alpha}$  photons (red).

as:

$$S_{E}^{ph} = \sum_{p} S_{p} \Delta E_{p} r_{p}^{ph} + \sum_{p} \sum_{q > p} C_{pq} \Delta E_{pq} r_{p}^{ph} - \sum_{p > 1} \sum_{q < p} F_{pq} \Delta E_{pq} r_{p}^{ph} =$$
  
=  $S_{1}E_{0} + \sum_{p > 1} \sum_{q < p} A_{pq} \Delta E_{pq} r_{p}^{ph} - \sum_{p > 1} B_{1p} n_{ph}^{1p} \Delta E_{1p},$   
 $r_{1} = 1, \quad E_{1} = 0, \quad \Delta E_{p} = E_{0} - E_{p}, \quad \Delta E_{pq} = |E_{p} - E_{q}|$  (4.28)

where  $E_p$  is the energy of the level p,  $E_0 = 13.6 eV$  is the ionization energy. The energy loss per one ionization event (that is  $S_E^{ph}/S^{ph}$ ) in the case if where only  $Ly_{\alpha}$  line is absorbed is shown in Figure 4.5. It does not depend on the photon absorption rate because the population factors for any specific line  $r_p^{ph}$  in both Formulas (4.23) and (4.28) are proportional to this rate. For the temperature below 1 eV the energy loss is negative. This means that the electrons effectively gain energy due to de-excitation from the photo-excited states. The energy loss for the "optically thin" ionization is shown on the same figure.

Power balance for ionization and recombination of atoms can serve as a run-time consistency check of the implementation. This balance reads:

$$S^{E} - E_{0}S^{N} = \sum_{p} \sum_{q} A_{pq}E_{pq}n_{1}r_{p} - \sum_{p} \sum_{q} B_{qp}E_{qp}n_{qp}^{ph} + \beta$$
(4.29)

Here  $S^E$  is the total energy loss of electrons for ionization of atoms,  $S^N$  is the total sink of atoms,  $\beta$  is the energy loss due to radiative recombination, other notations are the same as for Formula (4.28).  $S^E$  and  $S^N$  include both ionization and recombination (with corresponding signs). The right hand side of this equation is the radiated energy calculated directly. This balance is valid not only globally but for each control volume as well, e.g for each cell of the computational grid. For practical purposes it is not necessary to calculate the right hand side of Equation (4.29) exactly. It is enough to take only the photons whose transport is taken into account explicitly: in all studied cases the contribution of  $Ly_{\alpha}$  and  $Ly_{\beta}$  to the global balance is dominant.

The relation (4.29) can be used to calculate the radiation energy heat flux  $q_{rad}$ :

$$\operatorname{div}(q_{rad}) = Q_E - Q_A = S^E - E_0 S^N$$
(4.30)

Here  $Q_E$  is the volume source of emitted radiation energy and  $Q_A$  is the absorbed radiation energy. The Equation (4.30) shows that  $q_{rad}$  can be calculated in the same way as for the optically thin case using the difference  $S^E - E_0 S^N$  as the volume source of the radiated energy. It automatically takes into account the absorption. The radiation heat loads are calculated in B2PLOT in exactly this way which is thus correct for the optically thick case without modification.

Technical aspects of the implementation of the radiation transport coupled to CRM in B2-EIRENE code are described in Appendix A.5.

#### **4.3** The effect for the ITER divertor plasma

A series of calculations was performed for the ITER set-up described in Section 1.3. The initial model corresponds to the case ITER 1055 with full molecular kinetics and neutral-neutral collisions. The model was updated with the transport of the 5 first Ly-lines ( $\alpha$ .. $\delta$ ) coupled with CRM as described in the previous sections.

Two cases, referred below as the LP and HP cases, are considered in detail. The calculations with updated model are compared to the cases with a similar average divertor pressure. The LP (Low Pressure) case is the case with  $S_{puff} = 10 \cdot 10^{22} s^{-1}$ ,  $P_{PFR} = 7.0 Pa$  (Case 1055p1). It is compared with a case without photon trapping and with :  $S_{puff} = 7.6 \cdot 10^{22} s^{-1}$ ,  $P_{PFR} = 6.4 Pa$  (Case 1049). The HP (High Pressure) case has  $S_{puff} = 17 \cdot 10^{22} s^{-1}$ ,  $P_{PFR} = 10.7 Pa$ (Case 1055p3) and compared with a case with  $S_{puff} = 15.3 \cdot 10^{22} s^{-1}$ ,  $P_{PFR} = 11.3 Pa$  (Case 1055).

Trapping of photons can significantly increase the ionization source in the low temperature regions with high neutral density. Here and below "low temperature" means  $T_e < 2 \ eV$ . These regions in the inner and outer divertors are shown in Figure 4.6. The picture is made for the HP case. The filled domain there is the region where the photo-induced ionization rate exceeds the ordinary ionization (due to the electron impact only). It corresponds approximately to the domain with  $T_e < 2eV$  and with atom density  $n_D > 5 \cdot 10^{14} \text{ cm}^{-3}$ .



Figure 4.6: The regions in the inner and outer divertors for which the photo-induced ionization is greater than the ordinary ionization. Dashed line is the isotherm with  $T_e = 2 \ eV$ , solid line is the contour of constant atom density  $n_D = 5 \cdot 10^{14} \ cm^{-3}$ 

The extra particle source due to photo-induced ionization increases the plasma density in this region. The high density  $(n_e > 10^{15} \text{ cm}^{-3})$  region extends further towards the low temperature area, Figures 4.7, 4.8. The maximum electron density in the inner divertor rises by almost a factor two, Figure 4.7. The dominant recombination mechanism there is the 3-body recombination, which scales as ~  $n_e^3$ , whereas ionization scales approximately as ~  $n_e^2$ . As a result, the recombination source rises more strongly with density, compensating the extra photo-induced ionization source. It is predominantly the recombination source rather than the target recycling source that balances the increase of the ionization sources due to photon trapping, Figure 4.10.

The effect of photon trapping is stronger for the inner divertor where the plasma is cooler, although it can be seen in the outer divertor as well, Figure 4.10, Table 4.3. Figures 4.8 show that the increase of the plasma density is accompanied by a decrease of the temperature in front of the targets. The neutral density for a given  $P_{PFR}$  becomes higher,

following the increase of the plasma density, Figure 4.9. The degree of ionization does not change significantly, compare Figures 4.7 and 4.9. This may be due to a mitigation of the neutral diffusion (reduction of the diffusivity) from the targets to the channel underneath the dome because of the higher plasma density. Qualitatively a similar effect (increase of the plasma density and reduction of temperature near the target) was obtained in 1D modelling by Adams and Scott [119, 120]. They associated this with the shift in the balance of ionization and recombination to lower temperatures as the optical thickness increases.



Figure 4.7: Electron density near the inner target with (solid line) and without (dashed line) photo trapping. Dotted line is the result obtained with "totally opaque" rates. *x* is the (poloidal) distance from the target.

The global opacities and the contribution from individual lines to the total ionization sources are shown in Table 4.3. The main contribution to the total photo-induced ionization source is from the  $Ly_{\alpha}$  ( $\approx 90$  %) and  $Ly_{\beta}$  (the remaining  $\approx 10$  %) lines, and the effect of higher levels is negligible. A similar result was reported in [119, 125] and [117]. The global opacity for  $Ly_{\alpha}$  line is around unity (> 75 %) even for the LP case. The data in Table 4.3 suggest that higher lines (n > 3) can be neglected in the modelling for ITER conditions.

Table 4.4 shows the total population of individual excited levels in the inner and outer



Figure 4.8: Electron temperature near the inner target with (solid line) and without (dashed line) photon trapping. Dotted line is the result obtained with "totally opaque" rates. x is the (poloidal) distance from the target.



Figure 4.9: Neutral density near the inner target with (solid line) and without (dashed line) photon trapping. x is the (poloidal) distance from the target.

divertors associated with different populating mechanisms. The population originating from the ground state was calculated by CRM for a fixed plasma background with given photon absorption rates. Populations due to recombination of  $D^+$  and dissociation of  $D_2$ and  $D_2^+$  were calculated using the population factors from [106] (similar to that shown in Figures 4.4). The two latter mechanisms were not taken into account for the photon sources in the B2EIRENE modelling. According to Table 4.4, the main populating mechanism for the level n = 2 is the excitation of the ground state. For higher levels (n > 2) the recombination channel prevails. Population due to dissociation of  $D_2$  is negligible, because of very low relative population of D(n) originating from  $D_2$  in low temperature domain. The relative population of D(n) originating from  $D_2^+$  can be rather high (~ 10<sup>-3</sup>, the highest ratio is for n = 3). The corresponding processes were considered in Section 3.2.3. But the obtained density of  $D_2^+$  in the region in question is low ( $10^{10}..10^{12} \text{ cm}^{-3}$ ) and even for level n = 3it can support less than 10 % of the total population. This mechanism would be more important if the density of  $D_2^+$  was higher, which is the case e.g. in linear devices [126]. Transitions due to the absorption of Balmer series photons could increase the population of n = 3 level as well.

The figures in Table 4.3 suggest that the ITER divertor is almost completely opaque for the hydrogen line radiation. Therefore, it is plausible to assume that the modelling with ionization and recombination rates calculated with totally suppressed spontaneous transitions (see Formulas (4.26) in Section 4.2.2) will give approximately the same result as with explicit transport of photons. Such calculations were made for the cases with the same set-up as ITER1055p1 and ITER1055p3. The results are shown in Figures 4.7, 4.8 with dotted lines. As expected, the difference is not very large. The difference is small because for the ITER divertor most of the atoms are ionized in "optically thick" conditions.



Figure 4.10: Principal sources and sinks of D atoms in the inner (dark bars) and outer (open bars) divertors without (left side) and with (right side) photon trapping. R is the target recycling sources, VR is the volume recombination, I is the total ionization sources,  $I_{ph}$  is the photo-induced ionization sources.

	Opac	Opacity (absorbed/emitted), % Contribution to ionization, %						on, %	
Line	LP-	case	HP-	case	LP-	LP-case		HP-case	
	Inner <sup>1</sup>	Outer <sup>1</sup>	Inner <sup>1</sup>	Outer <sup>1</sup>	Inner <sup>1</sup>	Outer <sup>1</sup>	Inner <sup>1</sup>	Outer <sup>1</sup>	
Total <sup>2</sup>	—	—	—		66	28	80	54	
$Ly_{\alpha}^{3}$	96	79	98	90	88	90	88	88	
$Ly_{\beta}$ <sup>3</sup>	84	58	90	77	9.1	7.8	9.2	9.2	
$Ly_{\gamma}^{3}$	76	46	84	66	2.0	1.4	2.1	1.9	
$Ly_{\delta}^{3}$	65	35	75	56	0.64	0.40	0.72	0.61	
$Ly_{\epsilon}^{3}$	55	25	67	43	0.36	0.14	0.31	0.23	

Table 4.3: Opacity and ionization related to individual lines

<sup>1</sup> Integrals over the inner and outer divertors

<sup>2</sup> Contribution of the photo-induced ionization to the total ionization source

<sup>3</sup> Contribution of the individual lines to the photon-induced ionization source

For other parameters (lower densities) it can be that most of the atoms are ionized in "optically thin" conditions. In this case one has to distinguish at least two kinds of the ionization rates: "totally opaque" for one region and "optically thin" for another one. The (crude) role of taking into account the photon transport in EIRENE is in fact in finding the boundary between these two regions "automatically" without enforcing it by some external assumptions.

Practically all the calculations for ITER done in this work were performed on identical computational grid (28 radial and 74 poloidal cells, 12 cells in each divertor, 8 rings in the core) to exclude possible discretisation effects when comparing the different physical models, as well as for performance reasons. One test calculation was made for the same set up as the case ITER 1055p1 but with a finer grid. The refined grid had 96 poloidal and 36 radial cells, 24 poloidal cells in the inner divertor and 22 poloidal cells in the outer divertor. Therefore, doubling the poloidal resolution in the divertors.

The resulting plasma profiles in the divertor region have similar shape but the numbers can be somewhat different. Some examples are shown in Figures 4.11. These figures present distributions of some parameters along selected flux surfaces which are denoted by their distance from separatrix along the target *y*. For the temperature, the selected flux surface was the flux surface of the maximum incident heat flux. For the densities: the flux surfaces where the maximum of the electron density is reached.

The strongest difference can be seen for the densities, especially at the inner target, Figure 4.11b. The position of the maximum and the density drop are poorly resolved even with the refined grid. The same can be seen for the atom density, Figure 4.11c. However, the shape of the profile is similar in both cases. The effect is smaller for the outer target because the density peaking is less pronounced, Figures 4.11e, 4.11f. The

Population (%)		LP-	case				HP-ca	ase
originated from: <sup>1</sup>	D(1s)	$D^+$	$D_2$	$D_2^+$	D(1s)	$D^+$	$D_2$	$D_2^+$
n = 2, Inner	84	15	0.04	0.61	80	20	0.02	0.54
n = 2, Outer	88	10	0.43	1.6	83	16	0.14	0.85
n = 3, Inner	27	70	0.03	3.0	21	77	0.02	2.3
n = 3, Outer	35	56	0.39	8.0	26	70	0.14	4.0
n = 4, Inner	5.7	93	0.01	1.1	4.0	95	0.01	0.77
n = 4, Outer	9.6	87	0.16	3.5	5.7	93	0.05	1.5

Table 4.4: Comparison of the different mechanisms of populating the excited levels

<sup>1</sup> Fraction of the total population of excited state in the inner and outer divertors

difference observed for the temperature profile is much smaller: for the outer target the profile almost does not change, Figure 4.11d and for the inner target the same problem of resolving the position of the drop as for the densities is seen.

Despite observed differences in the poloidal profiles, the parameters in front of the targets calculated with different grids are not much different, Figure 4.12. No significant difference was found for the global particle and energy sources (total ionization, recombination etc.), neither as for the operational parameters of the divertor, see below in Section 5. The conclusion may be that it is desirable to make calculations with finer greed for the detached plasma where strong gradients in poloidal direction are observed. The relatively coarse grid is still used for the modelling because the finer grids needs more time for calculations and reduces numerical stability. However, the main features of the system and principal output parameters are found to be not very sensitive to the grid size.



Figure 4.11: Electron temperature and the density of electrons and atoms along selected flux surfaces in the inner and outer divertors calculated on the standard-size and refined grid. *y* is the radial coordinate of the flux surface (at the target). "Distance along separatrix" is the poloidal projection



Figure 4.12: Electron temperature and density in front of the targets and the total incident heat flux calculated on standard-size and refined grid.

## **Chapter 5**

## Impact on the ITER modelling

The main engineering output of the modelling are the parameters which characterise the effectiveness of impurity pumping and the target heat loads. As it was already mentioned in Section 1.3, extensive simulations made with B2-EIRENE code show that the principal parameter for the scaling is the neutral gas pressure in the divertor [50, 66, 68, 69]. Here it is represented by the average pressure at the edge of the Private Flux Region.

Four series of calculations with different models were performed for the ITER set up described in Section 1.3. The gas puffing rate was varied to obtain the pressure scans. The results are shown in Figures 5.1- 5.5. The first series was calculated with the old EIRENE 1996 model (calculations made by A. Kukushkin, ITER IT, Garching). It is shown in blue dashed lines. In the second series the Neutral-Neutral Collisions (NNC), Chapter 2, were added (green line with triangles). Series number three is the series with NNC and improved Molecular Kinetics (MK), Chapter 3, which is the standard model for ITER at the moment [50]. It is shown in red solid lines with diamonds. Finally, the photon transport coupled with CRM, Chapter 4, was added to this standard model: black solid lines with squares. In addition, the two points with totally opaque rates (solid black points) and the point obtained with refined grid (red circle) are shown in the figures as well, see Section 4.3.

The parameteres of the effectiveness of impurity pumping are shown in Figure 5.1. The effective charge at the separatrix, Figure 5.1a, does not change much for the different models. It is somewhat higher than the limit 1.6 (see Section 1.3) but does not exceed 2. The separatrix concentration of He, Figure 5.1b, becomes somewhat higher for the model with full molecular kinetics. But it still can be pushed well below the constrain 6 % for the high neutral pressures, Figure 5.1b. The radiation opacity decreases this concentration for the lower densities as well, possibly because of the high divertor densities, see Figures 4.7, 4.9, Section 4.3.

The peak incident heat flux density for the inner and outer targets is shown in Figures 5.2. Adding the NNC and then improved MK increases those peaks for the same neutral pressure compared to the old model. This can be also described as a shift of the scalings towards higher pressure. The shift can be explained by the fact that in the new model the temperature of molecules is much higher. Therefore, the same neutral pressure is achieved for the lower neutral density. A similar but less pronounced shift can be seen in Figure 5.1b as well. The increase of the neutral pressure reduces the heat flux. But even for the pressures almost twice as high as before (for the old model) the peak outer heat flux density is a factor of 2 higher than in the the old model: 4 MW/m<sup>2</sup> instead of 2 MW/m<sup>2</sup>. This is still below the allowed steady-state limit 10 MW/m<sup>2</sup>. The new model shows also some increase of the assimetry in the power loads between the inner and outer targets. The radiation opacity does not change the target heat loads at all.

The increase of the the peak heat flux density is related mainly to the higher peaking of the profiles of the plasma parameters in front of the targets, see Section 3.3.1. The total radiated power in all the considered cases is 60-70 MW. It is lower for lower pressures and its dependence on the used model is weak. This parameter (radiated power) is in fact an input parameter of the modelling because it depends mainly on the carbon sputtering yield which is specified externally (by the modeller).

The shift towards the higher pressures can be also clearly seen in Figure 5.3a which



Figure 5.1: Effectiveness of impurity pumping in ITER. Blue dashed line is the calculations with EIRENE 1996, green line (triangles) is the calculations with NNC, red line (diamonds) is the calculations with NNC and improved MK and the black line (squares) is the series with NNC, MK and the radiation opacity



Figure 5.2: Peak target heat flux density. See caption of Figure 5.1

shows the dependence of the divertor neutral pressure on the gas puffing rate. The separatrix electron density or the density at the Core-Edge interface is usually specified in the SOL modelling as the boundary condition. In this work it was not fixed but was obtained in the calculations. The result is shown in Figure 5.3b. This density is approximately the same for the model with EIRENE 1996 and for the new model. It varies in a relatively narrow range between  $2.4 \cdot 10^{19} m^{-3}$  and  $2.8 \cdot 10^{19} m^{-3}$ .

Some scalings of the target plasma parameters are shown in Figures 5.4, 5.5. For both targets the maximum electron density and temperature show "detachment-like" behaviour: they decrease when the gas pressure (or the separatrix electron density) increases. This indicates at least the partial detachment for both targets. With NNC added to the model, the densityes increase because more neutrals are retained near the target (higher ionization sources). Adding improved MK decreases the target density because, as shown in Section 3.3.1, Figures 3.11, the density does not increase monotonically towards the target any more. It forms a maximum away from the target and then drops. This can be associated with the extra momentum loss due to elastic collisions of molecules with ions. Finally, the radiation opacity leads to the increase of density. This effect was discussed in Section 4.3. The behaviour of the target temperature is more monotonic: it reduces with each new added model feature, Figure 5.5. The point calculated with the refined grid does not deviate much from the results of the reference model (coarse grid) for the engineering output parameters, Figures 5.1- 5.3. But some deviation can be seen for



Figure 5.3: Parameters related to particle balance. See caption of Figure 5.1

the calculated plasma parameters, Figures 5.4, 5.5.



Figure 5.4: Maximum electron density in front of the inner and outer target. See caption of Figure 5.1



Figure 5.5: Maximum electron temperature in front of the inner and outer target. See caption of Figure 5.1

## **Chapter 6**

# First experimental validation for JET

### 6.1 The experimental and model set-up

In this chapter the first confronting of the SOLPS4.2 package with experiment is presented. The benchmarking was done for JET (Culham, UK). It is a large tokamak with a major radius of about 3 m and with divertor magnetic configuration similar to ITER. The details on the device relevant for SOL modelling will be given throughout the text below. The series of shots #58353-#58357 was chosen for this study. These are the shots with plasma current 3 MA (toroidal field 3 Tesla) and relatively high line averaged density  $\approx 8 \cdot 10^{19} m^{-3}$ . Divertor structure is Mk2GB-SR with carbon targets. The magnetic equilibrium is the so called Diagnostic Optimised Configuration with Low X-point (DOC-L), see Figure 6.1. NBI heating power is 14..15 MW, gas puffing through inner divertor (GIM11), Figure 6.1b. The forward direction of the magnetic field ( $\mathbf{B} \times \nabla \mathbf{B}$  drift is directed downwards). A similar configuration was considered in [20].

The first shot #58353 with gas puffing rate  $S_{puff} = 2 \cdot 10^{22} s^{-1}$  was an H-mode. Then  $S_{puff}$  was increased to  $4 \cdot 10^{22} s^{-1}$  and an L-mode was obtained in the shot #58354. The shots #58355 and #58356 were similar H-mode shots with  $S_{puff} = 3 \cdot 10^{22} s^{-1}$ . The shot #58357 was an H-mode with lower density ( $S_{puff} = 10^{22} s^{-1}$ ). Type-I ELMs took place in all the H-mode shots in question. ELM frequency 10..15 Hz. The study was made for a quasi steady-state period of the discharges between 57 sec and 61 sec (between 57 and 59.5 for #58355).

Exactly the same code and the same model as for ITER (but without helium) were used, including neutral-neutral collisions and photon opacity. The only difference was that the neutral-neutral collisions for carbon atoms (all possible combinations,  $s_0 = 10^{10}$ , see Section 2.4, Table 2.1) were added. The grid was generated for the magnetic equilibrium of the shot #58355, time instant 60 sec. The equilibrium is reconstructed with EFIT code (routine diagnostic at JET). Identical grid, shown in Figure 6.1b, was used for the all shots. As in the case of ITER, it comprises a quasi-orthogonal grid for B2 and an additional triangular grid in the "plasma free" region. The model plasma consists of D<sup>+</sup> and the 6 charge states of C. The anomalous transport coefficients were specified according to the previous modelling experience [20, 129, 130]: diffusion coefficient  $D_{\perp} = 0.5 m^2/s$ , temperature diffusivity  $\chi_{\perp}^e = \chi_{\perp}^i = 1 m^2/s$ . The coefficients were fixed for the all modelling cases. All the results shown below were obtained after extra "smoothing runs" of B2-EIRENE (which followed each "main" run): 1000 steps with time step  $10^{-6}$  sec and 100 sec for EIRENE (approximately 10.000 histories for neutrals) to reduce the Monte-Carlo noises. Some noise still can be see, especially on the temperature profiles. The reason is partly the complicated shape of the B2 grid at the targets, Figure 6.1b.

The modelling in this work is fully steady-state. Therefore, the ELMs have to by eliminated from the analysis. The approach similar to that used in [131] was applied. The power flux from the core  $P_{SOL}$  was reduced by the estimated averaged power of ELMs  $P_{ELM}$ . It was assumed that in this case the simulations correspond to the inter-ELM period. The ELM peaks were removed from the all experimental signals.



Figure 6.1: a) General view of the vacuum chamber and magnetic configuration with lines of sight for some diagnostics. b) The grid and structure for numerical simulations

The algorithm of removing ELMs works as following. On the first step the mean square average  $\sqrt{S^2}$  and the time variance *var*(*S*) of the signal *S* are calculated:

$$\sqrt{\overline{S^2}} = \sqrt{\frac{\int_{t_{min}}^{t_{max}} S^2 dt}{t_{max} - t_{min}}}; \quad var(S) = \sqrt{\frac{\int_{t_{min}}^{t_{max}} (S - \overline{S})^2 dt}{t_{max} - t_{min}}}$$
(6.1)

After that all data points  $S_i$  for which:

$$|S_i - \sqrt{S^2}| > A \cdot var(S) \tag{6.2}$$

are taken out. The routine is repeated for the remaining points. The iterations continue until no points which satisfy the condition (6.2) are left. The parameter A should be small enough to ensure good filtering of pikes and at the same time not too small to ensure that a statistically significant amount of points will be left after the processing. It was found empirically that A = 1.5 provides good filtering and works sufficiently reliable.

This algorithm is heuristic and has no solid theoretical basis. In fact it looks for the value around which most of the points are concentrated. By visual analysis it was found that for most of the signals this method gives reasonable "inter-ELM" values. It effectively removes not only the ELM peaks but also the traces of arcing for Langmuir Probes and the post-ELM deeps for  $H_{\alpha}$  radiation. Some examples are shown in Figure 6.2. The raw signals are shown in blue and the red horizontal line shows the obtained inter-ELM level. For some signals, e.g. particle flux measured by the Pressure Gauge, this technique shows obviously overestimated values, Figure 6.2e. In the case of the data without strong peaks the average level can be slightly ( $\approx 10$  %) underestimated, Figure 6.2f. The quality of processing for the all signals was controlled visually. The values obtained from the Langmuir probes for #58354 for the inner target were cross-checked with smoothing which was made independently by S. Jachmich.

The data acquisition and processing is performed by the set of MATLAB scripts installed on JAC (JET Analysis Cluster). Those scripts use CODAS MATLAB interface (CO-DAS=Control and Data Acquisition Systems) [83].

The SOL input power  $P_{SOL}$  for the modelling was calculated as

$$P_{SOL} = P_{NBI} + P_{ohm} - P_{rad}^{core} - P_{ELM}$$

Here  $P_{NBI}$  is the NBI heating power,  $P_{ohm}$  is the ohmic heating power (it is an order of magnitude lower than  $P_{NBI}$ ),  $P_{rad}^{core}$  is the core radiation measured by the KB4 bolometry



Figure 6.2: Examples of the calculated average signals with removed ELMs. Figures (e) and (f) show negative examples when the smoothing technique does not work

system (vertical view),  $P_{ELM}$  is the average power of ELMs. This latter was estimated as the time average of the time derivative of the diamagnetic energy (signal MG3/WPD) taking into account only the negative part (the energy lost by plasma):

$$P_{ELM} = \frac{1}{t_e - t_s} \int_{t_s}^{t_e} \left| \frac{d(MG3/WPD)}{dt} < 0 \right| dt$$

The time interval for averaging was from t<sub>s</sub>=57 sec to t<sub>e</sub>=59.5 sec for all shots because for t>59.5 sec too strong oscillations in the MG3/WPD signal were found (indicating possible problems with measurements or data processing?). For the specified time interval the difference between integrals over the negative and the positive derivatives is less than 5 % (consistency check).  $P_{ELM}$  estimated in this way takes 20..24 % of the total input power  $P_{inp} = P_{NBI} + P_{ohm}$ . The data published elsewhere show somewhat higher figures [134, 135, 136]. If the technique which is used here is applied to the shots from those publications, then the obtained  $P_{ELM}$  takes 45-75 % of the ELM power which backs the consistency of the data processing. The  $P_{ELM}^{rad}$  is calculated as the difference between the unsmoothed and smoothed total radiation measured by bolometers (DDA BOL4/TOPI). The conclusion may be that the technique which is used in this work gives a reasonable estimate of  $P_{ELM}$  but should be used carefully.

The way of density control was similar to that used for ITER modelling. The density at the core boundary (at the separatrix) was not fixed but controlled via the neutral pressure in the divertor. A small particle influx from the core was specified  $S_{core} = 10^{21} s^{-1}$ to compensate the neutral influx to the core, to take into account the NBI flux and for the numerical stability. In a real device in addition to "intentional" pumping due to cryopumps the wall can absorb a significant amount of hydrogen. To take into account those two kinds of pumping the two albedo coefficients were introduced:  $A_p$  on the entrance to the cryo-pump slots, Figure 6.1b and  $A_w$  on all the other surfaces except targets.

The albedo  $A_p$  and  $A_w$  were adjusted to match the septum neutral flux  $F_n = 5.8 \cdot 10^{22} m^{-2}/s$  measured by the Pressure Gauge PG23, see Figure 6.1b. This ionization pressure gauge [132] measures the density of molecules inside itself. This density depends linearly on the incoming particle flux (measured in equivalent molecules). The accuracy of PG measurements is  $\pm 20$  % for L-mode in case of good calibration. It can be significantly perturbed by ELMs [133]. Therefore, the adjustment was made only for the L-mode shot #58354 and the same values of  $A_p$  and  $A_w$  were used for all modelling cases. The ratio between  $A_p$  and  $A_w$  was taken to keep the ratio of wall pumping to cryo-pump pumping approximately 2:1. This value was found in [137] for the similar JET shots. The gas puffing rate in the model was the same as in the experiments:  $S_{puff} = 1..4 \cdot 10^{22} s^{-1}$ . The possibility of wall outgasing was not considered.

The carbon sputtering yield  $Y_{chem}$  was adjusted to match the divertor and X-point radiation  $P_{rad}$  measured by the bolometry KB4. It was assumed that the all surfaces are covered by carbon. Therefore the total radiation  $P_{rad}$  is in fact an input parameter. This assumption is more or less arbitrary but the model for carbon which is used at the moment is rather primitive anyway (a constant sputtering yield, no molecules, perfect sticking). The obtained  $Y_{chem} = 0.45$  % for L-mode and  $Y_{chem} = 0.7$  % for H-mode are relatively low. This could be due to reduction of  $Y_{chem}$  for high incident fluxes [63].

The input data for all the modelling cases and corresponding experimental shots are summarised in Table 6.1. The match of the radiation power  $P_{rad}$  is relatively good (the difference is less than 10%) for all the cases except #58357. The measured control neutral flux  $F_n$  was matched well only for the shot #58354. For H-mode shots the discrepancy can be a factor 2..3, but it is not clear how reliable are the PG data in the presence of ELMs. For this diagnostics the corresponding figures for the H-mode were taken approximately from the plots, because the smoothing algorithm described above clearly failed to find the inter-ELM level.

The diagnostic signals were taken from the JET CODAS database. The list of the all signals used in this work is shown in Table 6.2. The last column shows the corresponding markers in the databases (DDA, Diagnostic Data Area). The experimental data which were compared to the calculations include: midplane electron density measured by Li-beam charge-exchange spectroscopy Ky63; divertor Langmuir Probes KY4D;  $H_{\alpha}$  spectroscopy KS3; the reconstruction of the incident target heat flux base on the infrared (IR) cameras

measurements (KL3) [134]; the tomographic reconstruction of the total radiated power (bolometers KB1). The lines of sight for Ky63 and KS3 are shown in Figure 6.1a. The Ky63 data including error bars were taken from the RADISP analysis application. In analysing the mid-plane profiles it has to be taken into account, that the error of the reconstruction of magnetic equilibrium (position of separatrix) can reach  $\pm 1$  cm.

Shot	#58357	#58353	#58355, #58356	#58354
$S_{puff}, s^{-1}$	$1 \cdot 10^{22}$	$2 \cdot 10^{22}$	$3 \cdot 10^{22}$	$4 \cdot 10^{22}$
$P_{inp}, MW$	15.9	16.2	14.5, 16.3	14.6
$P_{rad}^{core}, MW$	1.9	1.9	1.5, 1.8	0.9
$P_{ELM}, MW$	3.8	3.6	2.9	L-mode
$P_{ELM}^{rad}, MW$	2.2	2.7	1.3,1.9	L-mode
$P_{SOL}, MW$ (model)	10	10	10	14
$F_n, \ m^{-2}/s$	$\approx 3.0 \cdot 10^{22} *$	$\approx 3.0 \cdot 10^{22} *$	$\approx 4.55.0 \cdot 10^{22} *$	$5.8 \cdot 10^{22}$
$A_p, \%$	3.2	3.2	3.2	3.2
$A_w, \%$	1.4	1.4	1.4	1.4
$F_n, \ m^{-2}/s$ (model)	$1.5 \cdot 10^{22}$	$2.8 \cdot 10^{22}$	$4.2 \cdot 10^{22}$	$5.6 \cdot 10^{22}$
$P_{rad}, MW$	4.0	3.8	4.5, 4.4	4.7
Y <sub>chem</sub> , %	0.7	0.7	0.7	0.45
$P_{rad}, MW$ (model)	2.9	3.8	4.3	5.0

Table 6.1: Input data for modelling cases

\* approximate "inter-ELM" values from the time tracing plots

Unfortunately, signals from the high resolution CCD cameras KL2 were not available for the studied discharges. The low resolution spectroscopy KS3 has only 3 points in the inner divertor and 3 points in the outer divertor. The error of the spectroscopic measurements (for the total photon flux of the selected line) is estimated as  $\pm 10\%$  [140].

Quantity	Diagnostic	Signal
Divertor neutral flux	Pressure Gauges KY5	PG23/FLUX
Gas Puffing Rate	-	GASM/G11R
Total input power	-	MG3/YTO
Coupled NBI power	-	NBIP/GTT
Ohmic heating power	Magnetic diagnostic KC1D	MG2/YHO
Core radiation	Bolometry KB4	BOL4/TOPU
Divertor and X-point radiation	Bolometry KB4	BOL4/TXPN
Diamagnetic Energy (fast)	Magnetic diagnostic KC1D	MG3/WPD
Upstream density	Li-beam spectroscopy KY63	RADISPLAY
Target ion flux	Langmuir Probes KY4D	KY4D/JSAT
Target electron temperature	Langmuir Probes KY4D	KY4D/TE
Divertor H-alpha	Spectroscopy KS3	EDG7/DAPR
Incident Heat Flux	Infrared Cameras KL3	KL3J/J3D
Deposited Energy	Calorimetry KD1D	DVTC/ETJ
Total Radiation (tomography)	Bolometry KB1	-

Table 6.2: Diagnostic signals

The Langmuir Probes (LP) measure the target incident ion flux  $I_i$  and the electron temperature  $T_e$ .  $I_i$  is calculated directly as the probe ion saturation current divided by wetted area.  $T_e$  is restored from the I-U characteristics. It is well known, that LP always tend to overestimate  $T_e$  if it is lower than 3..5 eV [139]. This was the reason, why  $I_i$  but not the electron density  $n_e$  was chosen for the comparison. The calculation of  $n_e$  involves the temperature and is therefore unreliable for the low temperature region. 5 LP were available on the inner target and 6 LP on the outer target. The error of LP measurements can reach  $\pm 30 \%$  [139]. Like in the case of the mid-plane profile, the error of the reconstruction of magnetic equilibrium can be 1-2 cm. An analysis of the profiles obtained during a vertical shift of the strike points in the time intervals 50-52 sec and 62-65 sec was made by

S. Jachmich. It shows that the real position of the strike points is 1..1.5 cm lower than obtained from the magnetic reconstruction (for both targets).

IR cameras KL3 allow to restore the surface temperature by measuring the emitted infrared radiation. This temperature is then used to reconstruct the incident heat flux [134]. The KL3 measurements were available for all the studied shots except #58357. The total heat fluxes on the inner and outer targets were cross-checked with the divertor calorimetry KD1D [141], Table 6.3. In this table "inner" corresponds to the tiles 1 and 3 (inner target) and "outer" stands for the tiles 6 and 7 (outer target). The average power deposited on each tile was estimated as the deposited energy (DDA DVTC/ETJ, MJ) divided by the duration of the NBI heating (duration of NBIP/GTT signal). For KL3 the time averaged signals KL3I/GnSP (where 'n' is the index of the tile) were used. Table 6.3 shows that whereas the mismatch of two diagnostics for the inner target is 30 % and less, for the outer target KL3 gives a factor 2 higher power for #58355, #58356 and even a factor 3 higher for #58354. In the latter case the KL3 signal shows a constant increase of the heat flux density which finally reaches unrealistic values  $\approx 100 \text{ MW/m}^2$ . This indicates possible problems with KL3 data for the outer target. The possibility that the reconstructed outer heat flux could be overestimated should be kept in mind when comparing this diagnostics with the modelling. The divertor calorimetry allows also to estimate the global power balance: the fraction of the total input power which lands at each divertor target.

Shot	Inner Power, MW			Outer Power, MW		
	KL3	KD1D	KL3/KD1D	KL3	KD1D	KL3/KD1D
58353	1.8	2.3	0.78	6.7	5.8	1.16
58355	2.7	2.3	1.17	9.8	5.0	1.96
58356	2.8	2.4	1.17	11.0	5.5	2.0
58354	3.0	2.3	1.30	20.0	6.3	3.18

Table 6.3: Cross check between KL3 and KD1D diagnostics

The error bars shown on the plots below were calculated as  $\sqrt{var(S)^2 + \Delta^2}$  where  $\Delta$  is the prescribed experimental error (instrumental error) and  $var(S)^2$  is the variance of the signal, Formula 6.1 (on the last iteration of smoothing).

## 6.2 Comparison with experiment

The upstream density profile (mapped along the magnetic surfaces to the outer midplane) is shown in Figure 6.3. The experimental profiles were shifted by  $\leq 1.0$  cm to account for uncertainties in the reconstructed magnetic equilibrium. Applying such a shift, it is always possible to get a good match outside the separatrix. Near and inside the separatrix the discrepancy is large because no attempts were made to emulate the transport barrier in the modelling. Note, that for the density control procedure applied, the absence of the perfect match of the upstream profile is not crucial.

In Figures 6.4-6.7 the incident target ion flux  $I_i$  and electron temperature  $T_e$  are compared with LP measurements. The profiles are mapped to the outer midplane (the same as in Figure 6.3). The experimental points were shifted vertically by -1.5 cm for the outer target and by -1.0 cm for the inner target to account for the errors in the magnetic reconstruction. Applying this shift gives a good agreement for the outer  $I_i$  for all shots, Figure 6.5. Inner  $I_i$  profile is relatively well reproduced for the H-mode shots, Figures 6.5a-6.5c, but the drop of  $I_i$  above the separatrix in #58354 is not reproduced in the modelling, Figure 6.5d. Calculated  $T_e$  above the separatrix is always a factor 1.5-2 larger than the measured one, Figures 6.6, 6.7. The largest difference is found for the inner target for #58354, Figure 6.6d. It is very likely that the LP TR06 and S31C overestimate the temperature because it falls below 3 eV under the separatrix. The extremely high temperatures (> 20 eV) shown by S32B could be caused by the direct losses of the fast (suprathermal) particles in the vicinity of separatrix.

The comparison of the  $H_{\alpha}$  signal integrated over the lines of sight (see KS3 in Figure 6.1a) is shown in Figure 6.8. There are in fact only 3 points in the inner divertor which allow meaningful comparison because the data on the outer side do not touch the



Figure 6.3: Upstream density profile (experimental profiles were shifted outwards)



Figure 6.4: Ion flux density incident on the inner target



Figure 6.5: Ion flux density incident on the inner target



Figure 6.6: Electron temperature in front of the inner target


Figure 6.7: Electron temperature in front of the outer target

target region at all. The agreement is relatively good for the H-mode shots, Figures 6.8a-6.8d. For #58354 the calculated maximum is a factor 2 lower than the measured one, Figure 6.8d.

Figures 6.9, 6.10 show the comparison of the reconstructed and calculated incident heat flux. The agreement for the outer target looks good. One should recall, however, that the "measured (reconstructed) flux could be overestimated, see Section 6.1, Table 6.3. The reconstructed heat flux for the outer target for #58354 is not shown because it was obviously overestimated, see Table 6.3. For the inner target the calculated maximum is a factor 1.5-2.5 higher than the measured one. The calculated profiles are more peaked. Similar results: good agreement for the outer target and a factor 2 disagreement for the inner were shown in [20].

The asymmetry of the power distribution between two divertors  $P_{out}/P_{in}$  and the fraction of the total power which goes to the targets  $P_{targ}/P_{inp}$  are shown in Table 6.4. The experimental figures are obtained using divertor calorimetry. The measured asymmetry of 2.2..2.7 is somewhat higher than the calculated one (1.6..1.8). Recent studies show that this quantity can be better reproduced by the modelling if the parallel classical drifts are taken into account [129, 143, 144]. The measured  $P_{targ}/P_{inp}$  ( $\approx$ <60 %) is somewhat lower than  $\approx$ >70 % obtained in the simulations. No significant difference is seen for  $P_{out}/P_{in}$  and  $P_{targ}/P_{inp}$  for L- and H-mode shots.

Shot	$P_{out}/P_{in}$		$P_{targ}/P_{inp}$ , %		
	Experiment	Model	Experiment	Model	
58357	2.3	1.9	56	83	
58353	2.5	1.8	57	73	
58355	2.2	1.6	57	72	
58356	2.3		55		
58354	2.7	1.8	63	73	

Table 6.4: Power distribution

Examining the experimental data shown in Figures 6.4- 6.10 one can see that the dif-



Figure 6.8: Line integrated  $H_{\alpha}$  radiation (lines of sight are shown in Figure 6.1a)



Figure 6.9: Heat flux density incident on the inner target



Figure 6.10: Heat flux density incident on the outer target



Figure 6.11: Measured and calculated distribution of the radiated power (inter ELM) for the shot #58353 (Low Density)



Figure 6.12: Measured and calculated distribution of the radiated power for the shot #58354 (High Density)

ference between the H-mode shots with different gas puffing rate is very weak (subfigures a,b,c). A similar insensitivity is found in the modelling as well. Clear difference is seen between those shots and the L-mode shot #58354 (to compare subfigures a,b,c with d). In the modelling the "L-mode" and "H-mode" cases are differ only in input power  $P_{SOL}$ , Table 6.1. The measured outer  $I_i$  is higher for #58354, Figure 6.5d, and this increase is also seen in the modelling. The temperature above the separatrix increases as well, Figure 6.7d, but in the modelling it remains nearly on the same level.

The most significant discrepancy can be seen for the inner target. The experimental data show signs of detachment at the upper divertor tile. The ion flux drops several times, Figure 6.4d (compare with sub-figures a,b,c). The temperature also decreases by almost a factor 2, Figure 6.6d. At the same time, the intensity of the H<sub>a</sub> radiation increases, Figure 6.8d. All these three features are well known experimental characteristics of detachment [14, 16, 135]. The simulations do not reproduce them: the modelling results which correspond to #58354 are largely similar to those for the cases with lower density.

The difference in the results which is seen between #58354 and the H-mode cases is predominantly due to the different power input rather than the different gas puffing rate. To show this two extra cases were considered for #58354: with  $S_{puff} = 6 \cdot 10^{22} s^{-1}$  and with  $S_{puff} = 3 \cdot 10^{22} s^{-1}$ . The results are shown in Figures 6.8d, 6.9c marked as "model, HD" and "model, LD" respectively. The difference is small. The difference for  $I_i$  and  $T_e$  (not shown) is even smaller.

The comparison of the spatial distributions of the measured and calculated total radiated power is shown in Figures 6.11, 6.12. The shown experimental distribution is the tomographic reconstruction of the KB1 bolometry measurements made by A. Huber. This reconstruction was made for two time instants inbetween ELMs (in case of H-mode). The reconstructed distribution shows that the area of the dominant radiation is localised beneath the X-point and on the inner side in front of the upper divertor tile, Figure 6.11. In the high density case the light blob reaches the target tile, Figure 6.12. The modelling shows completely different picture: concentration of the radiated power along the separatrix with strong peaks near the strike points. However, the old KB1 diagnostic had very bad resolution and the error in the reconstruction can be very large, see e.g. [142].

Some effects which are not included in the model so far but can in principle be strong enough to help to explain the observed discrepancies with experiment. The explicit transport of vibrational excitations of molecules can significantly change molecular kinetics [43] and provide an extra channel for the cross-field energy transport [111]. Including classical drifts [129, 143, 144] and ballooning-like radial dependence for the transport coefficients (~ 1/r) could substantially change the in/out asymmetry of the particle and power flows. Finally, the neutral gas leakage from the sub-divertor volume can in some cases produce a strong effects as well [51, 89, 90].

#### 6.3 Comparison of different models

To study the influence of the individual new features in the model on the self-consistent solution, a series of calculations was performed with stepwise updates of the model. The corresponding modelling cases are described in Table 6.5. Model 1 corresponds to the initial version EIRENE 1996. In model 2 the improved molecular chemistry, Section 3.2, was added. Model 3 is the model 2 with added elastic collisions  $D_2 + D^+$ , Section 3.1. The neutral-neutral collisions (NNC), Chapter 2, were added in Model 4. Model 5 corresponds to the reference case including the photon opacity, Chapter 4. This latter model was used in the all calculations described above. The model 3 is the same as the model of EIRENE 1999 (the hydrogen part) which was used for example by M. Wishmeier [73].

The calculated target profiles of the electron temperature and density and the incident heat flux are compared in Figures 6.13, 6.14. The strongest effect is seen after the transition from Model 2 to Model 3. That is, after including the elastic collisions  $D_2 + D^+$ . For the electron temperature in the inner divertor the strongest effect is seen due to the updated molecular chemistry (transition from Model 1 to Model 2). The non-linear effects: NNC and photon opacity, yield only a very weak modification. The most pronounced effect of the NNC is a higher molecule temperature near the septum plate: 0.1..0.15 eV instead of the wall temperature of 0.05 eV.

Marker	Description	$F_n, m^{-2}/s$	$P_{rad}, MW$
1	EIRENE 1996, same input as $#58354$ , Table 6.1	$7.1 \cdot 10^{22}$	8.1
2	Model 1 plus improved Molecular Chemistry	$7.0 \cdot 10^{22}$	8.1
3	Model 2 plus elastic collisions $D_2 + D^+$	$6 \cdot 10^{22}$	5.9
4	Model 3 plus neutral-neutral collisions	$5.5 \cdot 10^{22}$	5.1
5	Model 4 plus photon opacity (reference model)	see Table 6.1	
HD	model 1 adjusted with #58354 case, Table 6.1		
	$A_p = 4.2 \%, A_w = 1.7 \%, Y_{chem} = 0.15 \%$	$5.9 \cdot 10^{22}$	5.3
LD	model 1 adjusted with #58353 case, Table 6.1		
	$A_p = 4.2 \%$ , $A_w = 1.7 \%$ , $Y_{chem} = 0.25 \%$	$2.9 \cdot 10^{22}$	3.8

Table 6.5: Modelling cases with stepwise update from EIRENE 1996 to the current version

The analysis shown above aimed at finding the model feature which produces the strongest effect (a sensitivity analysis). It was not intended to provide a physically meaningful comparison of the old and the new model because the parameters  $A_p$ ,  $A_w$  and  $Y_{chem}$  were fixed, hence  $P_{rad}$  and  $F_n$  could be different, Table 6.5. For a physically correct comparison, the same  $P_{rad}$  and  $F_n$  have to be matched for the old and new model. This was done for the two modelling cases: one corresponded to #58353 and another to #58354. They will be referred to below as "the low density" (LP) and "the high density" (HD) cases respectively, Table 6.5. The results of those calculations are shown in Figures 6.3- 6.10c,d with dashed lines (marked as "EIRENE 1996").

The calculations with EIRENE 1996 show broader density profiles, Figure 6.4 6.5c,d, and  $T_e$  profiles shifted upwards, Figure 6.6, 6.7c,d. The difference of the maximum heat flux density can reach a factor of 2, Figure 6.10c. The difference between the two models



Figure 6.13: Parameters in front of the inner target: comparison of different models, Table 6.5



Figure 6.14: Parameters in front of the outer target: comparison of different models, Table 6.5



Figure 6.15: (a) Contours of local opacity for  $Ly_{\alpha}$  line and atom density  $n_D$  near the inner target; (b) ionization rate  $S_i$  and the boundary below which the "photo-induced" (ionization from the photo-excited levels) ionization rate  $S_i^{ph}$  exceeds optically thin (ordinary) ionization  $S_i^{thin}$ . (c) "Optically thin" and "photo-induced" ionization rates in front of the inner target.

becomes smaller for lower density but does not vanish. The 2D distributions of the plasma parameters obtained with the two models are shown in Appendix E. The most striking difference is seen in the distribution of the atom density, Figures E.5, E.12 and the molecule density, Figures E.3, E.10. This difference is mainly due to the elastic collisions of the molecules with ions. The calculations made with EIRENE 1996 show that the ionization front detaches from the inner target, Figure E.5a, whereas in the new model it is attached, Figure E.5b.

Comparing with the available experimental data it is difficult to say which model (old or new) yields better agreement. The new model gives a better match for the incident ion flux, Figures 6.4, 6.4c, d. At the same time, the target temperature shown by the old model is closer to the experiment, Figures 6.6, 6.6c,d. Both models show similar  $H_{\alpha}$  profiles for the low density case, Figures 6.8b, and both of them failed to reproduce the measurements for the high density case, Figures 6.8d. The calculated incident heat flux is similar for both models for the low density case, Figures 6.9a, 6.10a. For the high density case the inner target profile obtained with EIRENE 1996 is close to the measured one. Note, that for the old model the correct total radiated power was achieved with only  $Y_{chem}$ =0.15-0.25 %, Table 6.5, which can be partly explained by higher (by 30-50 %) total incident ion and atom flux. The fact that the old model provides in some cases a better match for some parameters does not mean that it is more correct. The general philosophy is that all effects, which are known to be operative, have to be included in the modelling. The fact that sometimes it brings the results further away from experiment can not serve as the excuse to neglect those effects, due to the large number of remaining other uncertainties in the divertor plasma modelling.

The radiation opacity is the only effect which was included in the JET simulations but is currently not included (by default) in the standard ITER model [50], despite its availability. The global opacity for  $Ly_{\alpha}$  line is found to be close to unity, see Table 6.6. Here "global opacity" means the total number of absorbed photons divided by the total number of emitted photons of the specific line. This conclusion coincides with experimental observations [115]. The regions near the strike points where the atom density  $n_D$  is large  $(n_D > \approx 10^{19} m^{-3})$  and the Private Flux Region (PFR)  $(n_D \approx 10^{18} m^{-3})$  are opaque for the Ly<sub>a</sub> radiation, Figure 6.15a. But distinct from the ITER calculations, Section 4.3, the overall effect on the divertor performance is weak. The domain where ionization due to the photo excited levels can be comparable to, or larger than, the "ordinary" (optically thin) ionization occupies only a relatively small part of the ionization region, Figures 6.15b, 6.15c. It is the main mechanism of ionization in PFR but even for the case with the highest density its contribution comprises only 15 % of the total ionization source (22 % in the inner divertor alone). This is illustrated also in Figure E.7, Appendix E. As a result, the influence of the radiation opacity on the plasma parameters is weak. The key difference compared to ITER conditions is believed to be the higher temperature in the region of interest, which reduces the effect of extra ionization via photo-excited states. This can be seen from Figure 4.3, Section 4.2.2. For temperatures higher than 2 eV the recombination is very weak, therefore the effective ionization rate is represented almost purely by the opaque ionization  $S^{op}$ , see Equation 4.26, which is not much larger than the ordinary "optically thin" rate.

	#58354	#58355,6	#58353	#58357
Global Opacity, $Ly_{\alpha}$ , %	67	66	58	44
Global Opacity, $Ly_{\beta}$ , %	30	28	20	12
Photo-induced Ioniz., %	15	15	11	7

Table 6.6: Photon opacity effects

For the JET conditions the Molecular Activated Recombination (MAR) [109] can be even stronger than common 3-body recombination. For #58354 the total calculated ion sink due to common recombination is  $1.8 \cdot 10^{22} s^{-1}$  and the sink due to MAR is  $2.0 \cdot 10^{22} s^{-1}$ . For lower density shot #58353 the corresponding figures are  $0.4 \cdot 10^{21} s^{-1}$  and  $1.4 \cdot 10^{22} s^{-1}$  respectively. The maximum total rate of MAR reaches  $4 \cdot 10^{18} cm^{-3}/s$  for #58354 (the same value as for the 3-body recombination). The key difference compared to ITER, Section 3.3.2, is the lower density which reduces the ordinary recombination but is favourable for MAR. At the same time for the studied JET shots both MAR and 3-body recombination are not

important at all because they are at least an order of magnitude smaller than the recycling sources.

## **Chapter 7**

## Conclusions

In this work a new version of the coupled B2-EIRENE code packages SOLPS4.2 has been mounted and tested. The package comprises a 2D multispecies plasma fluid transport code B2.4 [25, 28] and a Monte-Carlo neutral transport code EIRENE [26, 27]. This version of the B2 code is adjusted specifically for meeting the demands of modelling the reactor scale ITER divertor plasma. In the new configuration the old version of EIRENE code from the year 1996 was replaced by the most recent version. This upgrade has made the model more relevant for the conditions of relatively cold (several eV) and dense ( $\approx 10^{21}$  m<sup>3</sup>) large divertor plasmas, i.e. for ITER.

The previous isolated upgrades of the EIRENE code have been combined together and implemented in the self-consistent (between plasma, neutral gas and radiation field) B2-EIRENE modelling. These isolated upgrades include the neutral-neutral collisions (C. May [38, 39]) and the model for the line radiation transport (S. Wiesen [45, 46, 47], P. Börner [48, 49]), coupled to atomic kinetics. The up to-date model for the hydrogen molecular chemistry is based on the Collision-Radiative Model of Sawada and Fujimoto [40, 41] for electron impact processes with H<sub>2</sub> molecules and H<sub>2</sub><sup>+</sup> molecular ions, which was revised and updated by D. Reiter and P. Greenland. It takes into account electronically and, in some cases, vibrationally excited states [42, 43, 106]. The Molecular Assisted Recombination (MAR) reaction chain initiated by the ion conversion process  $H_2 + H^+ \rightarrow H_2^+ + H$  [109] has been added to the model as well.

The new model also includes elastic collisions of the hydrogen molecules with ions based on the cross-sections of P. Bachmann and D. Reiter [44]. In frame of the present work the momentum and energy transfer rates between neutrals and plasma due to elastic collisions were calculated and applied in the Track Length estimator for the corresponding sources. Although it did not lead to the improvement of numerical accuracy for the ITER conditions, comparing Track Length and Collision estimators provides a good numerical test of the implementation.

To assess the effect of the new model features on the modelling results, three series of calculations have been made for ITER and one series for JET. The ITER reference model used in this thesis is the set-up with full carbon wall and 100 MW SOL input power. The choice of the chemical sputtering yield ensures that 60..70 % of the input power is radiated.

The strongest effect for the ITER modelling (in terms of the divertor plasma parameters and the ITER operational scalings) was found to be due to updated molecular reaction kinetics and neutral-neutral collisions. The obtained effect of MAR for the ITER conditions is insignificant because of high plasma densities (>>  $10^{20} m^{-3}$ ). The analysis showed that the molecule-ion elastic collisions were responsible for the strongest modification of the results. The elastic collisions (together with NNC) heat up the molecules and hinder their transport away from the divertor targets. The neutral density forms sharp peaks near the strike points. The plasma momentum sink due to its collisions with neutrals becomes a factor of 2-3 higher facilitating the onset of detachment.

The upgrades of the computational model result in a higher calculated peak flux density incident on the divertor targets even for the higher divertor gas pressure. The old model predicted that this peak can be reduced down to 2 MW/m<sup>2</sup> by increasing the neutral pressure (the gas puffing rate). For the new model this figure is  $4 \text{ MW/m}^2$  even for a factor

1.5..2 larger average neutral pressure in the divertor.

It is further shown that for ITER conditions the opacity of the hydrogen line radiation can lead to a significant (a factor of 2) increase of the plasma density in front of the targets. The maximum density can reach  $4..5 \cdot 10^{21} m^{-3}$ . The extra ionization via photoexcited states is compensated mainly by the enhancement of volume recombination: the calculated recombination sources become larger than the surface recycling sources. At the same time, the effect of the radiation opacity on the ITER operational parameters, e.g. on the target peak heat flux density, is weak.

The sensitivity analysis made for the JET case confirmed that the strongest effect of the new model appears due to the ion-molecule elastic collisions. The effect of the updated molecular chemistry can be also significant. On the contrary, the impact of the non-linear effects has found to be insignificant for JET conditions. The divertor plasma opacity with respect to the line radiation is high (up to 70 % of Ly<sub>a</sub> is absorbed). However, the extra photo-induced ionization is concentrated mainly below the separatrix providing no clear influence on the plasma parameters.

The calculations made for JET were compared with experimental data for 5 shots with the line average density  $\approx 8 \cdot 10^{19} m^{-3}$ , forward magnetic field, auxiliary heating power of 14..15 MW and a gas puffing rate of  $1..4 \cdot 10^{22} s^{-1}$  in the DOC-L (Diagnostic Optimised Configuration - Low) magnetic configuration. The following diagnostics were involved in the comparison: target Langmuir probes (incident ion flux and electron temperature), Li beam spectroscopy (upstream density), IR-cameras (reconstruction of the target incident heat flux), divertor calorimetry and divertor  $H_{\alpha}$  spectroscopy. The agreement is relatively good (within a factor of 2) for the outer tagret, but a significant discrepancy between the modelling and the experiment is seen in the inner divertor.

The SOLPS4.2 package is installed at the moment on computer systems at IPP, FZ-Jülich, at the ITER International Team, Garching and on the JET Analysis Cluster, Culham. It is now used routinely (version without photon opacity) for the ITER divertor modelling, see the recent publications [50, 51, 52].

Further development of the ITER divertor modelling tools will be driven by validation applications as the one for JET described in this work. Independent of that is it clear that all of the edge plasma physics elements, which are known to be operative, even if their experimental identification in tokamaks remains limited, will have to be implemented. Amongst these are the following features:

- Correct description of the transport of molecular vibrationaly excited states;
- Modification of the BGK algorithm for neutral-neutral collisions to get the correct Prandtl number: Elipsoidal-BGK, see e.g. [35, 36, 37, 84]);
- Including the hydrocarbon molecules;
- Replacing the old version of B2.4 by the state of the art version from the SOLPS5.0 package [28] which can take into account all kinds of classical drifts, electric currents at the edge and has improved numerics.

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## **Appendix A**

## **Technical notes**

#### A.1 Software and hardware

The version of the B2-EIRENE code which was used in this work comprises the B2.4 code of the ITER IT and the most recent EIRENE version (2003-2004). B2-EIRENE is only the computational kernel of the package called SOLPS (SOL Plasma Simulation). It includes also a number of tools for preparing the models and post-processing as well as service scripts. In frame of this work the almost identical copy of the configuration of ITER IT, Garching was installed on the computer system of IPP, FZJ. The package which was used for ITER simulations before 2004 has index SOLPS 4.0. The package, upgraded in frame of this work got the index SOLPS 4.2. All the software works under operating system Linux (SuSe Linux 9.0 in case of IPP, FZJ).

For creating the models SOLPS has a graphical (X-window) application DG [76]. It allows to define the geometry and the parameters of the model (including the properties of the surfaces, material etc.) in a user friendly "Windows-like" way. It also produces the data for grid generator. The quasi-orthogonal grid for B2 is generated by the code CARRE [77]. This is a rather robust grid generator for single-null divertor topology. It can also generate the grid for a double-null geometry but in this case it may work unstably.

The output of the DG code is processed by a driver UINP which produces the input files for B2 and EIRENE. This driver was updated for the new version of EIRENE. However, the preparation of the input files for the new version is still not completely automated. The user has to specify the new atomic physics data manually (or by "copy-paste").

In the new version of the package B2 and EIRENE work on different grids. The region between B2 grid and the wall (additional surfaces) is filled by triangular grid generated by the code TRIA [78]. The B2 grid is divided into triangles and connected with the TRIA-grid by the driver TRIAGEOM. The process of grid generation is controlled by a Korn Shell script TRIANG [79]. A similar script is used to operate CARRE.

B2.4 requires the following files to run. Input file "b2.parameters", CARRE grid file and database STRAHL (fort.25) which contains atomic data for impurities. The name of the EIRENE input file is not hardwired, usually "input.eir". The triangular grid is stored in three files: fort.33 (coordinates of nodes), fort.34 (table of triangles), fort.35 (table of neighbours). EIRENE also uses the atomic databases HYDHEL, AMJUEL, METHANE and PHOTON, a file with parameters for calculating sputtering coefficients SPUTER and TRIM tables for reflection of fast particles: for example "D\_on\_C" for reflection of D on carbon surface. For a stand alone run (without B2) EIRENE also needs files with B2 grid (fort.30) and with plasma background (fort.31). They are generated automatically by B2.

During the run B2 periodically stores the status of all its arrays in the file B2SXDR. Besides that the diagnostic information is stored in B2SDIAG and the information about the time behaviour in b2time.nc. B2 also produces ASCII files with time tracings of some variables (printed from subroutines DIAGNO). The time-tracings can be then plotted "on-line" by the script TRC. EIRENE also stores some data in file "fort.13". The data stored by both codes can then be used to continue the calculation from the point where it was stopped. Since the amount of data to be stored can exceed hundred megabites it would be too much load for the system to store them on each time-step (which usually takes less than one CPU minute). The data are stored periodically (for example every 4 hours). This

is controlled by the accompanying scripts which run in parallel with the code. In fact they make periodic back-ups of the whole state of the calculations. All the messages from both codes are piped into a log-file (usually b2.log).

The basic tool which is used in SOLPS for plotting and data processing is the separate application B2PLOT [81]. In particular, B2PLOT calculates the radiation loads on the wall. In addition to B2PLOT there is also a driver TIME\_DEP which is used to produce extra time-tracings (using the information stored in file "b2time.nc"). Special scripts are used to collect the results from several modelling cases to produce summary plots [80]. An example of such plots is shown in Section 5. To eliminate the noise produced by the Monte-Carlo code, the summary data are smoothed over a certain number of last time-steps (script "last\_2d")

In this work B2PLOT was used only to produce the ASCII text output. All the dataprocessing and plotting the 1D plots was performed with MATLAB 14 installed at IPP, FZJ. 2D colour plots were produced with free application GMSH [82] (version 1.58) using output of EIRENE tallies into separate files. A driver CNV11 was written to convert the data between different formats: in particular, between triangular and rectangular grids.

The current version of EIRENE is written in FORTRAN 90/95. The B2.4 and all accompanying software (UINPUT, B2PLOT) are written in FORTRAN 77. The compilation was done with Portland Fortran compiler PGF90. The calculations were mainly performed on several workstations (INTEL P4 3.2GHz based platform) in IPP FZJ and on JAC (JET Analysis Cluster, Culham UK) using remote access. A number of cases were run by A. Kukuskin on the facilities of ITER IT. The data acquisition and processing for the JET modelling was done using a set of specially developed MATLAB scripts and the CODAS MATLAB interface [83] (CODAS=Control and Data Acquisition Systems).

#### A.2 Some technical information about EIRENE



Figure A.1: Flow-chart of the coupled B2-EIRENE code

The main subroutine of the code is the subroutine MCARLO. Subroutine INPUT which is called prior to MCARLO reads the input file and makes some precalculations. In particular, the collision rates are calculated in each cell of the computational grid. After the particle sampling the printing routines (OUTEIR) and the user specified post-processing subroutine MODUSR can be called.

The relative position of the test particle regarding the grid and surfaces is controlled in subroutines TIMER (standard surfaces, triangular grid) and TIMEA (additional surfaces). EIRENE has a set of flag arrays for optimising the geometry module (IGJUM0, IGJUM1, IGJUM2). In some cases they can help to increase the performance significantly.

The sources are sampled in subroutine LOCATE. The truncated Maxwellian distribution for the particles incident to the wall (1.44) is sampled in subroutine VELOCS. Subroutine SHEATH is used to calculate the sheath acceleration (1.31). The sputtering is treated in subroutine SPUTER, reflection from the wall - in subroutine REFLEC.

Subroutine FOLNEUT performs the sampling of the trajectories of the neutral particles (including photons). The selection of the type of collision and the sampling of the type of secondary particles is done in subroutine COLLIDE. The estimators are calculated (updated) in subroutine UPDATE. The sampling of the post-collision velocity for the charge-exchange and elastic collisions is performed in subroutines VELOCX and VELOEL respectively.

The flow-chart of the coupled B2-EIRENE code is shown in Figure A.1. As it was mentioned in Section 1.1.1 EIRENE is used for calculating the particle, momentum and energy sources  $S_n$ ,  $S_{mu_{\parallel}}$ ,  $S_E^e$ ,  $S_E^i$ . In turn, B2 provides EIRENE with plasma background: electron and ion temperatures  $T_e$  and  $T_i$ , the density of ions  $n_\alpha$  and their flow velocities  $V_\alpha$ . The main data transfer is performed via two modules: BRAEIR to transfer the data from B2 to EIRENE and EIRBRA to transfer the data in the opposite direction. In addition, the module EIRDIAG transfers some extra diagnostic data to B2. The interfacing subroutine which processes the data from B2 on EIRENE side is INFCOP. Other subroutines related to the coupling are: UPTCOP, which updates the estimators of the coupling-specific parameters (momentum source  $S_{mu_{\parallel}}$ ); WNEUTRALS, which calculates diagnostic data transferred to B2 and produces the file fort.44 for B2PLOT (see also Appendix A.1); GEOUSR, which aligns some EIRENE additional surfaces with the corners of B2 grid (to avoid gaps). On the B2 side EIRENE is called in subroutine NEUTRALS via interface EIRSRT. Currently different versions of the module INFCOP and related subroutines have to be applied for different grid options. In the coupled code EIRENE is normally used to find the steady state neutral solution although a time-dependent mode of operation is also possible.

#### A.3 Implementing BGK in the EIRENE code

The BGK approximation for neutral-neutral collisions was implemented in EIRENE code by Christof May [38], [39]. To describe the implementation it is convenient to write the Equation (2.1) in the following form (using the notation  $v_{ij} = \langle \sigma v \rangle_{ij} n_j$ ):

$$St^{BGK}(f_i) = \sum_{j=1}^{N} \langle \sigma v \rangle_{ij} (T_{ij})n_j \cdot \left[n_i \hat{f}_{ij}^M(\mathbf{v}, \mathbf{r}; T_{ij}, \mathbf{u}_{ij}) - f_i(\mathbf{v}, \mathbf{r})\right]$$

Here  $\hat{f}_{ij}^M = f_{ij}^M/n_i$  (normalised Maxwellian distribution). For the cross collisions the number of collisions of species *i* with *j* is equal to the number of collisions of species *j* with *i*:  $v_{ij}n_i = v_{ji}n_j$ . Each term of this equation describes the scattering of the test particles *i* by the background of particles *j* with density  $n_j$ . The corresponding collision frequency is  $\langle \sigma v \rangle_{ij}$ . The test particles emerging after collisions have shifted Maxwellian velocity distribution  $\hat{f}_{ij}^M$ .

This nonlinear equation is simulated by EIRENE in an iterative way. On each iteration EIRENE samples trajectories of test particles taking into account collisions with artificial BGK background. The parameters of the BGK background are taken from the previous iteration (see below). Note that in general for cross-collisions  $\hat{f}_{ij}^M \neq \hat{f}_{ji}^M$ , therefore, the collisions of species *i* with *j* and collisions of species *j* with *i* have to be represented by two different artificial background species. For example, considering D and D<sub>2</sub> one introduces artificial species 'D' to simulate self-collisions of D atoms and artificial species 'D<sub>2</sub>' to simulate collisions of D with D<sub>2</sub>. For D<sub>2</sub> molecules one needs a species 'D<sub>2</sub>' for self collisions and a second species 'D<sub>2</sub>D' for collisions of D<sub>2</sub> with D. After sampling the trajectories the parameters of the self-collision terms (background) are calculated using relations (2.6). The cross-collision temperatures and average velocities are calculated using the relations (2.14) and (2.16) with  $\alpha = 1$ :

$$\mathbf{u}_{ij} = \frac{m_i \mathbf{u}_i + m_j \mathbf{u}_j}{m_i + m_j}, \quad T_{ij} = T_i + \frac{2m_i m_j}{\left(m_i + m_j\right)^2} \left(T_j - T_i\right) + \frac{m_i m_j}{3k \left(m_i + m_j\right)^2} \left(\mathbf{u}_i - \mathbf{u}_j\right)^2$$

After that EIRENE begins the next iteration. In case of B2-EIRENE the BGK iterations are combined with the time steps of the B2 code.

For the scoring of neutral trajectories EIRENE has a possibility to add an extra triangular grid in the region between the B2 grid and the wall of the vacuum vessel, see Section 1.3. The grid is generated by TRIA code [B. Küppers, FZJ] and combined with the B2 grid by TRIAGEOM driver [P. Börner, FZJ], see also Sections A.1.

The tests of the BGK approximation implemented in EIRENE are shown in [38] (see also [39]). Two problems with known analytical or numerical solutions were used: equilibration of two gases with different initial temperatures and Couette flow between two parallel plates (see e.g. [88]). An application conditions of a real tokamak was made for Alcator-C-Mod [89, 90]. In this case EIRENE was used to simulate the neutral pressure in the divertor plenum (gas box) with plasma background reconstructed from the experimental measurements. The first attempt to model it with DEGAS 2 code gave results a factor 10 lower than the measured pressure 25 mTorr. Including, in particular, neutral-neutral collisions lead to a calculated pressure 11 mTorr. However, neutral-neutral collisions were only one among the new features implemented in those calculations. It is difficult also to say what is responsible for the remaining discrepancy with experiment, especially taking into account uncertainties in the reconstruction of the plasma background.

### A.4 Implementing the Track Length Estimator for transfer rates

#### A.4.1 Technical description

The standard option in EIRENE is calculating the momentum and energy sources using the Collisional Estimator (CL). CL calculates directly the momentum and energy transferred in each collision. The resulting sources are the sums over all collisions. The approach described in Chapter 3.1 allows to employ the Track Length Estimator (TL). This could in principle decrease the level of Monte-Carlo noise in the sources in question. However, the numerical tests made so far have shown no clear evidence of such improvement (see Section 3.1.8).

For implementation of TL one first has to calculate the functions  $R_{pt}(E, T)$  and  $I^{(1,2)}(E, T)$  according to formulas (3.36) and (3.39) and to tabulate them. The standard double logarithmic parametric dependence (3.22) is used to fit the data. The corresponding fitting parameters were placed into AMJUEL database [106]: Section H.6 for  $R_{pt}(E, T)$  and Section H.9 for  $I^{(1,2)}(E,T)$ . The functions  $R_{pt}(E,T)$  and  $I^{(1,2)}(E,T)$  for H<sub>2</sub>+H<sup>+</sup> collisions are shown in Figure 3.4.

In the text below, in the names of subroutines and variables the suffix CX corresponds to the Charge Exchange and the suffix EL to the Elastic Collisions. The same markers are used in the EIRENE input file in Block 4 "Input Data for Species Specification and Atomic Physics Module". The main difference between CX and EL process in EIRENE is the following. For CX EIRENE assumes that the scattered particles have the velocity distribution of the incident background ions. It corresponds to the scattering of the particles with equal masses by the angle  $\pi$  in the centre-of-mass frame (subroutine VELOCX). For EL processes (subroutine VELOEL) EIRENE uses the approach described in Section 3.1 and Appendix B.2.

The usage of the pre-computed transfer rates is controlled in the input file, Block 4B, data for individual species, flags IESTCX=2, IESTEL=2 (variables NSECX4 and NSEEL4 inside the code). If this option is switched on, then EIRENE reads  $R_{pt}(E,T)$  and  $I^{(1,2)}(E,T)$  from AMJUEL in subroutines XSTCX and XSTEL and reduces them to dependencies on E only. The information is stored in arrays MOMCX3 and MOMEL3 for  $R_{pt}(E,T)$  and in EPCX3, EPEL3 for  $I^{(1,2)}(E,T)$ . The mass rescaling is performed. Formulas (A.1) and (A.3) are used for charge-exchange and formulas (A.2), (A.4) for elastic collisions. See discussion in Section 3.1.3 and [103]. The masses  $m_{p1}$  and  $m_{t1}$ , see Appendix A.4.2, are taken from the Block 4A, "Data for reaction rates" and  $m_{p2}$ ,  $m_{t2}$  are taken from Block 4B, "Specification of individual species".

During the particle sampling  $R_{pt}$  and  $R_E$  are calculated for the given kinetic energy of the test particle  $E^R$  (energy in the *rest frame* for plasma!) in subroutines FPATHA and FPATHM. The first one works with atoms and the second one with molecules. The energy  $E^R$  is mass-rescaled accordingly. The energy transfer rate in the laboratory frame  $R_E^L$  is calculated using formula (3.42).  $R_{pt}$  and  $R_E$  are stored in the arrays VSIGCX, VSIGEL and ESIGCX, ESIGEL respectively. Variables ESIG\* are used then in subroutine UPDATE to update the energy sources due to atom-plasma and molecule-plasma collisions: tallies EAAT and EAML respectively. Variables VSIG\* are used in subroutine UPTCOP to calculate the parallel momentum sources (tallies COPV) using formula (3.41).

#### A.4.2 Mass rescaling

As it was mentioned in Section 3.1.3 the cross sections calculated for one isotope can be scaled for other isotopes of this element. Two kinds of scaling for the cross-section are considered here:  $\sigma^{(l)}(v_r)$  (3.21) and  $\sigma^{(l)}(E_r)$  (3.21).

Let assume that the integral  $I_1^{(l,n)}$  has been calculated for masses  $m_{p1}$  and  $m_{t1}$  and one needs to calculate a similar integral  $I_2^{(l,n)}$  but for masses  $m_{p2}$  and  $m_{t2}$  assuming certain scaling law for  $\sigma^{(l)}$ .

For the scaling  $\sigma^{(l)}(v_r)$ ,  $v_r = \sqrt{\frac{2T}{m_p}\xi}$  following the definition of  $I^{(l,n)}$  (3.36) one finds:

$$\begin{split} I_{2}^{(l,n)}(E,T) &= \frac{1}{\sqrt{\pi}} \sqrt{\frac{m_{t2}}{2E}} \frac{2T}{m_{p2}} \int_{0}^{\infty} d\xi \xi^{2+n} \sigma^{(l)} \left( \sqrt{\frac{2T}{m_{p2}}} \xi \right) \\ &\left\{ \exp\left[ -\left(\xi - \sqrt{\frac{m_{p2}E}{m_{t2}T}} \right)^{2} \right] - (-1)^{n} \exp\left[ -\left(\xi + \sqrt{\frac{m_{p2}E}{m_{t2}T}} \right)^{2} \right] \right\} \\ &= \frac{1}{\sqrt{\pi}} \sqrt{\frac{m_{t1}}{2\frac{m_{t1}}{m_{t2}}E}} \frac{2\frac{m_{p1}}{m_{p1}}T}{m_{p1}} \int_{0}^{\infty} d\xi \xi^{2+n} \sigma^{(l)} \left( \sqrt{\frac{2\frac{m_{p1}}{m_{p2}}T}{m_{p1}}} \xi \right) \\ &\left\{ \exp\left[ -\left(\xi - \sqrt{\frac{m_{p1}\frac{m_{t1}}{m_{t2}}E}{m_{t1}\frac{m_{p1}}{m_{p2}}T}} \right)^{2} \right] - (-1)^{n} \exp\left[ -\left(\xi + \sqrt{\frac{m_{p1}\frac{m_{t1}}{m_{t2}}E}{m_{t1}\frac{m_{p1}}{m_{p2}}T}} \right)^{2} \right] \right\} \\ &= I_{1}^{(l,n)} (\frac{m_{t1}}{m_{t2}}E, \frac{m_{p1}}{m_{p2}}T) \end{split}$$
(A.1)

In the same way for the scaling  $\sigma^{(l)}(E_r)$ ,  $E_r = \frac{m_r T}{m_p} \xi^2$ :

$$I_{2}^{(l,n)}(E,T) = \frac{1}{\sqrt{\pi}} \sqrt{\frac{m_{l2}}{2E}} \frac{2T}{m_{p2}} \int_{0}^{\infty} d\xi \xi^{2+n} \sigma^{(l)} \left(\frac{m_{r2}T}{m_{p2}}\xi^{2}\right) \\ \left\{ \exp\left[ -\left(\xi - \sqrt{\frac{m_{p2}E}{m_{l2}T}}\right)^{2} \right] - (-1)^{n} \exp\left[ -\left(\xi + \sqrt{\frac{m_{p2}E}{m_{l2}T}}\right)^{2} \right] \right\} \\ = \frac{1}{\sqrt{\pi}} \sqrt{\frac{m_{r1}}{m_{r2}}} \sqrt{\frac{m_{t1}}{2\frac{m_{t1}m_{r2}}{m_{p2}m_{r1}}}} \frac{2\frac{m_{p1}m_{r2}}{m_{p1}}T}{m_{p1}} \int_{0}^{\infty} d\xi \xi^{2+n} \sigma^{(l)} \left(\frac{m_{r}^{1}\frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T}{m_{p1}}\xi^{2}\right) \\ \left\{ \exp\left[ -\left(\xi - \sqrt{\frac{m_{1p}\frac{1}{m_{t1}m_{r2}}E}{m_{t1}\frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T}}\right)^{2} \right] - (-1)^{n} \exp\left[ -\left(\xi + \sqrt{\frac{m_{p1}\frac{m_{t1}m_{r2}}{m_{p2}m_{r1}}T}}\right)^{2} \right] \right\} \\ = \sqrt{\frac{m_{r1}}{m_{t1}\frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T}} I_{1}^{(l,n)} \left(\frac{m_{t1}m_{r2}}{m_{t2}m_{r1}}E}, \frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T}\right) \right] \right\}$$
(A.2)

Formulas (A.1) and (A.2) for I-integrals allow to obtain the similar scaling for momentum transfer rate (3.39). For  $\sigma^{(l)}(v_r)$ :

$$\begin{split} R_{pl}^{2}(E,T) &= m_{r2} \sqrt{\frac{2T}{m_{p2}}} \left[ I_{2}^{(1,1)}(E,T) - \frac{1}{2} \sqrt{\frac{m_{t2}T}{m_{p2}E}} I_{2}^{(1,0)}(E,T) \right] = \\ m_{r1} \frac{m_{r2}}{m_{r1}} \sqrt{\frac{2\frac{m_{p1}}{m_{p2}}T}{m_{p1}}} \left[ I_{1}^{(1,1)} \left( \frac{m_{t1}}{m_{t2}}E, \frac{m_{p1}}{m_{p2}}T \right) - \frac{1}{2} \sqrt{\frac{m_{t1}\frac{m_{p1}}{m_{p2}}T}{m_{p1}\frac{m_{t1}}{m_{t2}}E}} I_{1}^{(1,0)} \left( \frac{m_{t1}}{m_{t2}}E, \frac{m_{p1}}{m_{p2}}T \right) \right] = \\ \frac{m_{r2}}{m_{r1}} R_{pt}^{1} \left( \frac{m_{t1}}{m_{t2}}E, \frac{m_{p1}}{m_{p2}}T \right) \end{split}$$

(A.3)

(A.4)

For  $\sigma^{(l)}(E_r)$ :

$$\begin{split} R_{pt}^{2}(E,T) &= m_{r2} \sqrt{\frac{2T}{m_{p2}}} \left[ I_{2}^{(1,1)}(E,T) - \frac{1}{2} \sqrt{\frac{m_{t2}T}{m_{p2}E}} I_{2}^{(1,0)}(E,T) \right] = \\ m_{r1} \sqrt{\frac{m_{r2}}{m_{r1}}} \sqrt{\frac{2\frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T}{m_{p1}}} \left[ \sqrt{\frac{m_{r1}}{m_{r2}}} I_{1}^{(l,n)} \left( \frac{m_{t1}m_{r2}}{m_{t2}m_{r1}}E, \frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T \right) - \\ \frac{1}{2} \sqrt{\frac{m_{t1}\frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T}{m_{p1}\frac{m_{t1}m_{r2}}{m_{t2}m_{r1}}E}} \sqrt{\frac{m_{r1}}{m_{r2}}} I_{1}^{(l,n)} \left( \frac{m_{t1}m_{r2}}{m_{t2}m_{r1}}E, \frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T \right) \right] = \\ R_{pt}^{1} \left( \frac{m_{t1}m_{r2}}{m_{t2}m_{r1}}E, \frac{m_{p1}m_{r2}}{m_{p2}m_{r1}}T \right) \end{split}$$

The energy transfer rate  $R_E$  does not need special rescaling because it can be calculated using  $R_{pt}$  and  $I^{(1,2)}$ , relation (3.40).

## A.5 Implementation of the photon transport coupled to CRM

The radiation transport option in EIRENE code was developed in the framework of the PhD Thesis by Sven Wiesen [47] and the Diploma Thesis by Petra Börner [48]. The coupling of photon transport and CRM was first implemented for Alcator-C-mod simulations [90] and is further revised in the present work. The current implementation has still a number of drawbacks because some design solutions were taken based on their convenience for programming rather than on the numerical efficiency.

The sampling of the photon trajectories is performed by the same subroutines LOCATE and FOLNEUT as the sampling of neutrals. The photon sources have to be defined as recombination sources in the Input File, Block 7. The spontaneous transition probability serves as a "recombination rate" and the excited states play the role of the "recombining species". They have to be defined in Block 6. Two "recombining species" for each line are considered: for the population coupled to continuum  $n_p^+$  and for the population coupled to the ground state  $n_p^1$ . This splitting into two parts is needed to sample the Doppler shift of the energy of emitted photons, see Chapter 4.2.1. The density  $n_p^+$  is calculated (in subroutine PLASMA\_DERIVE) using the pre-calculated population factors (two examples of them are shown in Figures 4.4a, 4.4a) tabulated in the AMJUEL database. The density  $n_p^1$  is taken from the previous time-step where it is calculated by the CRM, see below. The neutral background for the sampling of photon trajectories (the ground state density  $n_1$ ) is taken from the previous time-step as well. During the sampling the photon absorption rates  $Q_p = B_{1p} n_{ph}^{1p}$  are estimated.

These absorption rates are then used in CRM (4.15) to calculate the populations  $n_p^1$  and the effective ionization rate (4.18). This rate is used on the next time step for the atoms instead of the prescribed ionization rate AMJUEL H.4 2.1.5. Technically all the subroutines related to the CRM are contained (hidden) in the module CCRM. This module is semiself-closed: it uses global variables from other EIRENE modules but it has no own global (public) variables but only public subroutines. Subroutines of module CCRM are called in INPUT (READ\_CRMS) and FIND\_PARAM (FIND\_CRMS) to read the definition of CRM from the input file (Block 4E), in subroutine SETAMD (XSECTEE\_PARAM and XSECTEE) to overload the appropriate reaction rates. The CRM itself (subroutine MODPHT) is called from MODUSR (after MODBGK). MODPHT makes an explicit call of the reduced Sawada code H\_COLRAD (the part related to atoms only). The effective reaction rates are saved together with the background parameters in file FORT.13 (subroutine WRPLAM). On each time-step EIRENE does no extra iterations: the iterative solution of the non-linear problem for photon opacity is combined with the time steps in B2, like for the neutral-neutral collisions.

In the current implementation both the total ionization rate *S* and the total recombination rate *R* are calculated by the CRM and passed to the next time step. On one hand,

if *S* was calculated for the plasma parameters  $(n_e, T_e)$  from the previous step and *R* was calculated for  $(n_e, T_e)$  from the current step, then it could spoil the numerical stability because of appearance of an artificial particle sources (inconsistency between ionization and recombination). In the previous implementation only the photo-induced ionization  $S^{ph}$  was calculated using the CRM, and  $S^e$  and *R* were calculated on the current time-step using the data from AMJUEL. On the other hand, using the reaction rates from the previous time step could slow down the convergence because of introducing an artificial inertia. However, no difference in the numerical stability between these two approaches was found. The reason for this insensitivity is apparently the fact that B2-EIRENE has to use small time steps anyway.

One may feel a temptation to calculate  $S^{ph}$  and  $n_p^1$  before the Monte-Carlo sampling using the rates  $Q_p$  from the previous time step. An attempt to do this led to a numerical instability appearing as an onset of strong oscillations. The reason is not completely clear. It could be an inconsistency between the number of emitted and absorbed photons (artificial photon flux "from the past" or "to the future"). In principle, the fact that populations  $n_p^1$  and  $n_p^+$  are calculated on different time-steps can also produce the same inconsistency. But in the problems which were considered the total population of  $n_2^1$  was always an order of magnitude larger than that of  $n_2^+$  and this level (n=2) is the most significant in the particle balance.

Despite remaining inconsistencies the coupled code (B2-EIRENE) can work sufficiently stable even for severe ITER conditions ("severe" because of high density and large dimensions). The implementation of the iterations will have to be revisited in future. In particular, it will be probably better to sample photons and to calculate the effective rates before sampling the neutrals on each time step. It should be also mentioned that calling the CRM in the iterated code was found to be unpractical because it can take cpu-time comparable to the time needed for the Monte-Carlo sampling itself. The tabulated reaction rates and population coefficients have to be used in future.

### **Appendix B**

# Some details of the model for elastic collisions

#### **B.1** Sampling the incident velocity

To sample the collision event one needs to know the velocity of both colliding partners. The test particle velocity is known by definition. The velocity of the background particle has to be sampled from the distribution with the following probability density:

$$p(\mathbf{v}_p) = \sigma^t(v_r)v_r f_p(\mathbf{v}_p), \quad v_r = |\mathbf{v}_t - \mathbf{v}_p|$$
(B.1)

Here  $f_p(\mathbf{v})$  is the probability density for the velocity distribution of background particles (shifted Maxwellian, Formula (3.10)). It is clear that in general the distribution of the incident particles  $p(\mathbf{v}_p)$  is not the same as the velocity distribution of the background particles  $f_p(\mathbf{v}_p)$ . They are equal only if  $\sigma^t(\mathbf{v}_r)v_r = const$ .

To sample a random variable which has the probability density (B.1) one can use a rejection sampling technique, see e.g. [60], Chapter 7.3. The idea of the rejection sampling as it is applied to this particular case is the following. First, the velocity  $\mathbf{v}_t$  which obeys the distribution function  $f_p(\mathbf{v})$  is sampled. Then the quantity:

$$X = u \cdot \max \left| \left( \sigma(v_r)^t v_r \right) f_p(\mathbf{v}_t) \right|$$

is calculated. Here *u* is a random value distributed uniformly between 0 and 1. The points X fill uniformly the volume under the hypersurface  $Z = \max \left[ \left( \sigma^t(v_r)v_r \right) f_p(\mathbf{v}_t) \right]$  in  $(\mathbf{v}_t, Z)$  space. The hypersurface  $Z = p(\mathbf{v}_t)$  lies under this surface. The subset of the set *X* which meets the following inequality:

$$u \cdot \max\left[\left(\sigma^{t}(v_{r})v_{r}\right)f_{p}(\mathbf{v}_{t})\right] < p(\mathbf{v}_{t}) = \sigma^{t}(v_{r})v_{r}f_{p}(\mathbf{v}_{t})$$
(B.2)

will fill uniformly the volume under  $p(\mathbf{v}_t)$ . Therefore, the corresponding points  $\mathbf{v}_t$  will obey the distribution function (B.1).

This algorithm is implemented in EIRENE in subroutine VELOEL. The implementation is straightforward. The incident velocity  $\mathbf{v}_t$  is sampled from the shifted Maxwellian distribution. After that *u* is sampled. If this pair ( $\mathbf{v}_t$ , *u*) meets the inequality (B.2), then the sampled  $\mathbf{v}_t$  is accepted as the incident particle velocity. Otherwise the next pair ( $\mathbf{v}_t$ , *u*) is sampled and checked.

Instead of rejection sampling an alternative way would be to sample the incident velocity from the shifted Maxwellian and to apply an appropriate modification of the statistical weight, see [44], Section 6. This method was implemented in EIRENE before but it was found that it results in too strong variation of the particle weight causing very bad statistics.

A simplified approach, - sampling the incident velocity from the shifted Maxwellian distribution (that is assuming that  $p(\mathbf{v}_p) = f(\mathbf{v}_p)$ ), - is used in EIRENE as a default option. Although this issue was not studied properly, the experience of calculations shows that the result is not much different from that obtained with rejection sampling.

#### **B.2** Scattering angle

This description follows [44], Section 2. In the case of  $H_2 + H^+$  collision to describe the shot-range repulsive - long-range attractive interaction a Morse-like potential [100] is used:

$$V(r) = \epsilon \left[ e^{2g\left(1 - g\frac{r}{r_m}\right)} - 2e^{g\left(1 - g\frac{r}{r_m}\right)} \right], \quad g = \begin{cases} g_1, r < r_m \\ g_1 g_2, r \ge r_m \end{cases}$$
(B.3)

This function has four free parameters: the potential depth  $\epsilon$ , equilibrium separation  $r_m$  (radius of the minimum potential) and fitting parameters  $g_1$  and  $g_2$ . For  $H_2 + H^+$  collision they were taken from [101].

To calculate the deflection function (3.5) one first has to find the root of the equation:

$$r^2 \sqrt{1 - V(r)/E_r - (b/r)^2} = 0$$
(B.4)

to get the parameter  $r^*$ . The root-finding routine was optimised making use of the specific properties of the potential (B.3). The important characteristic parameters of this function are the root  $r_0$  and the point of inflection  $r_w$ :

$$r_0 = r_m \left( 1 - \frac{\ln 2}{g} \right), \quad r_w = r_m \left( 1 + \frac{\ln 2}{g} \right)$$
 (B.5)

If  $\alpha = E_r b^2$  is larger than a certain  $\alpha_c$  the potential (B.3) becomes monotonic function (without minimum). The critical parameters  $\alpha_c$ ,  $r_c$  are found by solving the algebraic equations:

$$V_{eff} = V(r) + \frac{\alpha}{r^2}, \quad \frac{dV_{eff}}{dr} = 0 \text{ and } \frac{d^2V_{eff}}{dr^2} = 0$$

Therefore, eliminating  $\alpha$  yields:

$$h(r) = \frac{3}{2}\frac{dV}{dr} + \frac{r}{2}\frac{d^2V}{dr^2} = 0$$

Solving this algebraic equation one finds  $r_c$ . Other parameters at the critical point can be calculated as:

$$p = \frac{r_c g}{r_m}, \quad E_{rc} = \epsilon \frac{(p-3)(p^2 - 3p + 3)}{(2p-3)^2},$$

$$b_c = \frac{pr_c}{\sqrt{p^2 - 3p + 3}}, \quad \alpha_c = E_{rc} b_c^2$$
(B.6)

For the known parameters  $r_0$ ,  $r_m$ ,  $r_w$ ,  $r_c$  the location of the root  $r^*$  is summarised in the scheme below:

$$\begin{cases} 0 < b \le r_0, & 1 \text{ root } b < r^* \le r_0 \\ r_0 < b \le r_w, & 1 \text{ root } r_0 < r^* \le r_w \\ \mu < 1, \begin{cases} \mu b_c < r_w, & 1 \text{ root } r^* > r_0 \\ \mu b_c \ge r_w, \begin{cases} r_w < b \le \mu b_c, & 1 \text{ root } r^* > r_c \\ b \le \mu b_c, & 1 \text{ root } r^* > r_c \end{cases} \\ \mu \ge 1, \begin{cases} r_w < b < \mu b_c, & 1, 2 \text{ or } 3 \text{ roots } r^* = \max(r_i) > r_w \\ b > \mu b_c, & 1 \text{ root } r^* \ge r_c \end{cases} \end{cases}$$
(B.7)

The sampling of the deflection angle  $\Theta$  (or deflection function  $\chi$ ) is implemented in EIRENE as following. The data array:

$$\mathbf{R} = \{\epsilon, g_1, g_2, r_m, r_0, r_w, r_c, b_c, E_{rc}, E_{r0}\}$$

is read from the datafile AMJUEL [106], Section H.0 (e.g. AMJUEL H.0 0.3T for H<sub>2</sub>). The energy  $E_r$  is calculated from the known  $\mathbf{v}_t$  and  $\mathbf{v}_p$ , see Section B.1. Here  $b_{max}$  is found from the condition:  $\sigma^t = \pi b_{max}^2$ . After that  $r^*$  is calculated by solving the algebraic equation (B.4) using its properties (B.7) (subroutine RSTERN, uses modified bisection method). To find the deflection function  $\chi$  the integral (3.5) is calculated using a Gauss-Mehler type quadrature rule with 16 nodes (subroutine GAUMEH), which is enough to achieve the relative error less than 1 % [44].

## **Appendix C**

# Notations for vector and tensor operations

To avoid misunderstanding the notations for the tensor and vector operations used in Chapter 2 of this thesis are listed in this appendix. Here "tensor" means tensor of rank 2. The notations are the same as in the monograph of Chapman and Cowling [58].

Dyadic of two vectors  $\mathbf{a} = (a_x, a_y, a_z)$  and  $\mathbf{b} = (b_x, b_y, b_z)$  is a tensor defined as:

$$\mathbf{ab} = \begin{pmatrix} a_x b_x & a_x b_y & a_x b_z \\ a_y b_x & a_y b_y & a_y b_z \\ a_z b_x & a_z b_y & a_z b_z \end{pmatrix} = a_\alpha b_\beta$$

Note that in general  $ab \neq ba$ . This operation should not be mixed up with the scalar product (!):

$$\mathbf{a} \cdot \mathbf{b} = (a_x b_x, a_y b_y, a_z b_z)$$

Let us define a tensor w:

$$\mathbf{w} = \begin{pmatrix} w_{xx} & w_{xy} & w_{xz} \\ w_{yx} & w_{yy} & w_{yz} \\ w_{zx} & w_{zy} & w_{zz} \end{pmatrix} = w_{\alpha\beta}$$

A tensor, conjugate to **w** is defined as  $\overline{\mathbf{w}} = w_{\beta\alpha}$ . Its matrix is transposition of that of **w**. A symmetrical tensor corresponding to **w**:  $\overline{\overline{\mathbf{w}}} = \frac{1}{2}(\overline{\mathbf{w}} + \mathbf{w})$ 

Divergence (Spur) of the tensor:  $w_{xx} + w_{yy} + w_{zz}$ 

Upon defined a unit tensor  $U = \delta_{\alpha\beta}$  (Kronecker Symbol, unit matrix), a non-divergent tensor corresponding to w can be written as:

$$\mathbf{\mathring{w}} = \mathbf{w} - \frac{1}{3}(w_{xx} + w_{yy} + w_{zz})\mathbf{U}$$

A product of a vector **a** and a tensor **w**:

$$(\mathbf{a}.\mathbf{w})_{\alpha} = \sum_{\beta} w_{\alpha\beta} a_{\beta}$$

The result is a vector with coordinates found from matrix multiplication.

A simple product of two tensors w and  $w^\prime\colon$ 

$$(\mathbf{w}.\mathbf{w}')_{\alpha\beta} = \sum_{\gamma} w_{\alpha\gamma} w'_{\gamma\beta}$$

The result is a tensor with coordinates found from matrix multiplication. A double product of two tensors:

$$\mathbf{w}:\mathbf{w}'=\sum_{\alpha}\sum_{\beta}w_{\alpha\beta}w'_{\beta\alpha}=\mathbf{w}':\mathbf{w}$$

The result is a scalar equal to the divergence (Spur) of w.w'

## **Appendix D**

# Hydrogen molecular chemistry in ITER: some examples



Figure D.1: Density of molecular ion  $D_2^+$  for the old and new model for molecular kinetics (on a fixed plasma background)



Figure D.2: The total ionization ( $D_2 \rightarrow D_2^+$ ) and dissociation ( $D_2 \rightarrow 2D$ ) sinks of D<sub>2</sub> molecules



Figure D.3: Processes relevant for molecular ion  $D_2^+$  and the rate of atomic recombination for comparison

## **Appendix E**

## **Results of the JET modelling**

 $2\mathrm{D}$  distributions of the plasma parameters in the divertor of JET calculated with EIRENE 1996 and new EIRENE.



### E.1 Shot #58354 ("High Density")

Figure E.1: Electron temperature



Figure E.2: Electron density



Figure E.3: Density of D<sub>2</sub> molecules



Figure E.4: Density of D atoms



Figure E.5: Ionization sink of D atoms



Figure E.6: Photo-induced ionization source and the temperature of molecules


Figure E.7: The effect of the line radiation opacity: zoom in the inner divertor

## E.2 Shot #58353 ("Low Density")



Figure E.8: Electron temperature



Figure E.9: Electron density



Figure E.10: Density of D<sub>2</sub> molecules



Figure E.11: Density of D atoms



Figure E.12: Ionization sink of D atoms