THE EIRENE AND B2-EIRENE CODES

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The EIRENE neutral gas transport Monte Carlo code has been developed initially for TEXTOR since the early 1980s. It is currently applied worldwide in most fusion laboratories for a large variety of different purposes. The main goal of code development was to provide a tool to investigate neutral gas transport in magnetically confined plasmas. But, due to its flexibility, it also can be used to solve more general linear kinetic transport equations by applying a stochastic rather than a numerical or analytical method of solution. Major applications of EIRENE are in connection with plasma fluid codes, in particular with the various versions of the B2 two-dimensional plasma edge fluid code. The combined code package B2-EIRENE was developed, again initially for TEXTOR applications, in the late 1980s. It too has become a standard tool in plasma edge science. It is currently mainly used for divertor configurations, such as by the ITER central team, to assist the design of the ITER divertor. Both the EIRENE and B2-EIRENE concepts are introduced and illustrated with sample applications.

KEYWORDS: *neutral gas transport, EIRENE code, B2-EIRENE code*

I. INTRODUCTION

Neutral particle effects play a key role in fusion edge plasma physics because they influence and sometimes dominate the plasma dynamics and the experimental identification. Monte Carlo treatments are often preferred because they allow straightforward inclusion of many details and because they remain transparent despite complexity of the physical model. They are subject to statistical noise rather than numerical discretization errors or unjustified simplifications, but this noise level is readily available. Error estimates are obtained from the method itself.

The three-dimensional EIRENE neutral gas Monte Carlo code[1] has been developed initially for TEXTOR (Ref. 2) applications, since the early 1980s, as a stand-alone kinetic neutral particle transport model.[3,4] Since then it has had many applications in a large number of fusion research projects and by a large number of people, for tokamaks other than TEXTOR, for stellarators, and even for outside fusion research. Since about 1987 major applications of the EIRENE code have also been in connection with two-dimensional and later also with three-dimensional plasma edge fluid codes, in particular with the various versions of the two-dimensional B2 code and the three-dimensional EMC3 code. The low recycling conditions in TEXTOR with its ALT limiters[5] did not require special numerical attention other than the internal consistency between plasma flow and neutrals dynamics via boundary conditions at the recycling targets. This turned out not to be the case for the very strong recycling (highly nonlinear) conditions studied for the ITER (INTOR) (Ref. 6) divertor at that time. Special semi-implicit iterative coupling methods had been developed to deal with this numerical complexity with the computing power available then, until first converged two-dimensional plasma fluid neutral kinetic B2-EIRENE had been obtained for high recycling ITER conditions.[7–9] Since then coupled neutral Monte Carlo plasma fluid ("micro-macro") models have become a standard tool in edge plasma science, although semianalytic[10] or numerical (diffusion- or Navier-Stokes approximation) neutral models[11] often result in an overall much more robust code package. In any case the statistical approach may describe a physical process more faithfully, even partially, by indirectly modeling underlying small-scale phenomena. Some correlations and fluctuations vanish in the thermodynamical limit. However, if a system is close to instability or has more than one possible solution (such

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as high recycling/detached divertor states), such fluctuations may affect the loss of stability, cause bifurcations or jumps between two admissible solutions, and cause occurrence of singularities that cannot be detected by studying a deterministic model of such processes.

We close this introduction with a short historical overview. The main concept of the EIRENE code will briefly be described in Sec. II. Some stand-alone EIRENE applications, in a given, e.g., from experimental data reconstructed, plasma background are summarized in Sec. III.

The B2-EIRENE concept of consistently coupling a Monte Carlo kinetic neutral gas treatment with an edge plasma fluid code is outlined in Sec. IV, again with some sample applications in Sec. V.

Very recent developments and an outlook to possible future extensions of EIRENE and its interfaces to plasma codes are given in the concluding Sec. VI.

Historically the EIRENE work began in 1980 as an extension and upgrade of the then-famous (and probably first in fusion science) one-dimensional AURORA neutral particle Monte Carlo code.[12] The aim was a quantitative assessment of recycling effects in possible limiter and/or divertor configurations discussed for TEXTOR, prior to its operation, in those days. It was referred to as "NAurora" in its first published applications[3] and references therein.

This was roughly parallel in time with a similar code project (also based on AURORA) at Princeton Plasma Physics Laboratory[13] that had resulted in the DEGAS code there.

And, again roughly at the same time, a third neutral particle Monte Carlo code for fusion applications, NIMBUS, was adapted from a neutron shielding and transport package to fusion edge plasma atomic physics studies for the Joint European Torus[14] (JET).

These three codes, together with the Monte Carlo neutral gas package in the two-dimensional edge code DDC83 (former Soviet Union, A. Kukushkin), have later been benchmarked during the INTOR phase and, if run on identical reference cases and atomic data, also led to satisfactory agreement.[15–18]

The codes differed at that time by the description and options of geometrical details and by the statistical estimating technique but not significantly by their physical model, which, moreover, was carefully compared and exchanged between the then-responsible authors.

The EIRENE code resorts to a combinatorial discretization of general three-dimensional computational domains using unions and intersections of first- and second-order surfaces to construct cells and cell boundaries. This has made it particularly flexible for geometry optimization studies of vacuum pumping systems (pump limiters) because complex three-dimensional boundary structures (internal or external) could easily be implemented into structured grids without necessity to construct complex unstructured three-dimensional meshes for discretization. All surface-averaged quantities (fluxes) are estimated correctly without need for a spatial discretization of the volumes first (see Fig. 1).

In the mid-1980s the first two-dimensional plasma edge fluid codes became available, notably also the B2 (Braams) code.[19] A number of efforts had then been undertaken to couple these two-dimensional plasma fluid models to the neutral particle kinetic Monte Carlo codes in order to achieve computational self-consistency between the edge plasma transport and the recycling process. In Europe the "Next European Torus" (NET) team (EURATOM) had started with B2-NIMBUS (a development carried out jointly at JET and at AEA Culham), at IPP Garching a B2-DEGAS coupling was attempted for ASDEX (Ref. 20), and at KFA Jülich (now Forschungszentrum Jülich) the B2-EIRENE code package was developed for TEXTOR and ITER. Later the Culham group (G. Maddison, E. Hotston) joined the TEXTOR team, and B2-EIRENE became a NET (EURATOM)–sponsored project among KFA Jülich, AEA Culham, and ERM Brussels (M. Baelmans[21]). Since then the B2-EIRENE code has been applied to many other existing tokamaks, mainly to divertor edge plasma configurations, such as ASDEX, ASDEX-Upgrade (Ref. 22), JET (Ref. 23), and many others. It is, since the early 1990s, also used by the ITER team, both in the ITER physics design phase and currently still in the engineering design phase,[24] to quantify

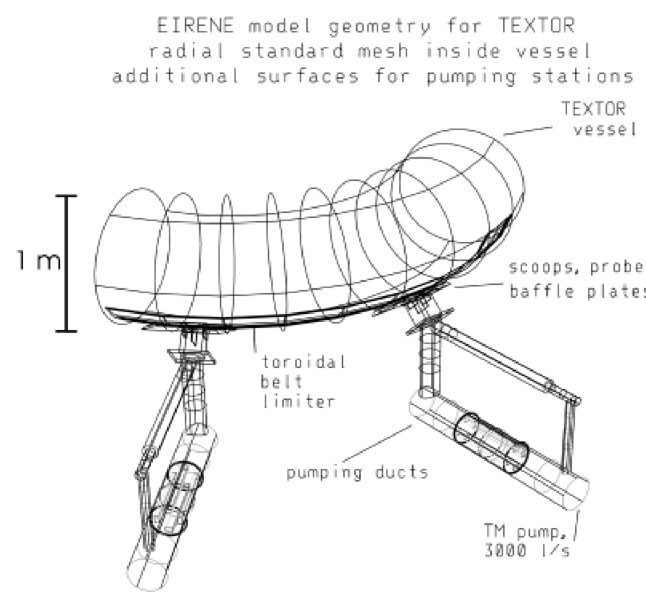

Fig. 1. An early three-dimensional EIRENE geometry for the TEXTOR–ALT-II configuration (about 1985). Two-dimensional spatial discretization inside the vacuum vessel by structured grids (see Fig. 3) supplemented with additional surfaces to describe detailed three-dimensional pumping stations at eight toroidal locations outside the vessel (only two of the pumping stations are shown here).

the possible role of at least those plasma edge effects, which have been identified already, in a most consistent and detailed way of complex bookkeeping possible today.

II. CONCEPT OF THE EIRENE CODE

EIRENE is a multispecies code solving simultaneously a system of time dependent (optional) or stationary (default) linear kinetic transport equations of almost arbitrary complexity in a given host medium (background). A crude model for transport of ionized particles along magnetic field lines was also included in the mid-1980s because of applications to hydrocarbon breakup via intermediate charged states (hydrocarbon molecular ions). EIRENE is coupled to external databases for atomic and molecular data and for surface reflection data, and it calls various user-supplied routines, e.g., for exchange of data with other (fluid-) transport codes. The main goal of code development was to provide a tool to investigate neutral gas transport in magnetically confined plasmas. But, due to its flexibility, it also can be used to solve more general linear kinetic transport equations by applying a stochastic rather than a numerical or analytical method of solution. In particular, options are retained to reduce the model equations to the theoretically important case of the one-speed transport problem (photon transport, i.e., radiation transfer, in particular). A tree of flowcharts on the code structure is maintained at the Internet site http://www.eirene.de (Ref. 1). The lowest and most general level of these flowcharts is shown in Fig. 2. The iterative mode indicated also in Fig. 2 is needed for treatment of any kind of nonlinear effects within the neutral particle model on fixed plasma (background) conditions, such as for accounting of neutral-neutral collisions.[25] These internal iterations become redundant if the plasma background response on the neutral gas transport is explicitly taken into account because then the coupled neutral-plasma problem is solved by iterations between EIRENE and the plasma code anyway (see Sec. IV).

II.A. The Generic EIRENE Equation

Details of the physical, mathematical, and numerical concept of the EIRENE code can be found on its home page: http://www.eirene.de (Ref. 1). In this section only some very brief general aspects are summarized. The EIRENE code solves the well-known system of Boltzmann equations for the one-particle distribution functions f_i in full six-dimensional phase space $[\vec{r},\vec{v}]$, but usually with linear collision operators only (test-particle approximation); i is a species labeling index. It mostly uses conventional Monte Carlo methods for linear transport problems,[26] as originally developed for neutron transport problems in the middle of the 20th century.

By adding, in a quite symmetric fashion with the velocity coordinates, a discrete species index i (labeling the chemical species and/or the internal excited state) to the phase space, this coupled system of equations becomes just a single Boltzmann equation, now in "6.5-dimensional phase space" $[\vec{r},\vec{v},i]$. Similarly, time t can be added to the phase space, formally symmetric with the spatial coordinates, to render the phase space 7.5-dimensional. Complexity of Monte Carlo schemes is usually quite insensitive to such increased dimensionality of phase space.[27]

By formally integrating the characteristics for this equation for f it can also be written in integral form. For example, for the precollision density Ψ, with $\Psi = \Sigma \cdot v \cdot f$ (density of particles in phase space volume entering a collision, per unit time) this prototypical equation of the EIRENE code reads

$$\Psi(x) = S(x) + \int dx'\,\Psi(x') \cdot K(x' \to x) \ . \tag{1}$$

Here, x is the independent phase space variable, e.g., $x = [\vec{r},\vec{v},i,t]$, and Σ is the "macroscopic cross section" (inverse mean free path). This equation has the general form of the backward integral equation of a Markovian jump process with initial distribution S and transition kernel K. It is therefore particularly well suited for a Monte Carlo method of solution. A direct intuitive interpretation of the integral equation is already sufficient to understand the Monte Carlo method of solution, which is employed in the EIRENE code.

In Eq. (1) x' and x are the states at two successive collisions (jumps). The integral $\int dx$ is to be understood as an integral over physical space and over velocity space and a summation over all species indices. The transition kernel K is usually decomposed, in our context, into a collision and a transport kernel, i.e., into C and T, where

$$K(\underline{r}',\underline{v}',i' \to \underline{r},\underline{v},i) = C(\underline{r}';\underline{v}',i' \to \underline{v},i) \times T(\underline{v},i;\underline{r}' \to \underline{r}) \ . \tag{2}$$

The kernel C is (excluding normalization) the conditional distribution for new coordinates $[\underline{v},i]$ given that a particle of species i' and with velocity $\underline{v}'$ has undergone a collision at position $\underline{r}'$ [or at $(\underline{r}',t')$]. This kernel can further be decomposed into

$$C(\underline{r}',\underline{v}',i' \to \underline{v},i) = \sum_k p_k\, C_k(\underline{r}';\underline{v}',i' \to \underline{v},i) \ ,$$

$$p_k = \frac{\Sigma_k}{\Sigma_t} \ , \tag{3}$$

with summation over the index k for the different types of collision processes (charge exchange, elastic, dissociation, etc.) under consideration and p_k defined as the

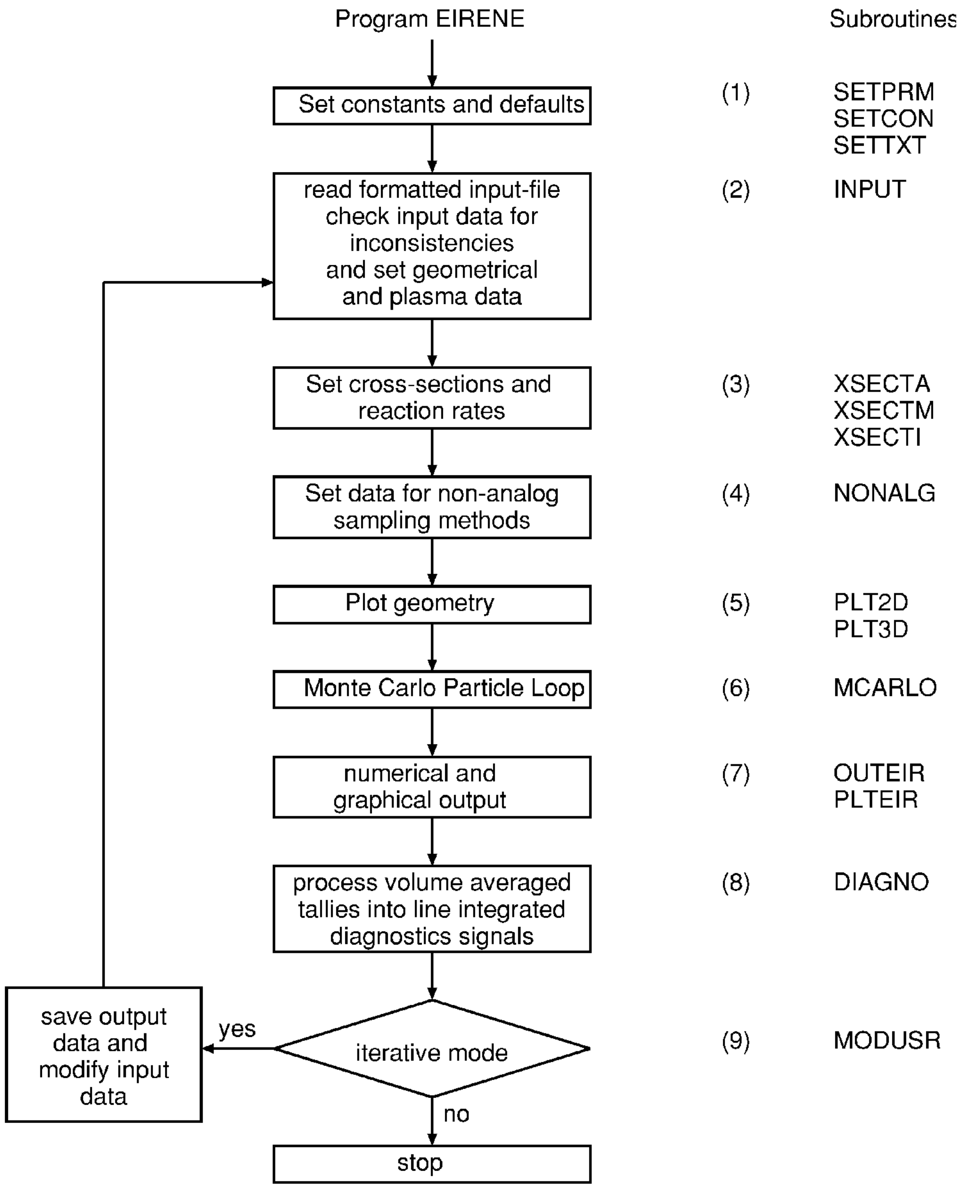

Fig. 2. Flowchart of EIRENE Monte Carlo Solver for Boltzmann equation, lowest level, showing only the basic structure. The numbers and names of programs on the right refer to further flowcharts at higher levels of an entire tree of flowcharts.

(conditional) probability for a collision to be of type k. The normalizing factor

$$c_k(x') = \sum_i \int d\underline{v}\, C_k(\underline{r}', \underline{v}', i' \rightarrow \underline{v}, i) \qquad (4)$$

gives the mean number of secondaries for this collision process k. For example, due to dissociation of H_2 molecules into two H atoms we are dealing here with a branching process. Absorption (ending a particle history) is due to either escape from the system (e.g., pumping at selected surfaces) or due to ionization (loss from the community of test particle species, into the host medium, here mostly: the edge plasma of fusion devices).

All parameters in this kernel are determined by the collision kinetics, i.e., from the local plasma data at $\underline{r}$, the test particle velocity $\underline{v}$, and the data in the atomic and surface data files (see Sec. II.B).

The kernel T describes the motion of the test particles between the collision events, and it is determined, again, by the local plasma data, the test particle velocity, and the collision rates from the atomic data files.

The inhomogeneity S in Eq. (1) is, excluding normalization, the distribution density of first collisions, whereas the integral term in Eq. (1) describes the contribution to Ψ from all higher generations ("secondary source"). The quantity S can be written as

$$S(x) = \int dx' \, Q(x') \cdot T(x' \to x) \ , \qquad (5)$$

with the "true physical" primary source density Q (such as recycling, gas puff, etc.). As the problem is linear, Q can be normalized to 1 and, thus, Q can be considered a distribution density in phase space for the "primary" birth points of particles.

It can be shown that a unique solution $\Psi(x)$ exists subject to appropriate boundary conditions and under only mild restrictions (basically on the constants c_k and p_a) to ensure that the particle generation process stays subcritical.

Usually, detailed knowledge of f or Ψ is not required, only a set of linear functionals of the dependent variable ("responses"), R, defined by

$$R = \langle \Psi | g_c \rangle = \int dx \, \Psi(x) \cdot g_c(x)$$

$$\left(= \langle f | g_t \rangle = \int dx f(x) \cdot g_t(x) \right) \ , \qquad (6)$$

where $g_c(x)$, $g_t(x)$ are weighting functions (so-called "detector functions") that can freely be chosen depending on the particular quantity of interest.

For example, all terms in the plasma fluid equations resulting from neutral plasma interaction can be written in this way. This fact is used when coupling EIRENE to plasma fluid models, for example, as in the B2-EIRENE code system (see Sec. IV). Equation (6) also shows that Monte Carlo source terms in coupled micro-macro models are integrals over cells of the computational grid and therefore particularly well suited for finite volume– or finite element–discretized fluid models.

II.B. Atomic and Surface Processes

The EIRENE code was the first neutral particle fusion code with an automated interface to external atomic, molecular, and surface databases. About 1987 it was linked to the data collection[28] for hydrogen (atomic and molecular) and helium particles in plasmas, and the collision processes to be included in a particular application could be picked, via the EIRENE-input file, from the table of contents of that book. In the same year the Ehrhardt-Langer database[29] for methane breakup also was added in a similar fashion, as well as a number of collisional radiative models (helium, hydrogen atoms and molecules, etc.) to separate fast (transitions between excited states) from slow (neutral gas transport) timescales. Surface reflection databases consisting of precomputed surface reflectivities as functions of material, incident energy and angle, and emerging energy and angle have been compiled and also linked to the EIRENE code.[30] These very general options to define a particular simulation model have made EIRENE a rather difficult tool to use because any user needs to decide by himself about the relevant processes. On the other hand it resulted in a very high level of flexibility with respect to the physics model.

Recently the collision databases for the methane, ethane, and propane families of hydrocarbons[31] as well as for hydrogenic particles ($H, H_2, H^-, H_2^+, H_3^+$), including also their electronic and vibrationally excited states, have been critically assessed, completed, and re-compiled.[32] These have already partly been implemented into the EIRENE code atomic databases. The current goal, as in other plasma edge particle codes specialized for impurity transport (ERO-TEXTOR), must be to simplify the kinetic schemes without sacrificing accuracy by developing appropriate operator splitting schemes to separate the fast and slow timescales.

Elastic collisions between neutral particles and plasma ions have long been neglected in tokamak neutral gas transport modeling. In the early 1990s a database for such collisions suitable for Monte Carlo schemes was both established (Ref. 33 and references therein) and implemented into EIRENE. The relevance in particular of the elastic helium-proton system for helium pumping was identified, caused by the absence of any other significant competing entropy-producing process (such as resonant charge exchange in case of the hydrogen-proton collision system) for neutral helium in edge plasmas. The classical collision formulation adopted in EIRENE proved to be in fairly good agreement with later quantal calculations.[34] Actually, the agreement of the physically most relevant momentum transfer cross section is better than indicated there (Fig. 14 on p. 48 in Ref. 34), if one corrects the labeling of the curves (exchange the viscosity cross-section label with the momentum transfer cross-section label) and properly accounts for the fact that the energy scale in Ref. 33 has been the proton energy but that in Ref. 34 is the (reduced mass) collision energy.

Of course, the issue of indistinguishability of "true" elastic and resonant charge exchange collisions (e.g., the p + H collision system) had to be carefully addressed to avoid double counting. In the terminology of the full quantum mechanical approach in Ref. 34, "elastic cross section" already refers to the sum of both components, whereas in neutral gas modeling it was common practice to add individual cross sections or rate coefficients of all specific reaction channels. Furthermore, it is important to note that the total cross section in the classical formulation has no physical meaning at all (it is infinite), and a formally introduced finite total cross section is instead just needed to define a numerical step size or a mean free path of Monte Carlo histories.[33] This had led to misunderstandings, e.g., when comparing this purely numerical parameter with the total cross section evaluated from quantal calculations. The latter, of course, does have a clear physical significance.

III. SAMPLE APPLICATIONS OF EIRENE

The EIRENE code has been applied to a number of issues related to TEXTOR experiments since the early 1980s. Interpretation of ion temperature measurements as inferred from the high-energy tail of charge exchange spectra has been carried out (as already outlined in Ref. 12) using a precomputed large set of modeled spectra with known correlation to the central ion temperature and a principal component analysis for data reduction. Later this method was also used for the low-energy spectra (edge ion temperature measurements) obtained by time of flight analysis at the ASDEX tokamak.[35]

The ALT-I and ALT-II pump limiter experiments have been analyzed using detailed three-dimensional models comprising the scoop and the neutral plasma interaction there as well as the entire pumping system.[5,36–38] The beneficial effect of plasma plugging (enhanced pumping efficiency due to reionization of neutrals inside the scoops) could be quantified correctly. This "validated" EIRENE ALT-II modeling strategy was then used during the pump-limiter study at JET (1985 to 1988) (Ref. 39) and contributed significantly to the final strategic decision of not installing a pump limiter at JET. The Tore-Supra "CIEL" pump limiter also has been designed and is currently being analyzed with the help of dedicated three-dimensional EIRENE applications along similar lines.[40]

The bulk of the TEXTOR scrape-off layer (SOL) outside the ALT-II scoops is typically modeled in a two-dimensional, toroidally symmetric approximation for the neutral gas transport, i.e., ignoring, for convenience, any protruding elements (antennas, test limiters). Such a computational grid for TEXTOR is shown in Fig. 3.

For example, in Ref. 41 a comparison of such two-dimensional experimental and simulated Balmer light emissivities near the ALT-II limiter blade is discussed; see Fig. 4 for a typical H_α pattern resulting from these studies.

These, and most other applications of EIRENE to neutral particle transport in the TEXTOR SOL and core, for example,[42] are usually based on a numerical reconstruction of the two-dimensional edge (and one-dimensional core) plasma host medium from the available diagnostic data. Under more complex conditions, e.g., for divertors, this edge plasma reconstruction can also be carried out by so-called "onion skin modeling" linked with EIRENE (OEDGE modeling[43]).

The goal in such stand-alone EIRENE applications to TEXTOR is typically not to match experimental results but instead to identify possible missing physics in edge plasma science by detailed bookkeeping of all known processes.

The numerical challenge for modeling the TEXTOR–ALT-II boundary plasma has an origin quite different from that when modeling high recycling or even detached divertor SOLs. In the former case the strong nonlinear coupling between neutral gas and plasma, as is typical for the latter, is absent. Instead the target surfaces are often very strongly inclined (almost parallel) to the magnetic field direction. This results in pronounced sensitivity to (still unresolved) basic physical questions such as those of appropriate boundary (sheath) conditions there.

For example, having eliminated all potential configurational and two-dimensional neutral particle transport effects by the detailed Monte Carlo simulation and comparing figures like Fig. 4 with experimental H_α patterns for a series of shots,[41] the remaining discrepancies in H_α intensity profiles had led to the clear identification of "incomplete edge physics understanding" with respect to recycling at (near) parallel target surfaces (i.e., also at the important baffling structures in divertors). This issue was later further investigated using the TEXTOR version of the B2-EIRENE code system (Sec. IV), applied to idealized model conditions dedicated to isolate this particular question.[44] It had required a significant generalization of the B2 code with respect to its numerical finite volume implementation to cope with the locally strongly nonorthogonal grids near the ALT-limiter blades and the inner bumper limiter. This scheme was employed for studying the effect of a possible "funneling action" of parallel (aligned or nearly aligned) surfaces on ALT-II in TEXTOR (Ref. 44). It had led to some clear modeling support of an earlier simpler ad hoc "funneling" model (Ref. 45, Sec. 25.2), but the entire issue still does not seem to be finally settled.

Knowing the full distribution in phase space of the neutral gas from an EIRENE solution [solution of Eq. (1)], further parameters can be obtained by integration over a proper lower dimensional manifold [proper choice of detector function g in Eq. (6)], which can directly be compared to experimental data. Balmer-α light emission from specified observational volumes near recycling surfaces (as shown in Fig. 4) is one example. Matching absolute intensities between modeling and experiment can then be used to infer the correct conversion factor between light emission and recycling particle fluxes for any specific configuration and condition.

The general concept of detector functions and responses [Eq. (6)] allows a quite flexible shifting between achievable resolution in physical and velocity space for fixed CPU storage requirements. Three-dimensional recycling effects from local "rail limiters" have been studied already from the very beginning of the EIRENE applications at TEXTOR (Refs. 3, 4, and 46). Resolution has always been limited by the computing systems available at each time, for example, to about (30, 20, 30) cells in radial, poloidal, and toroidal direction in the early 1980s. In Ref. 46 a comparison of experimental and simulated Balmer-α frequency resolved line shapes, as observed near a test limiter in TEXTOR, is carried out. Here, the spatial resolution was restricted to the observational volume of the spectrometer, and the gained storage was used for velocity space resolution in the direction

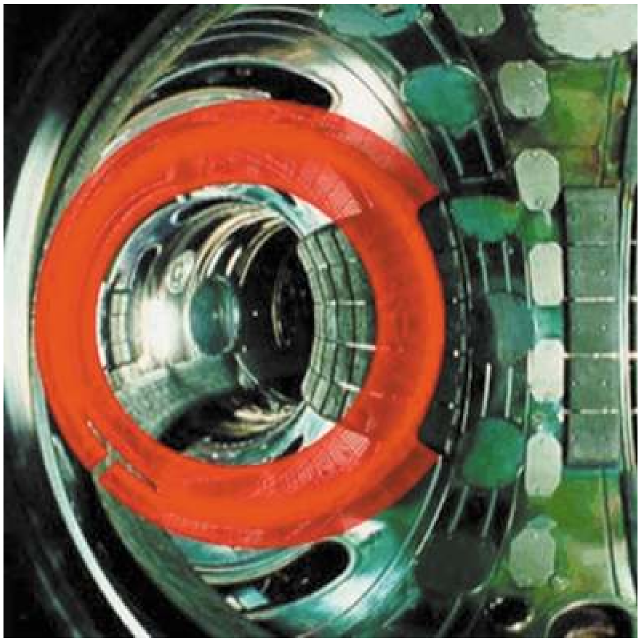

Fig. 3. Two-dimensional spatial grid in poloidal plane of TEXTOR (minor radius: 50 cm) with detailed discretization of the region near ALT-II belt limiter.

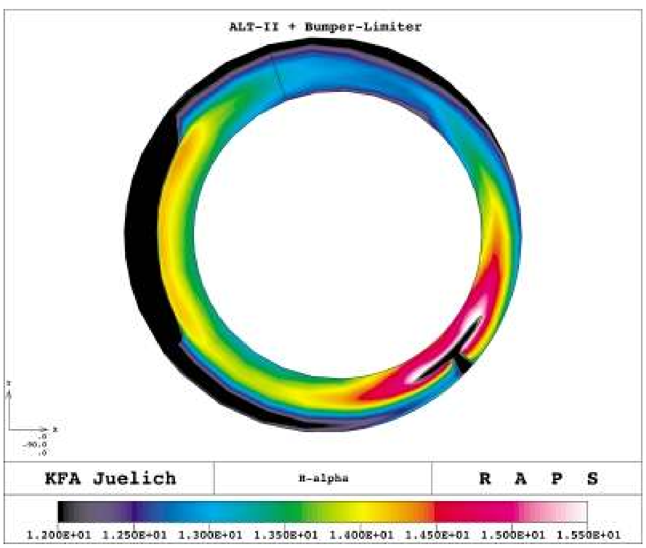

Fig. 4. Typical Balmer-α emission pattern near ALT-II limiter blade, as used for two-dimensional edge model assessments (color shading corresponds to a logarithmic scale, arbitrary units). The clear identification of some missing physics in present edge codes concerning recycling at almost parallel surfaces, here midway between the limiter tips, was possible by computationally eliminating most other possible complicating effects with EIRENE.

of the lines of sight. Using this combination of high-resolution spectrometer and the EIRENE code had allowed a rather direct assessment of both surface reflection models and hydrogen molecule breakup kinetics in neutral transport models.[46]

The observed velocity space effects are consistent with a rather subtle effect of neutral gas recycling near target surfaces, which is shown in the two-dimensional profile (averaged over toroidal direction and velocity space) in Fig. 5. In simple estimates the neutrals are usually assumed to cool the edge plasma because of ionization and radiation losses. As seen here, locally, at least for the ion component, the opposite may be true because of sheath acceleration of ions, reflection as energetic atoms and subsequent charge exchange between atoms and ions, or ionization, with atoms having an energy higher than the average ion energy (3/2 Ti) (see also Ref. 45, Sec. 2.9i). Peak ion heating terms near the upper ALT-limiter tip can be of the order of 1.5×10^5 W/m^3 in TEXTOR.

Similar studies on Balmer-line shapes have subsequently been carried out at other machines, for example, at JT-60U for a divertor configuration but with similar plasma temperatures as in the TEXTOR cases, using the DEGAS code[47] there, and with findings consistent to those from the earlier TEXTOR studies.

Only much more recently have the effects of hydrogenic molecules on edge plasma conditions become accessible through Fulcher band spectroscopy (see also Sec. V). Using a similar three-dimensional modeling strategy near the test limiter in TEXTOR as above, the spatial profiles of this band emission were obtained and compared with experimental data.[48] Spatial emission profiles

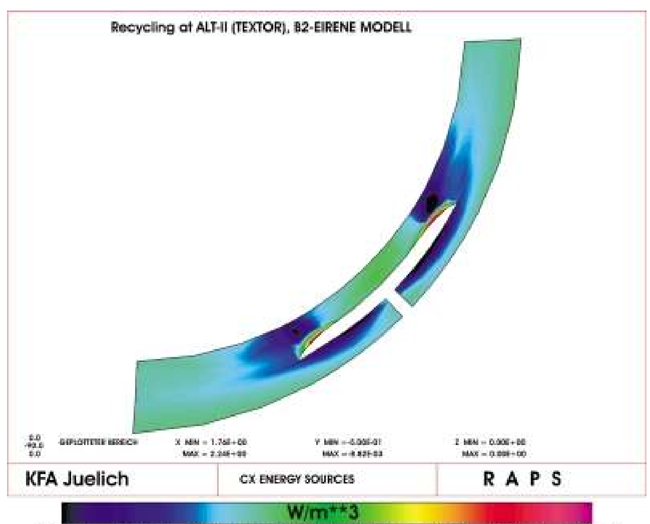

Fig. 5. Charge exchange energy loss/gain for ions near ALT-II blade because of recycling, showing a change in sign (a gain region) very near the target, with a charge exchange ion heating source of $\sim 1.5 \times 10^5$ W/m^2.

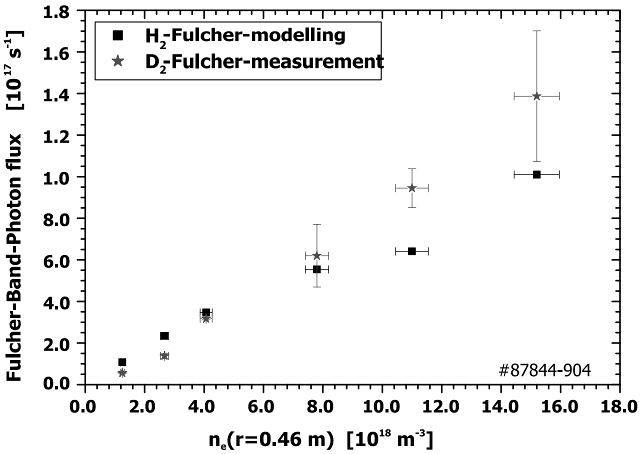

Fig. 6. Comparison of total Fulcher band photon fluxes near a test limiter from TEXTOR spectroscopy (asterisks) and EIRENE simulation (squares) versus electron density.

are again found to be quite sensitive to plasma and sheath conditions near the limiter (same as with the Balmer lines near limiters; see above). By integration over the observational volume (both in simulation and in experiment), quite satisfactory agreement can robustly be achieved under moderate plasma density conditions also for these molecular bands. This is indicative for a roughly correct set of cross-section data used in the collisional radiative models for molecules employed here.[48] Figure 6 shows such a comparison of Fulcher fluxes for a scan of electron densities, and this is to be compared with the corresponding results for the Balmer-α emission (same discharges) in Fig. 7.

Experiments (on deuteron plasmas) and modeling (using hydrogen cross-section data) show for both cases the same qualitative behavior: a rise of photon fluxes with density. Up to a density of $n_e = 1 \times 10^{18}$ m^{-3} there is even quantitative agreement. Above this density there is a significant departure in both the atomic (Balmer) and molecular (Fulcher) intensities. However, systematic departures of both photon fluxes in the same direction point toward a problem in the reconstruction of the edge plasma data near the three-dimensional limiter structure rather than to the neutral gas recycling or atomic physics part (e.g., an isotope effect in molecular data) of the model.

A major upgrading of the three-dimensional (in physical space) capabilities of EIRENE, from its early regular three-dimensional grid options toward a fully unstructured three-dimensional discretization based on tetrahedrons, has been carried out for the first stellarator applications of EIRENE in the late 1990s, in collaboration with CIEMAT, Spain. See, for this first example, a full three-dimensional prescription of vessel and host medium (plasma) from the TJ-II stellarator (Madrid) in Fig. 8 (private communication, A. Salas, CIEMAT, Spain, 1999).

These options have meanwhile led to the development of the fully three-dimensional stellarator edge plasma transport code system EMC3-EIRENE, with current applications to the W7AS, W7X, and recently, LHD stellarators, as well as for the three-dimensional TEXTOR dynamic ergodic divertor configuration (see Refs. 50 through 53 and references therein). These options have recently also become the basis for the first industrial

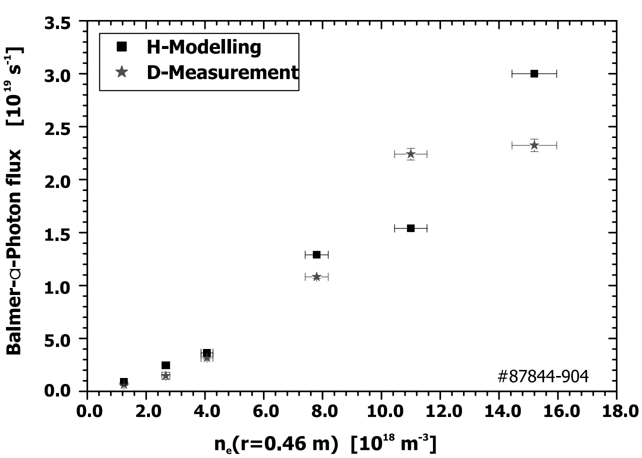

Fig. 7. Comparison of total Balmer band photon fluxes near a test limiter from TEXTOR spectroscopy (asterisks) and EIRENE simulation (squares) versus electron density.

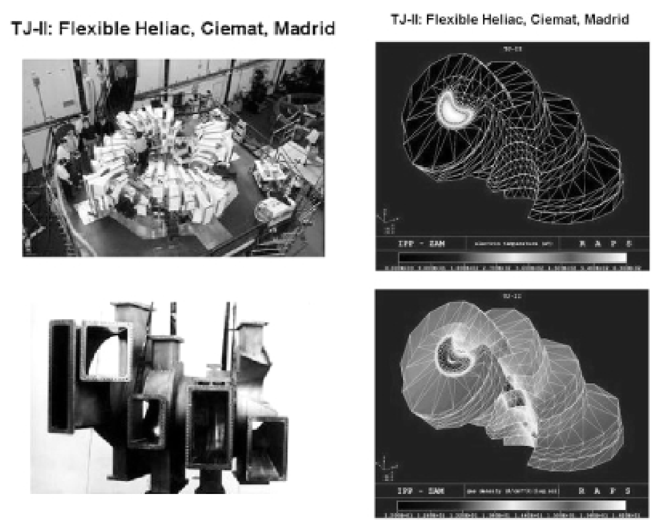

Fig. 8. Vacuum vessel of the TJ-II stellarator[49] (left), $R = 1.5$ m, $a \leq 0.22$ m, and three-dimensional host plasma profiles used as input for EIRENE (right, top), as well as the resulting three-dimensional neutral gas distribution in the vessel and edge plasma, showing a clear separation of core (no neutrals) and edge plasma even in this rather small device.

application of the EIRENE code: Detailed three-dimensional radiation transfer studies are carried out by the lighting industry for the design of high intensity discharge lamps with, for example, automotive applications.[54]

IV. B2-EIRENE

The B2 code[19] is a two-dimensional plasma multifluid code. It has been derived initially from the Braginskii equations (the Navier-Stokes equation counterpart in magnetized plasma physics), employing a significant but apparently quite clever chosen number of simplifications and even ad hoc assumptions. Its great success and acceptance, until these days, is largely based on the transparency and availability of the code. In later years there have been many attempts to reinstall some of the omitted terms, such as improved transport models, or electrical fields, drifts, and currents. The first significant upgrade in this latter direction was achieved with the EB2 code in the mid-1990s (Refs. 55 and 56 and references therein), initially developed and applied to TEXTOR. Inclusion of strongly nonlinear boundary conditions for the electric potential at targets and implementation of a neoclassical expression for the radial current did somewhat facilitate the evaluation of the electric potential inside the last closed flux surface.[56] It also facilitated the study of asymmetries in heat power load, density, temperature, and pressure, as well as the interpretation of biasing experiments.[57]

However, achieving convergence was very difficult at that time and required frequent manual intervention by the person running the code on a case-by-case basis. Some of these problems, meanwhile, have apparently been overcome in present edge codes, partially also due to the explicit cancellation of divergence-free terms in the balance equations, which was formulated only after the EB2 work had come to an end at TEXTOR. But this entire matter of a computationally robust implementation of drifts and electrical currents in two-dimensional edge codes, and the formulation of a set of consistent boundary conditions, has remained a still ongoing major field of active edge physics research since then.

A method for consistently linking the EIRENE code to a fluid model for the background medium such as B2 or EB2 has been developed initially in the late 1980s with many refinements since then. Basic steps included the following:

1. development of common numerical grid structures to avoid any interpolation between the results of the two codes when iterating. In particular, the recycling fluxes have to be consistent between the two codes because typically only a very small fraction (1% or less) constitutes the pumped fraction, yet this can be decisive for the overall SOL dynamics in strong recycling regimes.

2. a unified formulation of expressing sources and sinks in the plasma balance equations in terms of Monte Carlo responses (to avoid any bias resulting from reformulating, fitting, etc., in those terms). Strictly, the kinetic distributions f_{pl} of the host medium fluid (here: plasma) have to be used to evaluate the collision terms

$$\int dv_n \int dv_{pl}\, \sigma(v_{rel}) v_{rel} A(v_i, v_n) f_n(v_n) f_i(v_i) \ ,$$

where v_{rel} is the relative velocity between collision partners and A is the mass, momentum, or energy exchanged between neutrals and host medium in an elastic or inelastic collision with cross-section σ. The neutral particle distribution function f_n is directly related to the solution of the Boltzmann equation (1). Therefore, these source terms are, indeed, of the form of responses given in Eq. (6). Consistent formulations, avoiding independent integrations, and fitting of the A-moments over f_{pl} have been derived in Ref. 58.

3. a particular implicit scheme of iteration to cope with the rather limited CPU power available in these days and the subtle combination of statistical and numerical errors involved in the iterative scheme (see Fig. 9).

One should note that this implicit scheme can be significantly faster than the explicit schemes typically used today in most B2-EIRENE versions, but it does require some detailed monitoring by the person running the case. As machine time has become much cheaper than manpower, meanwhile, it seems to have become less relevant now. However, it was essential to obtain the first converged solution in the late 1980s and early 1990s for high recycling (strongly nonlinear coupled) cases such as ITER applications then. Coupled three-dimensional EIRENE-FIDAP simulations employed by the lighting industry for coupled radiation hydrodynamics[54] have recently led to a revival and further upgrading of these historically first B2-EIRENE schemes in present days.

The methods developed and implemented in this regard resulted in the EIRENE "sandwich"-code package EIRCOP and have been described in Ref. 59. These methods have been kept fairly general, and the mathematical formulation of the terms in Eq. (6) and their known convergence behavior [with $O(1/\sqrt{\mathrm{CPU}})$] allowed to prove convergence of the coupled scheme, however, in a manner quite different from that for purely numerical procedures.

Basically, for a given permitted time-step size δt_B of the plasma code the numerical problem consists in finding an optimal choice between number of internal iterations (i.e., size of the implicit time step $\Delta t = n_s \cdot \delta t_B$ with many n_s "short cycles" to EIRENE for an implicit adaptation of source terms but without new Monte Carlo trajectories) and the number of Monte Carlo histories N_{MC} to be followed in each full EIRENE run with a completely new evaluation of source terms. The coupled code

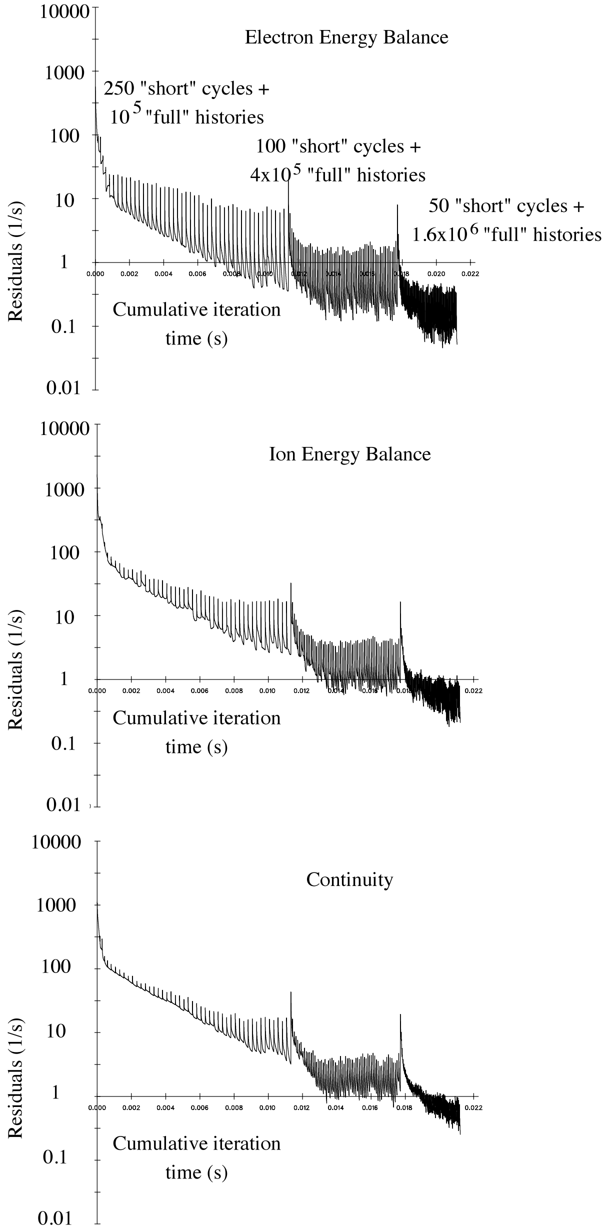

Fig. 9. Convergence of B2-EIRENE showing the typical "saturated residuals behavior" versus cumulated iteration "time" and numerical and statistical control parameters n_s and N_{MC} for the electron energy, ion energy, and continuity equations, respectively. Residuals (1/s) are plotted here on a logarithmic scale. The inverse of the shown residuals can be regarded as the typical physical time constant (s) on which the temperatures and densities, respectively, would continue to change in further iterations.

usually converges with order $O(\Delta t + 1/\sqrt{N_{MC}})$. Figure 9 shows the reduction of "residuals" (normalized errors in the balance equations) with iteration number. If there is a saturation after a certain number of iteration time steps, then the (normalized) noise in the Monte Carlo source terms has become comparable to these numerical balance errors (bias). Further reduction of residuals can then only be achieved by increasing N_{MC}, the number of Monte Carlo histories, and by reducing Δt, i.e., n_s, the number of internal B2 iterations between two full EIRENE runs (termed short cycles[59]). The overall run time of a particular coupled B2-EIRENE case can therefore easily vary by more than an order of magnitude depending on the criterion (the "metric in solution space") employed to measure the level of convergence and on the path chosen in $(\Delta t, N_{MC})$ space to reach these conditions.

V. SAMPLE APPLICATIONS OF B2-EIRENE

Although the historically first applications of B2-EIRENE have been to TEXTOR–ALT-II limiter conditions,[60] most of the effort went into developing a procedure also suitable for high recycling divertors (later: even detachment scenarios). All limiter SOLs modeled so far confirmed the quite robust linear, purely convective isothermal and sheath limited flow conditions expected also from simple models. Deviations from these simple, robust model predictions do exist sometimes in two-dimensional limiter edge models, but these are then usually because of details beyond the predictive quality even of the most authentic edge code models available. The first converged B2-EIRENE results for a high recycling divertor have been presented in connection with a helium removal study for ITER (see Ref. 7, and some of the numerical details have been detailed in the accompanying paper[8]). It was clear from the very beginning of the B2-EIRENE history that the typical convergence behavior of this combined stochastic/numerical tool is fundamentally different from that of the pure numerical edge code known up to then.

Among all existing tokamaks to which B2-EIRENE has been applied since then (interpretative mode), the ASDEX-Upgrade applications are probably the most detailed and systematic ones (Refs. 22 and 61 and references therein). Figure 10 shows a typical two-dimensional (polygonal) grid used by both EIRENE and B2. For more recent applications the outer volume between the computational domain for the plasma flow ("B2-grid") and the vacuum vessel has also been discretized, using an independent finite element grid generator there. In applications since about 2000 a toroidal rather than a periodic cylindrical symmetry was chosen on the EIRENE side, leading to a more consistent treatment of volume recombination under detached divertor conditions.

Figures 11 and 12 show a typical distribution of the molecular and atomic neutral gas, here under plasma conditions with a detached inner divertor and semi-detached outer divertor,[62] corresponding to the cases with upstream (midplane) density of 5×10^{19} m^{-3} described

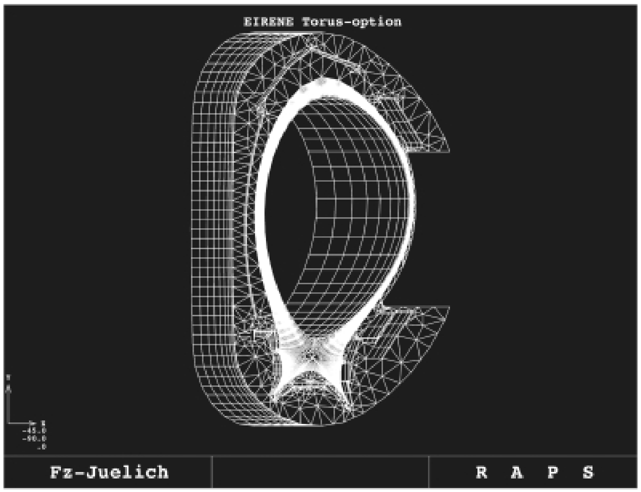

Fig. 10. Typical ASDEX-Upgrade grid in recent B2-EIRENE applications (major radius: 1.65 m; absolute divertor dimensions: see Fig. 13). The structured grid part is used by EIRENE and B2 to solve the plasma conservations equations consistent with recycling; the unstructured outer part is only seen by EIRENE and needed to account for possible nonlinear (neutral-neutral or neutral-photon) interactions there.

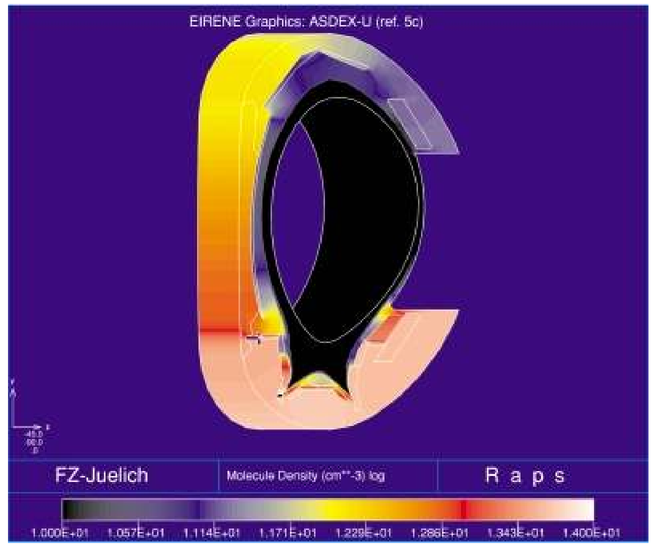

Fig. 12. Same as Fig. 11, but for the atomic component of the neutral gas, with the same logarithmic scale and color code. Substantial atomic pressure can only be found near the targets and in the subdivertor region because of the efficient surface recombination of atoms to molecules.

there. A strong self-sustained neutral cushion (density 10^{20} m^{-3}) in front of exposed target surfaces resulting from the self-consistent coupling of the plasma fluid equations with the neutral gas kinetic equations protects the divertor target from overexposure by the plasma. Details of the physical conditions [upstream (input) parameter range, hydrogenic chemistry in this cushion, pumping, etc.] are currently a subject of significant edge science research, both to identify the driving basic physical processes and to incorporate them into the edge plasma modeling code package.

A detailed B2-EIRENE transport modeling analysis of Fulcher band molecular spectroscopy in the ASDEX-Upgrade divertor has led to a revision of opinion on the role of the so-called "molecular activated recombination" (MAR) on detachment in divertors[6,62] as compared to simple zero-dimensional collisional radiative model predictions. Figure 13 shows the experimental arrangement of the Fulcher band spectroscopy in the ASDEX-Upgrade divertor with the position of the lines of sight (ZOV and ROV) in the outer divertor indicated relative to the configuration used in the computations.

A comparison of experimental and computed Fulcher fluxes along these lines of sight, both for the detached and the later attached phase in discharges with density ramp up, is shown in Fig. 14. Fulcher fluxes (and hence molecular densities) had been systematically overestimated in simulations until the effects of vibrational excitation of the electronic ground state of H_2 had been included. These led to the reduction of the self-sustained molecular density (and the associated frictional effects on the plasma flow in the divertor), mainly because of the quasi-resonant ion conversion reaction acting as a

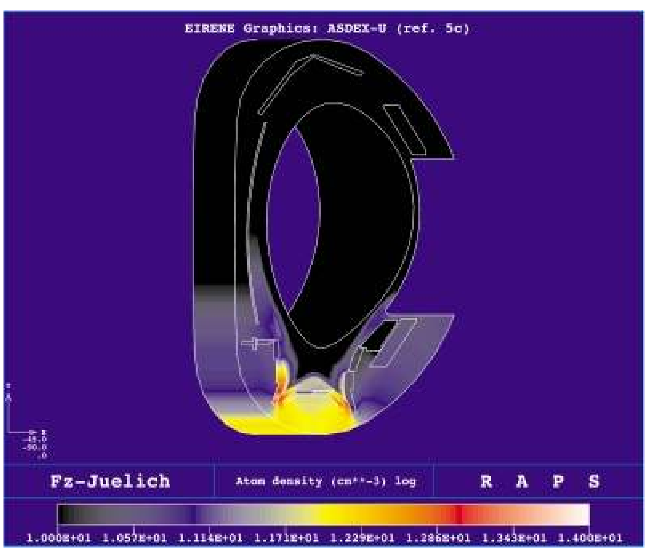

Fig. 11. Typical molecular gas density distribution in ASDEX-Upgrade, self-consistently computed with detached inner and weakly detached outer divertor conditions, plasma conditions as in Ref. 62. Color shading corresponds to a logarithmic scale, with peak values (bright colors) of $\sim 10^{14}$ cm^{-3}.

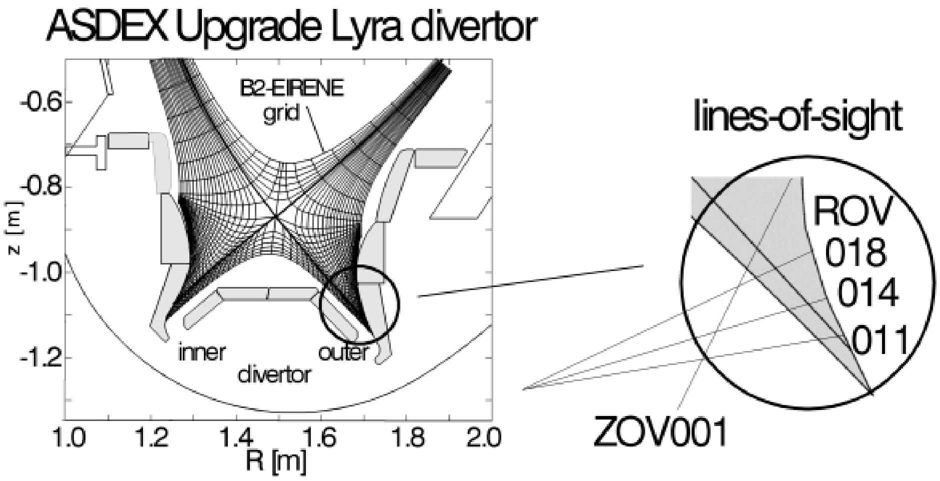

Fig. 13. Schematic of ASDEX-Upgrade divertor, absolute dimensions, including the lower part of the two-dimensional computational B2 grid. The position of the lines of sight used for Fulcher spectroscopy is shown in the window on the right, from Ref. 62.

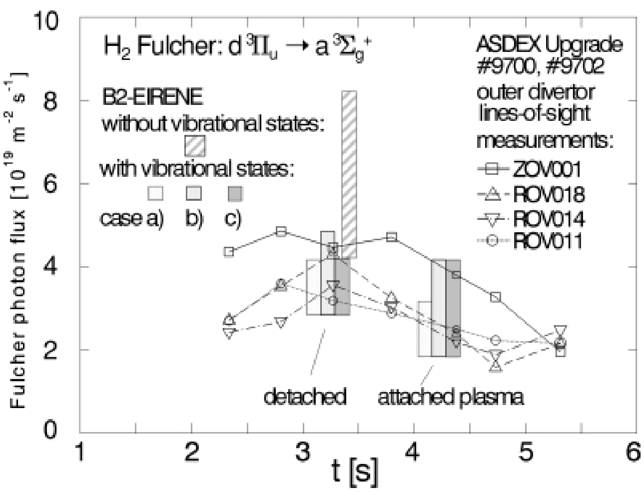

Fig. 14. Fulcher photon fluxes along selected lines of sight, experiment and modeling. The outer divertor was detached and later reattached during the time slot shown here. Modeling results are fairly insensitive to details of assumption on vibrational excitation/de-excitation at surface collisions (labeled cases a, b, and c).

precursor for MAR. The self-consistent response of the plasma on these distinct neutral gas cushion parameters has, in these cases, even led to an overall reduction of the volume recombination rate, although an additional volume recombination process (MAR) had been activated by allowing for vibrational excitation.

The molecular chemistry in cold detached divertors is sensitive to the vibrational population because of the resonances in the vibrationally resolved cross sections. Figure 15 shows a comparison of the computed and measured vibrational distributions, again for the lines of sight shown in Fig. 13. It seems that these are (a) matched rather well by the code calculations and (b) quite insensitive to different assumptions regarding vibrational state transitions at wall collisions, as indicated in Fig. 14. Volume processes [electron and proton impact on $H_2(v)$] apparently are dominant for establishment of the resulting vibrational distribution under divertor conditions.

Similar applications (sometimes with the B2-plasma solver replaced by other edge plasma codes) of EIRENE and its sandwich package EIRCOP are presently used in many laboratories, including by the ITER team.[24] In this latter case, where no experimental data exist to judge the correctness and completeness of the model, the code package at least serves to quantify the known, identified pieces of edge plasma science in a new, far more collisional and therefore perhaps different environment: the ITER divertor.

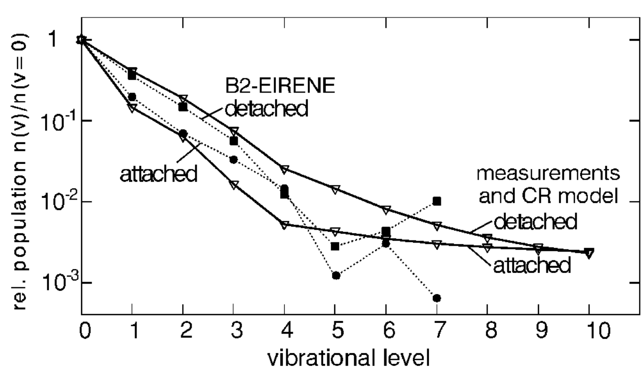

Fig. 15. Distribution of vibrational quantum number of ground state molecules, averaged along lines of sight. Comparison of experimental data and modeling.

VI. SUMMARY AND OUTLOOK

In summarizing it can be stated that the EIRENE Monte Carlo code presently provides a standard tool for solving neutral particle transport problems in fusion devices, without any essential restriction in geometrical and physical detail, but at the expense of statistical noise in the results. It has been and currently still is being applied worldwide to a large number of questions related to either plasma edge data interpretation, quantification of known atomic and surface effects in complex situations, and also for predicting neutral particle effects in future experiments. EIRENE has been linked to a number of plasma-fluid models, such as the various versions of the B2 two-dimensional plasma fluid code for tokamak edge plasmas, the two-dimensional edge interpretation (onion-skin) code OEDGE (P. C. Stangeby et al., University of Toronto), the EMC3 three-dimensional plasma edge stellarator fluid code (Greens function Monte Carlo for diffusion-advection edge equations, Y. Feng, IPP Greifswald), or the three-dimensional finite element plasma code FIDAP for technical plasma applications by the lighting industry.

Future developments will focus on the chemical richness of detached divertor plasma states, i.e., on an optimized treatment of systems with a very large number of species and corresponding automated atomic data-reduction techniques beyond the present "collisional radiative model" concepts. Intrinsic low-dimensional manifolds in composition space to simplify chemical kinetics will have to be implemented. This is because the strict separation between fast processes and slow processes by assigning species as fast and others as slow may not be tolerable in the future. Already the vibrational states of H_2 molecules seem to provide a rather wide spectrum (smooth) of relaxation timescales. In particular, if the carbon option is to be kept open for future divertor designs, then the hydrocarbon chemistry now seems to require a more sophisticated procedure to deal with complexity in composition space as, for example, already quite common in numerical combustion and flame simulation.

Radiation transfer problems (including Doppler-, Stark-, and Zeeman-broadening effects) are presently being implemented also in the nonlinear regime in which the population of excited states is calculated consistently with particle transport and the radiation field. This is made possible because of the mathematical analogy between the linear Boltzmann equation for classical particles (binary collision approximation) solved by EIRENE and the radiation transport equation for the specific intensity (nothing else but a strangely normalized photon-Boltzmann equation). Radiation trapping effects of resonance radiation (Lyman lines) have long been believed to be relevant for the ITER divertor dynamics simply because of the size of the divertor and the gas density there. Numerical studies with the CRETIN code [fluid neutrals self-consistently coupled to radiation transport and one-dimensional plasma transport (Ref. 63 and references therein)], first modeling applications of OSM-EIRENE (OEDGE), and experimental observations from the Alcator C-Mod tokamak seem to confirm the relevance of this mechanism that has hitherto received little attention for edge transport.

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