Journal of Nuclear Materials 196–198 (1992) 80–89
North-Holland

journal of nuclear materials

Progress in two-dimensional plasma edge modelling

D. Reiter

Institut für Plasmaphysik, Forschungszentrum Jülich GmbH, Association Euratom – KFA, Postfach 1913, W-5170 Jülich, Germany

A review is given of the status of various approaches dealing with tokamak edge related issues by employing two-dimensional numerical fluid codes for the main components of the edge plasma. The predictive capabilities of these models are assessed, in particular with regard to their completeness and the reliability of the transport coefficients. As the plasma edge characteristics in the favourable high recycling regime are determined by the mutual interaction of charged and neutral particle transport effects, sophisticated kinetic (often Monte Carlo) models for the neutral particles have been built into several of these 2D fluid programs. This allows for the first time consistently to study intrinsically 2D and multispecies effects, such as flow reversal or decoupling of plasma and impurity or helium ash flows.

1. Introduction

The key role of plasma edge physics on the path towards economic fusion power reactors has become increasingly evident in the past few years, in particular recently during the ITER physics phase study. Since plasma edge conditions are expected to be very different there from those in present day experiments, predictive computer simulations take on an essential role.

Computational studies referred to as "two-dimensional plasma edge modelling" have become a standard tool in tokamak edge physics and have been described frequently. For a recent review the reader is referred to the paper by Vold et al. [25], which covers the physical models and numerical implementations of most of the computational models used for boundary plasma transport studies. A further assessment of the status of such codes will result from the 3rd Int. Workshop on Plasma Edge Theory in Fusion Devices, Bad Honnef, later this year, and the proceedings to be published in the journal Contributions to Plasma Physics.

Such models simulate, in general, the following physical aspects: fluid equations for the plasma (electrons and ions) define conservation equations for basic plasma properties: particle continuity, momentum balance and electron and ion energy balances. Termination of the moment series is achieved by appropriate closure conditions, e.g. the microscopic heat flux density vector is approximated in terms of the mean energy (temperature), for the isotropic scalar pressure an equation of state is adopted, etc.

Without exception the approach followed is that of Braginskii [5] for the Boltzmann moment equations. This classical work is basically a reformulation of the Chapman and Enskog transport theory for ordinary gases to a two-species plasma (electrons and one ion species), in particular accounting for the long range nature of the Coulomb interaction.

Assumptions to obtain closure conditions and to simplify some expressions are typically a strong field limit, ie. $(\omega\tau) \gg 1$, plasma quasi-neutrality, a linear local perturbation method is used to estimate transport coefficients, and the small mass ratio (m_e/m_i) is exploited to expand some terms.

These classical expressions are typically adopted, for the parallel to the $\boldsymbol{B}$ field coefficients. Parallel conductivities, notably for electrons, are occasionally "flux limited", i.e. reduced below classical values. Such empirical modifications for even the classical parallel coefficients are motivated by collisionality and scale length considerations, which, in particular in low density/high temperature cases, render the validity of the fluid approximation questionable.

Anomalous (i.e. phenomenological) expressions are conventionally taken for cross-field coefficients. Furthermore the transverse momentum relation is replaced by a simple expression of (anomalous) diffusion type. In some codes (e.g. Simonini et al. [27]) the most important classical transverse terms are also kept. Choices of coefficients vary from dimensional constants to Bohm-like (Te/B) representations. Experimental information on scalings to large tokamak conditions (ITER) is still very scanty.

Various models then tend to diverge concerning extra simplifications introduced to reduce the transport coefficients and moment equations to simpler forms. A fundamental choice must be made between statement as a time-dependent (parabolic) initial value problem

0022-3115/92/$05.00

or a time independent (elliptic) boundary value problem. Steady states are intrinsically easier to resolve, and complex behaviour of highly nonlinear time-dependent problems may be more difficult to ascribe to physical origins (e.g. ELMs). However, a time-dependent approach will be needed ultimately, to resolve startup, ramping and transient effects.

Source terms, often nonlocal, arising from interaction of the plasma particles with neutral particles or with other ions not included in the fluid equations (e.g. hydrogenic molecular ions, or impurity ions with low collisionality) are obtained from separate kinetic equations.

In section 2 we will discuss physical issues in various computational models, and confine attention to those topics which have been subjects of considerable recent development efforts.

The numerical implementation of such models has been carried out in the past by resorting to various finite difference or finite volume techniques described in standard textbooks. This has been assessed e.g. in the review paper by Vold et al. [25]. Axisymmetric geometries naturally involve an ignorable coordinate (the toroidal angle) and the two-dimensional realisation is constructed by considering transport parallel and transverse to the field. SOL transport is dominated by behaviour parallel to the magnetic field, but two-dimensionality occurs even while transverse effects are orders of magnitude slower than parallel ones, because parallel lengths are also orders of magnitude longer than transverse ones. This extreme contrast in physical time scales is a fundamental difficulty for stable numerical integration and had restrict code development to only the much simpler orthogonal systems. Consequently realistic limiter and divertor configurations with oblique magnetic fields and target surfaces could be modelled only in the sometimes over-simplistic orthogonal target approximation.

In section 3 we discuss possible solutions to this problem, including finite element methods, which have recently gained renewed attention in plasma edge modelling.

One other major distinction in plasma edge transport codes concerns their capability to communicate with satellite codes, such as numerical grid generators, core transport models, external impurity transport codes, kinetic or particle codes for the collisionless sheath region and in particular with neutral gas transport codes. The most detailed description of the source terms in the fluid equations due to neutral–plasma interactions is achievable by employing Monte Carlo codes, and such codes have been available for fusion plasma application for many years.

As in other fields of computational physics in which a combination of Monte Carlo and finite difference methods has been attempted, such as in the analysis of nonlinear radiation transport problems, convergence and stability behaviour remains a critical issue.

In section 4 we describe a method of combining two-dimensional plasma fluid codes with Monte Carlo neutral gas transport codes, which has proven to provide stable solutions even for until recently numerically inaccessible regimes of very localized and strong recycling, as e.g. envisaged for the ITER poloidal divertor plasma.

2. 2D plasma edge modelling: physical models

The last years have seen a proliferation of 2D computational models for tokamak edge plasmas and in what follows we comment only on some of the more recently reported developments.

The most common presently in use is the B2-code [4]. It simulates a quasi-neutral plasma in steady state, employing general orthogonal curvilinear coordinates. Neglecting all electric currents and electron inertial terms allows electric field forces to be described in terms of the electron pressure gradients. Furthermore all diamagnetic terms are omitted, and the code contains a default "minimal" recycling model which gives a very crude treatment of the sources. But the key feature is its flexibility with regard to configuration and incorporation of various transport and source models.

From such a basis, Knoll [28], Prinja [29] and Koesoemodiprodjo [30] have formulated alternative (perhaps more robust) numerical solution methods and substituted a first flight corrected diffusion model for the neutrals. Rognlien et al. [31], Petravic et al. [32] and Simonini et al. [27] have followed the alternative time-dependent initial value approach. Furthermore, in all these cases, parallel electric currents and generically diamagnetic flows (i.e. flows in the $\nabla\Psi \times \boldsymbol{B}$ direction) have been addressed, sometimes, e.g. by Vold et al. [25], via an a posteriori estimation decoupling drift effects from parallel and anomalous transport. All these models include sophisticated neutral source term evaluations using fluid diffusion approximations and/or Monte Carlo procedures.

The B2-code itself is presently the subject of extensive application [33,34] and enhancement. In particular Baelmans et al. [1] have incorporated a diamagnetic momentum relation and consistent Ohm's law yielding fluid drifts and all components of divergence-free electric currents. However, the revised set of equations (similar to those used earlier by Gerhauser et al. [11] in the TEXTOR-configuration specific SOLXY code), exhibits unstable behaviour, necessitating a reducing factor of about 0.3 for the diamagnetic flow velocity. Since exactly the same instability was observed with the numerically distinct SOLXY code (loc. cit.) a physical origin is suggested. A possible explanation is the absence from the equations of viscosity associated with diamagnetic flow.

Finally, until recently, the correct form of the fluid equations, and in particular of the energy equations, involving radial anomalous transport has remained unclear. Only earlier this year a generally accepted form was derived [22]. The linear perturbation ion energy equation, using standard notations, may be written as

$$\frac{\partial}{\partial t}\left(\tfrac{3}{2}\bar{p} + \tfrac{1}{2}mn\overline{v^2}\right) + \boldsymbol{\nabla}\cdot\bar{\boldsymbol{Q}} = e\bar{\boldsymbol{\Gamma}}\cdot\bar{\boldsymbol{E}} + e\overline{\delta\boldsymbol{\Gamma}\delta\boldsymbol{E}} + \bar{\boldsymbol{R}}\cdot\bar{\boldsymbol{v}} + \overline{\delta\boldsymbol{R}\cdot\delta\boldsymbol{v}} + \overline{Q_{\mathrm{ie}}} + \overline{S_{\mathrm{E}}}, \quad (1)$$

with the generalized heat flux vector (loc. cit.)

$$\bar{\boldsymbol{Q}} = \tfrac{5}{2}\bar{p}\bar{\boldsymbol{v}} + \tfrac{5}{2}\overline{\delta p\delta\boldsymbol{v}} + \boldsymbol{q}_{\mathrm{cl}} + \left(\tfrac{1}{2}mn\overline{v^2\boldsymbol{v}}\right) + \tfrac{1}{2}m\overline{\delta\boldsymbol{\Gamma}\delta v^2} + \bar{\boldsymbol{\Pi}}\cdot\bar{\boldsymbol{v}} + \overline{\delta\boldsymbol{\Pi}\cdot\delta\boldsymbol{v}}. \quad (2)$$

Barred quantities here indicate fluctuation averages. $\boldsymbol{q}_{\mathrm{cl}}$ is the classical microscopic heat flux density vector. That is, given the spectra of specified fluctuating quantities, the correct form of the fluid transport equations is uniquely determined. However, by assuming phenomenological anomalous transport relations, it remains undetermined precisely what terms are actually being represented, e.g. what fraction of the term $e\boldsymbol{\Gamma}\cdot\boldsymbol{E}$ (often related to pressure gradients, see also the discussion by Baelmans et al. [1]) is already included in the empirical heat flux expression and what fraction should be retained in the energy balance equation.

Eliminating the other major source of uncertainty in plasma edge modelling, namely the source distribution due to neutral particle recycling, by applying powerful Monte Carlo descriptions in conjunction with the plasma models, allows then attention to be focused on the preceding anomalous transport issue.

Up to this point, only a single ion fluid (as in the fundamental work of Braginskii [5]) has been considered. The first, and until now only well documented, generalisation to more than one ion fluid retaining full geometrical flexibility has been carried out by Braams [4]. Application of this multifluid model e.g. to ASDEX divertor plasma conditions have been described by Neuhauser et al. [16], or by Reiter et al. [20] for the ITER operating scenario A1 [18].

This model is characterized by ion fluids with distinct flow velocities but a common temperature, which, however, may be different from the electron temperature. Coupling between species is through ionization, recombination, friction, electric and thermal forces and temperature equilibration. A strongly simplified set of equations for the parallel transport is derived, which is consistent with the standard classical one ion fluid case in the limit when all but one fluid are trace impurities.

Also the parallel transport coefficients are obtained from the one ion fluid formulae with appropriate replacements such that they have the correct limit in the case when one species dominates.

Recently, Claaßen et al. [6] have provided a complete multispecies transport theory, based on Grad's 21 moment approximation. This model takes full account of the finite mass ratios and arbitrary concentration (in the collision dominated limit). This 21 moment approximation based on Hermite polynomials has exactly the same level of accuracy as the (Sonine and Laguerre) polynomials expansion of the Chapman–Enskog approach used by Braginskii for the one fluid expression.

A similar approach is at present being followed by Radford [19] to provide the classical longitudinal transport coefficients, particularly for plasma impurity ions, for the JET boundary plasma transport codes EDGE1D and EDGE2D. Simultaneously, these equations are used to derive "natural" kinetic corrections for the fluid equations, allowing elimination of the empirical "flux reduction" factors mentioned in the previous section.

In reality, one would expect a transition from fluid-like behaviour to kinetic behaviour in approaching a material boundary, in particular for impurity ion species.

Certainly, the multifluid models available so far ignore this by applying a fluid model unmodified all the way to some perfect Debye sheath edge, which may result in over-estimate of associated parallel gradients in the plasma. A totally different approach, most flexible with regard to model details for release and redeposition, transport and inelastic collisions, is the description of impurity ions by a Monte Carlo procedure. Clearly, the validity of such an approach would not be restricted to the high collisionality regime. Automated interfacing routines between the two-dimensional version of the linear Monte Carlo impurity transport code DIVIMP developed by Stangeby [24] and B2–EIRENE plasma and neutral edge transport code system have been developed at KFA Jülich.

3. Numerical implementations

The "Braginskii" moment equations [5] are originally derived in an invariant (tensor) formulation. Numerical solution requires introducing a coordinate system. Natural 2D coordinates are, given axisymmetry, a radial and a poloidal coordinate. Both the parallel to $\boldsymbol{B}$ and the diamagnetic fluxes can be projected into a poloidal plane by scaling them with appropriate pitch angle factors.

Such 2D geometries are specified by a discretized metric tensor. Since all existing computer codes up to now are restricted to orthogonal coordinate frames, this tensor is always diagonal. Corresponding to such a set of metric coefficients is the specification of the physical coordinates of each node of the computational mesh. The former set of data enters the discretized form of the fluid equations, the latter is needed e.g. for a Monte Carlo computation of neutral or trace impurity ion transport. Magnetic interpolation codes, generating such datasets from given plasma edge equilibrium data, have been available for a few years already (e.g.

ref. [15,17]) but seem to have become sufficiently flexible and accurate only recently [23,33] to permit routine assessment of configurational aspects, at least within the orthogonal target surface approximation.

The domain of calculation, usually, consists of (some part of) the SOL, some portion of the private flux region for divertor configurations, and, often, an annulus of closed surfaces interior to the separatrix. This is motivated by a supposed greater certainty regarding symmetry of boundary conditions on a closed interior surface. Numerical grids for a finite difference type of discretisation for such domains necessarily must include discontinuities (grid cuts), which means that neighbouring cells in the numerical grid may physically be far apart and vice versa.

As long as a "categorical" approach is followed in code development, i.e. a particular code is set up for just one configuration (up to topological equivalence) and plasma model, these grid cuts do not pose a serious problem (e.g. refs. [17,27,11]). For the geometrically universal B2-code, linkage of flows across such grid cuts, retaining the full implicitness of the numerical scheme, has been achieved only very recently [23].

In this same work and resorting to a newly developed very powerful grid generator (loc. cit.) effects of realistic nonorthogonal divertor targets are approximately included in 2D plasma edge modelling for the first time. It is stated (loc. cit.) that these calculations are valid at least under conditions in which radial transport is dominated by the recycling neutral particles in the near target region.

Another approach, probably more consistent but computational more demanding, is being followed by Maddison et al. [15], resorting to a "staircase representation" of the oblique surface. Computational studies are presently being carried out, but results have not been obtained so far.

Most two-dimensional edge plasma transport codes employ more or less standard finite difference techniques to solve the plasma fluid equations. One exception is the B2-code, which is based on a more conservative formulation, called finite volume technique. Its results are averages over each mesh cell, whereas in finite difference approaches the results are obtained at grid points.

An alternative approach would be finite element techniques. These techniques are known to be extremely flexible with regard to geometrical details, whereas the above mentioned two schemes are not.

Finite element (FEM) techniques have reached a very high standard for conduction dominated problems and a vast number of elaborate algorithms is available in the literature and in computer libraries. On the other hand, the understanding for convection dominated phenomena (e.g. near sonic flow) is still marginal and this is a field of active research. For the plasma edge transport equations, both transport mechanisms have to be considered simultaneously. At present at least two different approaches look promising. Zanino [26] has started to develop from scratch an implicit FEM code based on the Galerkin method, for a two fluid magnetized boundary plasma. First results have been obtained, for idealized cases and on simple rectangular geometry (loc. cit.).

A different approach is followed by Pütz [37]. Here a three-dimensional FEM code, developed originally for jet engine design at the RWTH Aachen, is adapted for 2D plasma edge transport problems. For this code, based on linear triangular elements and an explicit predictor–corrector scheme developed by Donea [9], adaptive mesh refinement procedures, controlled by gradients arising in the edge plasma parameters, are already in place. Further due to the peculiarities of tokamak edge transport, a hybrid explicit–implicit technique is envisaged at present. In particular, for the longitudinal energy transport, the characteristic times for conduction are about 10 to 100 times faster than for convection, for ions, and about 1000 times faster for electrons (just opposite to the convection dominated parallel momentum transport, for which the explicit method is appropriate).

Using a fixed temperature field inferred from coupled B2–EIRENE calculations for TEXTOR typical plasma boundary conditions as well as the same transport coefficients and boundary conditions [1], the continuity and momentum equations have been solved with the explicit FEM method accounting for the detailed shape of the TEXTOR ALT-II toroidal pump limiter head. Both code optimisation, and employing some standard implicit techniques for the conduction dominated temperature equations within an otherwise explicit code, are the basic aims of present work.

The time scale for FEM code development, despite the recent progress and demonstration of feasibility, up to the same degree of completeness as existing finite difference codes, has to be estimated in years.

4. Neutral particle transport models

One significant difference between 2D plasma edge modelling and 1D radial plasma transport analysis is the fact that the plasma edge characteristics are highly sensitive to neutral gas transport details, in particular to the near target conditions.

In most applications the characteristic geometrical and physical scale lengths compared to neutral particle mean free paths prohibit a fluid description of the neutral particle transport and necessitate a kinetic treatment. All existing neutral particle recycling models (analytic kinetic, diffusion approximation or Monte Carlo kinetic) have neglected neutral–neutral collisions. In particular the newly reconsidered divertor concepts (radiative divertors, gas target or gaseous divertors), for next generation fusion experiments and reactors [35] will require neutral gas transport models for the transition flow regime between the presently considered linear (Knudsen) regime and the viscous flow limit. A brief discussion of the status of such models is given at the end of this section. If neutral–neutral interactions can be neglected, the neutral particle distribution $f_\nu(\boldsymbol{r},\boldsymbol{v})$ for each neutral particle species ν scales linearly with the total source strength Γ (dimensions: particles per unit time). This flux Γ is given by the total neutralized ion particle flux onto a target surface. Let A_p be the transport quantity in the fluid equations for the plasma species p (ions, electrons), i.e. $\mathsf{A}_\mathrm{p} = n_\mathrm{p}$ (particle density), $\mathsf{A}_\mathrm{p} = m_\mathrm{p} n_\mathrm{p} V_\mathrm{p}$ (momentum density) or $\mathsf{A}_\mathrm{p} = \frac{3}{2} n_\mathrm{p} T_\mathrm{p} + \frac{1}{2} m_\mathrm{p} n_\mathrm{p} V_\mathrm{p}^2$ (energy density). The source term due to one particular neutral–plasma interaction process, characterized by a cross section σ_k, then reads

$$S_{A_\mathrm{p},\nu,\mathrm{k}} = \Gamma \int \mathrm{d}^3 \boldsymbol{v}\, f_\nu(\boldsymbol{v}) \langle \sigma_\mathrm{k}(v_\mathrm{rel}) v_\mathrm{rel} \Delta \mathsf{A}_\mathrm{p} \rangle. \tag{3}$$

Here $\Delta\mathsf{A}_\mathrm{p}$ is the change of A_p per collision.

For convenience, the neutral particle density $n_{0,\nu} = \int \mathrm{d}^3\boldsymbol{v}\, f_\nu(\boldsymbol{v})$ is assumed to be normalized to the number of particles per unit volume per unit source strength. $v_\mathrm{rel} = |\boldsymbol{v}_\nu - \boldsymbol{v}_\mathrm{p}|$ is the relative velocity between the neutral and the individual charged particle and the brackets $\langle\ \ \rangle$ denote averaging over the plasma particle velocity distribution $f_\mathrm{p}(\boldsymbol{v}_\mathrm{p})$. This function is always taken to be a Maxwellian distribution, at the local plasma temperature T_p, shifted by the fluid flow velocity V_p. Such terms $S_{A_\mathrm{p},\nu,\mathrm{k}}$, summed over all neutral species ν and collision processes k considered, arise as (nonlocal) source terms in the plasma fluid equations.

The expression for S_{A_p} happens to be precisely of the format in which results are obtained from linear neutral particle Monte Carlo codes. Such codes, in general terms, estimate "responses" $R_\mathrm{g} = \int fg$, where f is the solution of the kinetic equation for the neutral particles and g is a "detector function", which can be arbitrarily specified (this nomenclature originates from neutron transport applications). The detector functions, in our case the ΔA_p-weighted rate coefficients, have to be evaluated along the neutral particle random walks generated by the Monte Carlo code (e.g. at the points of collision in the DEGAS code [13], or along the free flights between two collision events in the NIMBUS [8] and in the EIRENE codes [21], in order to obtain unbiased estimates of R_g. Using the same discretisation mesh in the Monte Carlo code as in the 2D plasma code and collecting all contributions of the random walks to each source term in each cell, allows incorporation of almost arbitrarily complex atomic, molecular and surface processes consistently in the two-dimensional plasma edge models. Atomic and molecular data for all relevant processes between hydrogenic and helium particles have been compiled and fitted to polynomials e.g. by Janev et al. [14]. These are also used as the database for results presented in section 5. Unfortunately, only the zeroth and first moments are given there, ie. the cross-sections and rate coefficients (for $\Delta A_\mathrm{p} = 1$). Including similar and consistent data fits also for the next two higher moments in the database would considerably facilitate and speed up the Monte Carlo procedure.

The CPU time needed to estimate the source term profiles from about 10^4 random walks on a mesh of order 10^3 cells with present day computers is in the range of 10 to 100 s. Typical time steps in 2D plasma edge codes are of the order of 10^{-6} to 10^{-5} s. Depending on the slowest time constant of the particular model under investigation, up to 10^5 such time steps Δt may be necessary to obtain steady-state solutions. It is obvious from this that a Monte Carlo source term estimation cannot be carried out at each time step, but only at some (10^2 or so) selected steps, $t_0, t_1, \cdots, t_n$, with $t_{i+1} = t_i + k_i \Delta t$ and $k_i \approx 1000$.

Freezing the source term profiles inbetween and only rescaling them at each time step with total particle flux Γ is a standard technique employed frequently, and works, e.g. for not too high recycling divertor plasmas or for rather open limiter plasma boundary configurations. It leads to numerical instabilities (often unphysical temperature collapses or peaks), though, under conditions with extremely highly localized recycling and large flux amplification factors.

Under such circumstances, as for example envisaged near the ITER divertor target plates, a more implicit source term rescaling is required. By this it is meant that as much information as possible on the new plasma state at $t_0 + \Delta t$ should be used to recompute $S_{A_\mathrm{p}}(t_0 + \Delta t)$ from $S_{A_\mathrm{p}}(t_0)$, $n_\mathrm{p}(t_0 + \Delta t)$, $T_\mathrm{p}(t_0 + \Delta t)$, $V_\mathrm{p}(t_0 + \Delta t)$, in order to render the calculation more stable.

In one particular case of coupling a 2D plasma edge code with a Monte Carlo neutral transport code, developed recently by Reiter et al. [20], this implicit technique was consequently applied in the sense described in the following.

To facilitate presentation we first discriminate between precollision rates S'_{A_p}, and postcollision rates S''_{A_p}, such that $S_{A_\mathrm{p}} = S'_{A_\mathrm{p}} + S''_{A_\mathrm{p}}$. The corresponding weighting factors, $\Delta A'_\mathrm{p}$ and $\Delta A''_\mathrm{p}$, stand respectively for the (taken negative) change in particle, momentum and energy density of plasma particles going into a collision and for the same quantities (taken positive) for plasma particles emerging from the collision event.

Let us assume that at one time t_0 during the relaxation towards steady state, all the source terms $S_{A_\mathrm{p}}(t_0)$ are computed, and that we wish to estimate such terms at $t = t_0 + \Delta t$.

We first consider neutral–plasma interactions with rate coefficients which, to a very good approximation, do not depend explicitly on the neutral particle velocity

v, such as e.g. electron impact collisions (ionisation and dissociation). In this case, the weighted collision rate coefficients can be taken out of the integral:

$$S_{A_p} = \left[\Gamma\langle \sigma v_{\rm rel}(\Delta A'_p + \Delta A''_p) \rangle (n_p, T_p, V_p) \right] \Big|_{t_0+\Delta t} \times \int \mathrm{d}^3 v\, f(v) \Big|_{t_0}. \tag{4}$$

The second factor is of the format of a typical Monte Carlo response, here with detector function $g \equiv 1$. It represents the normalized neutral particle density n_0, evaluated at time t_0. The first factor is recomputed at each plasma code time step from the actual plasma parameters and using only a so-called "short cycle" call to the atomic data routines of the Monte Carlo code without generating new random walks.

A somewhat more involved procedure results if there is an explicit dependence on neutral velocity in the rate coefficients, as e.g. for neutral–ion interactions between particles of comparable speed and mass. We demonstrate the technique using the most important example, namely the charge exchange process. Let the index q label the single ionised plasma species corresponding to the neutral atom species ν. For the particle source term the decomposition into one factor evaluated at $t_0 + \Delta t$ and one factor computed as Monte Carlo response at t_0, yields:

$$S'_{n_p} = \left[-\Gamma n_p \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v\, f_\nu(v) \langle \sigma v_{\rm rel} \rangle \Big|_{t_0} \tag{5}$$

and

$$S''_{n_q} = \left[\Gamma n_p \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v\, f_\nu(v) \langle \sigma v_{\rm rel} \rangle \Big|_{t_0} \tag{6}$$

For the momentum source term, we take

$$S'_{m_p v_p} = \left[-\Gamma m_p n_p V_p \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v\, f_\nu(v) \langle \sigma v_{\rm rel} \rangle \Big|_{t_0} \tag{7}$$

and

$$S''_{m_q v_q} = \left[\Gamma m_p n_p \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v\, f_\nu(v) \langle \sigma v_{\rm rel} \rangle v \Big|_{t_0}. \tag{8}$$

Lacking fits for the weighted rate coefficients, we have used the approximation $\langle \sigma v_{\rm rel} v_p \rangle \sim \langle \sigma v_{\rm rel} \rangle V_p$ in eq. (7), i.e. we have neglected the contribution from the integral $\langle \sigma v_{\rm rel} v'_p \rangle$ with $v'_p = v_p - V_p$. Since the product $\sigma v_{\rm rel}$ is almost constant for the charge exchange collision between hydrogenic atoms and ions, this integral is very small and the approximation made here is very good. If other atom–ion interactions (e.g. charge exchange between hydrogenic ions and excited helium atoms are to be considered accurately, such coefficients $\langle \sigma v_{\rm rel} v'_p \rangle (v, T_p)$ have to be computed first (in addition to σ and $\langle \sigma v_{\rm rel} \rangle$).

Finally, for the ion energy source rate we obtain:

$$S'_{E_p} = \left[-\Gamma n_p \frac{m_p}{2} V_p^2 \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v f_\nu(v) \langle \sigma v_{\rm rel} \rangle \Big|_{t_0} + \left[-\Gamma n_p \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v\, f_\nu(v) \langle \sigma v_{\rm rel} \frac{m_p}{2} v_p'^2 \rangle \Big|_{t_0}, \tag{9}$$

$$S''_{E_q} = \left[\Gamma n_p \right] \Big|_{t_0+\Delta t} \int \mathrm{d}^3 v\, f_\nu(v) \langle \sigma v_{\rm rel} \rangle \left(\frac{m}{2} v^2 \right) \Big|_{t_0}. \tag{10}$$

A double polynomial fit for the Maxwellian rate $\langle \sigma v_{\rm rel} (\frac{1}{2} m_p) v_p'^2 \rangle$ in eq. (9) had first been computed, from the cross section σ for charge exchange given by Janev et al. [14]. Again, the terms in S'_{E_p} involving $\frac{1}{2} m_p V_p \langle \sigma v_{\rm rel} v'_p \rangle$ are neglected for the same reasons as above.

For the applications in section 5 we have used a Monte Carlo code in which the choice of detector functions is left to the user, and, therefore, all the relevant responses could easily be estimated without need for modifying or extending the code [21].

Clearly, because of the peculiar combination of a Monte Carlo with a finite difference or finite volume calculation, there is no formal proof that the algorithm will converge to the actual solutions of the system of partial differential and integral equations.

Related issues, using similar methods, have been discussed quite extensively for a long time, e.g. already in 1963 for nonlinear radiation transport calculations carried out by Fleck [10].

For applications to consistent neutral–plasma edge modelling, we have found the following procedure useful (further results can e.g. be found in these proceedings in the papers by Baelmans et al. [1] and Schneider et al. [23]).

By comparing some aspects of source term profiles estimated from a full Monte Carlo run at time t_0 with the derived source term profiles computed during the short cycle at some later time t, one can derive a dynamical (i.e. depending on the evolution of the flow) criterion to interrupt the short cycle and to perform a full Monte Carlo calculation of the source terms for the next step. We have found it sufficient to compare the integrals

$$\int \mathrm{d}^3 r\, S_{n_p}(r) \quad \text{and} \quad \int \mathrm{d}^3 r\, S_{E_p}(r),$$

taken over the whole 2D computational mesh, and to prescribe a certain maximum tolerable percentage for the relative change in each of these quantities during the short cycle. Allowing too large such changes sometimes drives the numerical system unstable, in particular for extremely high recycling conditions. For example, we have found adequate 5%, 10% and 10% as limits for changes of the global particle, ion energy and electron energy source rates respectively, even for the

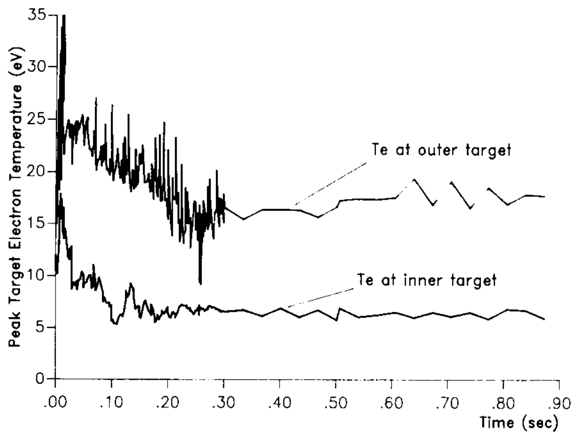

Fig. 1. Typical evolution of peak target-facing electron temperatures (eV) versus integrated time steps (s) for ITER conditions.

very high recycling regime in applications to ITER relevant conditions.

Convergence of the coupled transport code system has a well defined meaning only with respect to each particular choice of dynamical stopping criterion: if the short cycle stopping condition is not met anymore during the relaxation, then no further information can flow between the neutral gas model and the 2D fluid model, and the cycling can be stopped. This definition of convergence is specific to the coupling of (relatively fast, per time step) plasma fluid codes with the (relatively slow, per time step) Monte Carlo neutral gas models. Clearly, different and more restrictive criteria can be derived, if the neutral gas source terms can be computed at each time step, e.g. by using approximate analytic or diffusion like models. This, however, is then often at expense of completeness of the physical model, and in particular in high recycling divertors some detailed aspects of the simulation (such as flow patterns) may be less relevant. This will be demonstrated in section 5.

Fig. 1 shows a typical evolution of peak electron temperatures immediately in front of the divertor (orthogonal) targets for conditions representative of ITER [18]. There is a characteristic initial phase of very frequent recourse to full Monte Carlo calculations and during which plasma parameters fluctuate significantly. There is subsequently a marked transition to a more quiet phase with very infrequent Monte Carlo calls, i.e. a converged state in the previously defined sense.

The significance of a realistic recycling model also for less severe conditions and much less convergence problems is e.g. discussed by Baelmans et al. [1].

The method outlined so far is restricted to low neutral gas densities, typically below 10^{13} cm^{-3}. At larger densities, e.g. in very high recycling or gaseous divertors, neutral–neutral interactions start to compete with the inelastic neutral–plasma processes and surface collisions. Nonlinear Monte Carlo methods for such transition flow regimes (characterized by Knudsen numbers of the order of 1) have been developed since the early sixties, for problems in rarefied gas dynamics. The essence of the method is that intermolecular collisions may be treated separately from particle motions over timesteps that are small compared to the mean time between two such collisions. One such algorithm, generally referred to as "direct simulation Monte Carlo method" in the literature, proposed and developed originally by Bird [3], has recently been implemented into the EIRENE neutral gas Monte Carlo code by Behringer [2]. This extended code has been tested against experimental and theoretical results. Applications to idealized cases have shown trends similar to those resulting from elastic neutral–ion interactions [36]. An effective heating of molecules (here at the expense of the energy of neutral atoms), a resulting deeper penetration of these molecules into the plasma, and significant increases in vacuum transmission factors, in very good agreement with conductance measurements for cylindrical pipes in the transition flow regime, are reported by Behringer (loc. cit.).

5. Application to ITER conditions

Two examples of application of the B2–EIRENE code system, each of which addresses different aspects of 2D plasma edge modelling, are described in these proceedings. The first [1] can be taken to be representative for toroidal belt limiter tokamaks, as e.g. TEXTOR with the ALT-II pump limiter system, or JET.

Full convergence in the sense defined above was achieved after only five full Monte Carlo cycles. This uncritical behaviour is typical for open plasma edge configurations, in which the neutral source terms spread considerably over the computational area. In another paper [23], Schneider et al. discuss an application to typical poloidal divertor conditions using ASDEX and ASDEX-UPGRADE as examples. In particular, plasma flows from inboard to outboard divertor legs and neutral flows between plasma and first wall components are studied.

In this section we describe an application to a plasma edge configuration and physical conditions expected to be relevant for ITER scenarios. Although divertor plasmas often are expected to be strongly one-dimensional in character, with friction forces assisting impurity retention (see e.g. ref. [27]), intrinsically 2D effects have been identified in extensive 2D modelling studies, such as radial decoupling of helium versus hydrogenic transport. For a survey of ITER related edge plasma modelling studies, including discussion of such effects, the reader is referred to the summary report by Post et al. [18], and to the extensive scaling studies by Pacher et al. [34].

The example discussed next has been chosen to illustrate both typical two-dimensional and also multi-species effects. It has been pointed out for a long time, basically using strongly simplified models and analytical arguments, that the mutual effects of neutral and plasma transport can drive the bulk hydrogenic plasma flow away from target surfaces back towards the confined plasma region. This phenomenon, referred to as "flow reversal", has been re-investigated using the fully two-dimensional consistent plasma and neutral particle transport model described above, in collaboration with Stangeby, Univ. of Toronto, Canada. An ITER plasma edge simulation was carried out, using the "ITER operating scenario A1, reference ignition" prescription for an ELMy H-mode edge transport model [18]. The starting point was an initial plasma state obtained by employing a reduced analytical recycling model. After about 150 full Monte Carlo cycles and about 50000 implicit short cycles, the code system had converged in the above defined sense. Each Monte Carlo run generated 15000 neutral trajectories, although for the final 20 full cycles this number was increased to 60000 to damp any remaining small fluctuations caused by the statistical procedure.

Fig. 2 shows a typical plasma flow pattern for ITER-like conditions, superimposed on the outline of the computational domain (up–down symmetry is assumed). Each arrow is parallel to the local flow vector in the poloidal cross-section. Note the extended region of reversed plasma flow adjacent to the separatrix in the outside SOL.

Fig. 3 shows an enlargement of the outside target region, fig. 4 shows an equivalent case except for an arbitrarily increased pumping speed (from 500 m^3/s in figs. 2 and 3 to 10000 m^3/s in fig. 4 at the duct entrance). Note the strong impact on the magnitude of reversed flow by this seemingly marginal alteration of conditions. (In both cases the effective pumping speed at the divertor target is almost the same.)

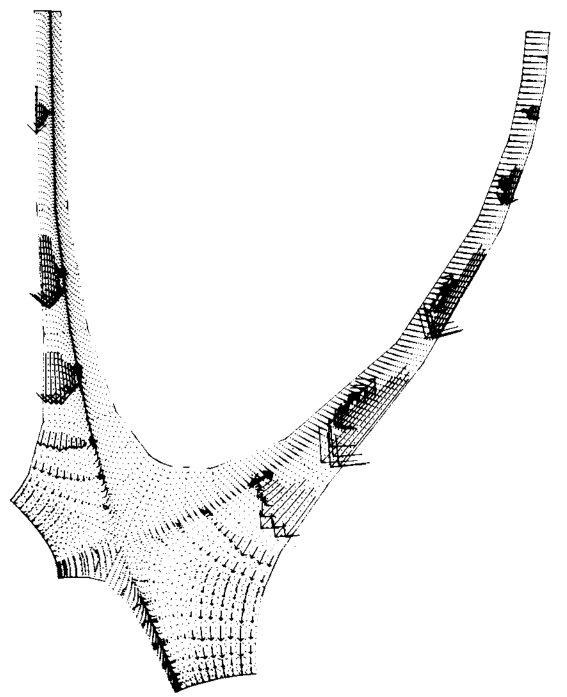

Fig. 2. ITER-like computational domain with typical plasma flow pattern superimposed.

Inspecting the flow pattern revealed the following features: the flow is directed towards the target plates in the first few zones (a few millimeters), clearly because this is enforced by the Bohm-like target sheath conditions imposed there. However, a channel near the separatrix had formed, starting at this poloidal distance of a few millimeters and ranging up to the symmetry plane, in which the flow was reversed.

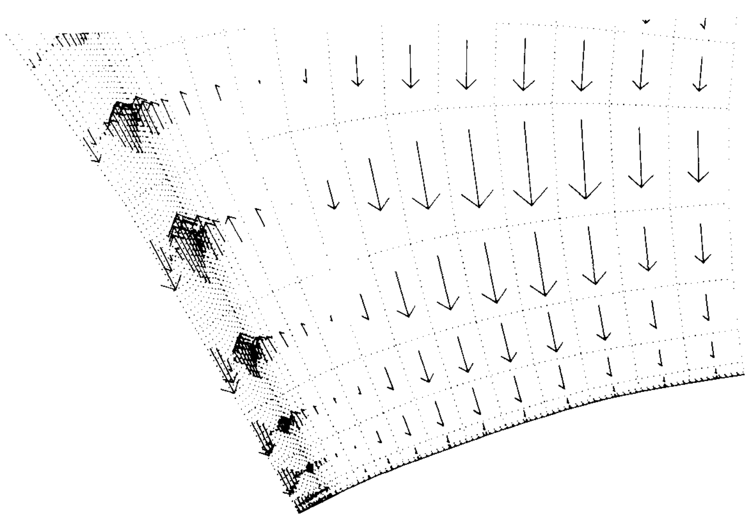

Fig. 3. Enlargement of outer target of fig. 2.

The key feature contributing significantly to this flow reversal was an excess reionisation of neutral particles originating from the left and the right wings of the footprint about the separatrix. These particles are preferentially reionised near the separatrix, because the plasma is hottest there. It was precisely this effect predicted from highly simplified analytic treatments, e.g. by Cooke and Prinja [7] which originally had led to prediction of the possibility of flow reversal caused by reionisation in tokamak edge plasmas.

For example, using the "minimal" B2 recycling model for the same case rather than the EIRENE model fully allowed us to eliminate or create reversed flow zones depending on choices made for "fudge factors" introduced to superimpose radial neutral transport effects on the only longitudinal treatment. This fully consistent computational analysis confirms this picture, and leads to the following immediate conclusions:

(1) The details of radial transport of neutral particles in the SOL determine the formation and location of reversed flow regions. This aspect of neutral transport in particular is often very crudely included in simplified analytic recycling routines in 2D plasma fluid codes.

(2) Whether or not impurity (and helium ash) retention by frictional forces will be efficient in high recycling divertors will depend critically on whether impurities are reionised before, or within, the reversed flow zone. In the latter case friction would act in just the opposite way and drive impurities back to the main plasma.

(3) Detailed experiments addressing such predominantly parallel transport issues under reactor relevant conditions are urgently needed, possibly with large linear devices in order to isolate the various parallel transport related divertor issues from the unknown and experimentally not easily accessible anomalous radial transport in tokamaks.

6. Summary

A significant amount of work was recently focused on 2D plasma edge code developments and applications. In these proceedings alone there are 11 papers dealing with this subject.

Apart from one documented "universal" code, the B2-Braams code, most other approaches seem to be addressing special issues, often more complete in their physical model but less flexible. Work on relaxing geometrical restrictions and on completing the physical model in the B2-code is reported in these proceedings, and in particular significant efforts are described to recover nonzero electric currents (and associated contributions in the expressions for the tensor fluxes and the inhomogeneous terms), which have been neglected often in plasma edge codes at the early stage of development. The same statement holds true for generically diamagnetic fluxes.

Longitudinal impurity ion transport coefficients have been rederived from higher moment equations (based on Grad's 21 moment method) recently. This same approach is believed also to help in reducing uncertainties introduced by kinetic corrections to the set of fluid equations used presently (nonlocal electron heat transport, "flux limiters"). 2D finite element codes are being developed and encouraging first results have been obtained. In general their state of development is still far behind the existing finite difference codes in terms of completeness of the physical model, but they have already proven their superiority as far as geometrical flexibility is concerned. Refined magnetic interpolating and grid generating codes have been developed,

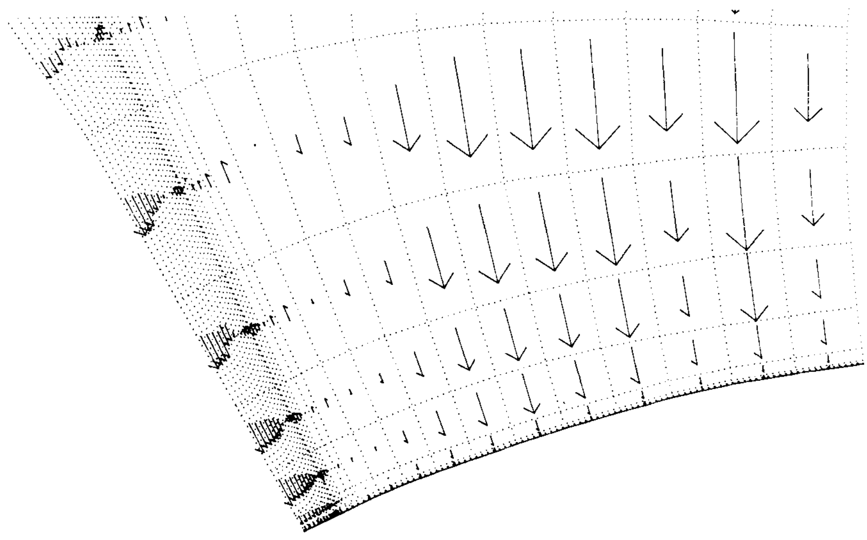

Fig. 4. As fig. 3, for arbitrary increased pumping speed at the duct aperture.

providing simultaneously consistent information for Monte Carlo neutral gas and for finite difference plasma fluid codes. This allows both a rapid interpretation of experimental results based on the actual magnetic configuration in the shots, and predictive studies on the scaling of plasma edge characteristics with geometrical parameters (connection lengths, etc.).

The regime of stable operation of coupled plasma fluid and Monte Carlo neutral particle codes has been significantly extended and such code systems have now become applicable even to the extremely high recycling conditions envisaged for some ITER divertor concepts.

Extensions of such neutral gas transport models to remain valid under radiative or gaseous divertor plasma conditions are presently being carried out, e.g. inclusion of elastic neutral–neutral and neutral–ion interactions. First numerical and experimental validations of these extended models are described in these proceedings.

Future 2D plasma edge code developments will include continuing adaptation and optimisation of FEM techniques, for the highly anisotropic and neither conduction nor convection dominated plasma transport in tokamak boundary regions. Furthermore, kinetic corrections to fluid equations, clarification of the role of anomalous transport in classically derived equations and coupling of Monte Carlo impurity ion transport models into existing neutral–hydrogenic plasma code systems for consistent evaluations of the erosion, redeposition and impurity retention will be addressed by various modelling teams.

References

[1] M. Baelmans et al., these Proceedings (PSI-10), J. Nucl. Mater. 196–198 (1992) 466.

[2] Th. Behringer, Nonlinear effects on neutral gas transport in tokamaks, KFA Jülich rep., JÜL-2637 (1992), in German.

[3] G.A. Bird, Phys. Fluids 13 (1990) 2676; and the monograph: Molecular Gas Dynamics (Clarendon, Oxford, 1976).

[4] B. Braams, A multi-fluid code for simulation of the edge plasma in tokamaks, NET rep. EUR-FU IXII-80-87-68, Comm. of the European Communities (1987).

[5] S.I. Braginskii, Rev. Plasma Phys. 1 (1965) 205.

[6] H.A. Claaßen, H. Gerhauser and Y.A. Sayed, Numerical evaluation of longitudinal ion transport coefficients in magnetized D-He and H-C plasmas, KFA Jülich rep., JÜL-2548 (1992).

[7] P.I.H. Cooke and A.K. Prinja, Nucl. Fusion 27 (1987) 1165.

[8] E. Cupini, A.De. Matteis and R. Simonini, NIMBUS–Monte Carlo simulation of neutral particle transport in fusion devices, EUR XII-324/9 rep. (1983).

[9] J. Donea, Int. J. Numer. Meth. Eng. 20 (1984).

[10] J.A. Fleck, Jr., in: Methods in Computational Physics, eds. B. Alder and S. Fernbach (McGraw–Hill, 1963) vol. 1, p. 43.

[11] H. Gerhauser and H.A. Claaßen, Proc. 18th EPS Conf. on Controlled Fusion and Plasma Physics, Berlin, 1991, Europhysics Conf. Abstr., vol. 15C, part III, p. 13.

[12] M.F.A. Harrison, E.S. Hotston and G.P. Maddison, Modelling of NET/ITER Edge Plasmas, NET rep. EUR-FU/80/91-100, Comm. of the European Communities (1991).

[13] D.B. Heifetz et al., A Monte Carlo model of neutral particle transport in diverted plasmas, PPPL-1843 (1981).

[14] R.K. Janev et al., Springer Series on Atoms and Plasmas, vol. 4 (1987).

[15] G.P. Maddison et al., Proc. 18th EPS Conf. on Controlled Fusion and Plasma Physics, Berlin, 1991, Europhysics Conf. Abstr., vol. 15C, part III, p. 197.

[16] J. Neuhauser et al., Contrib. Plasma Phys. 30 (1990) pp. 1, 95.

[17] M. Petravic and G. Kuo-Petravic, Nucl. Fusion 30 (1990) pp. 6, 1148.

[18] D.E. Post et al., ITER Physics, ITER Doc. Ser. 21, (IAEA, Vienna, 1991).

[19] G. Radford, Proc. 3rd Int. Workshop on Plasma Edge Theory in Fusion Devices, Bad Honnef, Germany, 1992, to be published in Contrib. Plasma Phys.

[20] D. Reiter et al., Plasma Phys. Control. Fusion 33 (1991) 1579.

[21] D. Reiter, The EIRENE code, Version Jan. 92, User manual, KFA Jülich rep., JÜL-2599 (1992) and KFA Jülich rep., JÜL-1947 (1984).

[22] D.W. Ross, Plasma Phys. Control. Fusion 34 (1992) 137.

[23] R. Schneider et al., these Proceedings (PSI-10), J. Nucl. Mater. 196–198 (1992) 810.

[24] P.C. Stangeby and C.M. Farrell, Description of the LIM and DIVIMP codes, Univ. of Toronto, 1992, unpublished.

[25] E.L. Vold, F. Najmabadi and R.W. Conn, Phys. Fluids B3 (1991) 3132.

[26] R. Zanino, 2-fluid modelling of magnetized plasma transport in axisymmetric domains with Galerkin finite elements, IPP Garching rep. IPP 5143 (1991), and these Proceedings (PSI-10), J. Nucl. Mater. 196–198 (1992) 326.

[27] R. Simonini et al., these Proceedings (PSI-10), J. Nucl. Mater. 196–198 (1992) 369.

[28] D.A. Knoll, ibid., p. 352, and references therein.

[29] A. Prinja, ibid., p. 340, and references therein.

[30] C. Koesoemodiprodjo, presented at this Conference (PSI-10) and references therein.

[31] T.D. Rognlien et al., ibid., p. 347.

[32] M. Petravic et al., ibid., p. 883.

[33] D. Stodler et al., presented at this Conference (PSI-10).

[34] H. Pacher et al., ibid., p. 457.

[35] R.W. Conn, presented at this Conference (PSI-10).

[36] G. Haas et al., ibid., p. 481.

[37] T. Pütz, Assessment of applicability of finite element methods for 2D plasma edge modelling, KFA Jülich, rep., in preparation.